

NMST539

Mnohorozměrná analýza
Multivariate Analysis

Lecture notes I (classical topics)

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Some basics first: quantitative data

Data matrix

The typical organization of the data in many problems in multivariate analysis is into a data matrix \mathbf{Y} , in which

- rows corresponds to different objects (“cases”)
- and columns to different attributes of the data (“variables”)

Example: Track Records for Men

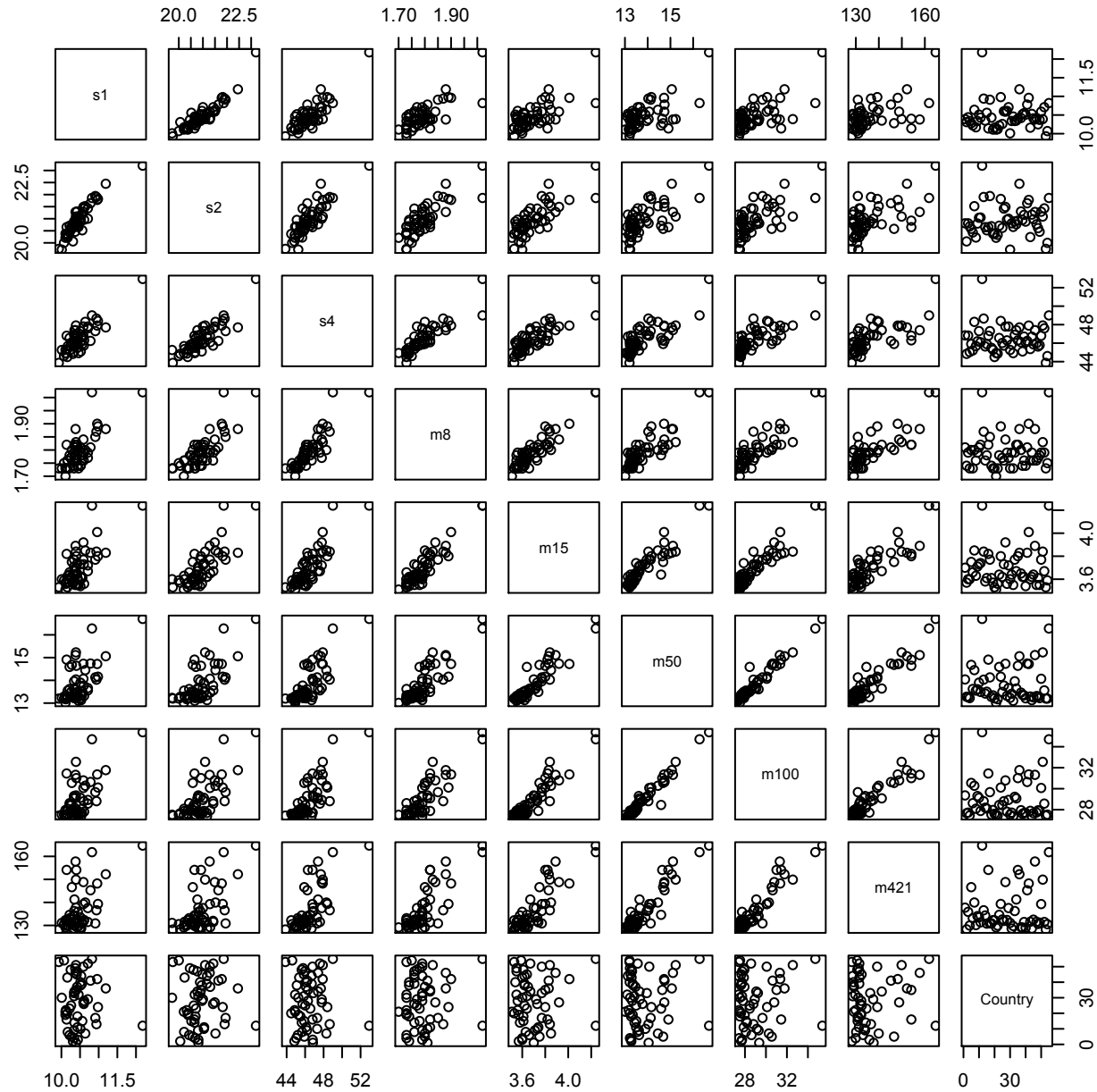
The data give best achieved times by men in various countries, and various running disciplines

```
> tram
```

	s1	s2	s4	m8	m15	m50	m100	m421	Country
1	10.39	20.81	46.84	1.81	3.70	14.04	29.36	137.72	argentin
2	10.31	20.06	44.84	1.74	3.57	13.28	27.66	128.30	australi
3	10.44	20.81	46.82	1.79	3.60	13.26	27.72	135.90	austria
4	10.34	20.68	45.04	1.73	3.60	13.22	27.45	129.95	belgium
5	10.28	20.58	45.91	1.80	3.75	14.68	30.55	146.62	bermuda
...									

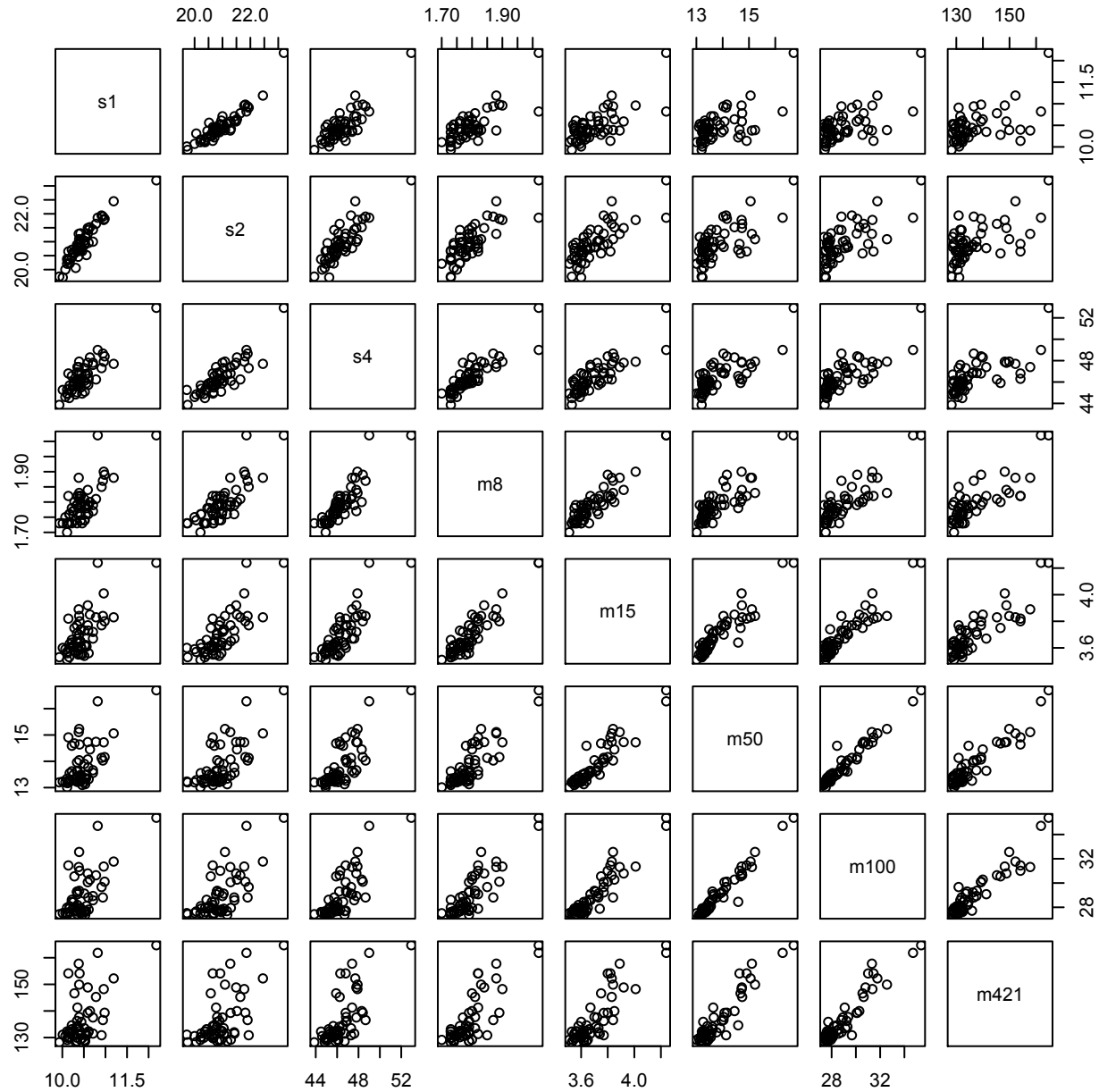
Any graphical representation for that? Well, we can try (all) projections into the coordinate directions...

...but not like this...



```
> pairs(tram)
```


...but rather like this!



```
> pairs(tram[,1:8])
```

Some preprocessing of the data may help too

```
> tram
      s1      s2      s4      m8      m15      m50      m100      m421      Country
1  10.39  20.81  46.84  1.81  3.70  14.04  29.36  137.72  argentin
2  10.31  20.06  44.84  1.74  3.57  13.28  27.66  128.30  australi
3  10.44  20.81  46.82  1.79  3.60  13.26  27.72  135.90  austria
...
> trackmen = tram[,1:8]
> row.names(trackmen) = tram[,9]
> trackmen
      s1      s2      s4      m8      m15      m50      m100      m421
argentin 10.39  20.81  46.84  1.81  3.70  14.04  29.36  137.72
australi  10.31  20.06  44.84  1.74  3.57  13.28  27.66  128.30
austria   10.44  20.81  46.82  1.79  3.60  13.26  27.72  135.90
...
```

Some more preprocessing perhaps

We often want to **center** the data: subtract the (corresponding) column means

```
> trackmenc = sweep(trackmen,2,apply(trackmen,2,mean))  
> apply(trackmenc,2,mean)
```

s1	s2	s4	m8	m1
-3.552625e-16	1.033536e-15	2.196231e-15	-6.459578e-17	-6.459677e-1
m50	m100	m421		
5.167584e-16	7.751770e-16	5.684247e-15		

and also **scale** them: divide by the (corresponding) column standard deviations

```
> trackmens = sweep(trackmenc,2,apply(trackmenc,2,sd),"/")
```

Another dataset: electrodes

Various electrodes have been tried successively on arms of 16 subjects. The question whether electrodes have different characteristics or not.

```
> read.table("electro.d",header=T,row.names=1)
```

	E1	E2	E3	E4	E5
1	500	400	98	200	250
2	660	600	600	75	310
3	250	370	220	250	220
4	72	140	240	33	54
5	135	300	450	430	70
6	27	84	135	190	180
7	100	50	82	73	78
8	105	180	32	58	32
9	90	180	220	34	64
10	200	290	320	280	135
11	15	45	75	88	80
12	160	200	300	300	220
13	250	400	50	50	92
14	170	310	230	20	150
15	66	1000	1050	280	220
16	107	48	26	45	51

If there were two electrodes only, we would just compare the results on those: as they may likely for a given subject be dependent, we rather form differences and then compare those to zero: paired t-test, for instance, if we can assume normal distribution for the data

Variance-covariance matrix of a random vector

Suppose that \mathbf{y} is a random vector - a collection of random variables y_1, y_2, \dots, y_p . The **variance-covariance matrix** (often they say just variance matrix or covariance matrix) of \mathbf{y} is defined to be

$$\begin{aligned}\text{Var}(\mathbf{y}) &= (\text{Cov}(y_i, y_j))_{ij} \\ &= \begin{pmatrix} \text{Cov}(y_1, y_1) & \text{Cov}(y_1, y_2) & \dots & \text{Cov}(y_1, y_p) \\ \text{Cov}(y_2, y_1) & \text{Cov}(y_2, y_2) & \dots & \text{Cov}(y_2, y_p) \\ \dots & \dots & \dots & \dots \\ \text{Cov}(y_p, y_1) & \text{Cov}(y_p, y_2) & \dots & \text{Cov}(y_p, y_p) \end{pmatrix} \\ &= \begin{pmatrix} \text{Var}(y_1) & \text{Cov}(y_1, y_2) & \dots & \text{Cov}(y_1, y_p) \\ \text{Cov}(y_2, y_1) & \text{Var}(y_2) & \dots & \text{Cov}(y_2, y_p) \\ \dots & \dots & \dots & \dots \\ \text{Cov}(y_p, y_1) & \text{Cov}(y_p, y_2) & \dots & \text{Var}(y_p) \end{pmatrix}\end{aligned}$$

where $\text{Cov}(y_i, y_j) = E[(y_i - E(y_i))(y_j - E(y_j))]$

and $\text{Cov}(y_i, y_i) = \text{Var}(y_i) = E[(y_i - E(y_i))^2]$

Matrix notation

In the matrix notation, \mathbf{y} is a vector - which we like to be a *column* one: $\mathbf{y} = (y_1, y_2, \dots, y_p)^\top$, that is

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \dots \\ y_p \end{pmatrix} \quad \text{and then} \quad \text{Var}(\mathbf{y}) = E(\mathbf{y} - E(\mathbf{y}))(\mathbf{y} - E(\mathbf{y}))^\top]$$

In particular, when $E(\mathbf{y}) = \mathbf{0}$, then $\text{Var}(\mathbf{y}) = E[\mathbf{y}\mathbf{y}^\top]$

This formalism is a neat way to observe that $\text{Var}(\mathbf{y})$ is always nonnegative definite (or positive semidefinite, if you wish), and also to obtain the formula

$$\text{Var}(\mathbf{A}\mathbf{y}) = \mathbf{A} \text{Var}(\mathbf{y}) \mathbf{A}^\top$$

holding true for any (nonrandom) matrix \mathbf{A} that can be multiplied with \mathbf{y} as indicated (that is, it has p columns). Its special case is the elementary formula

$$\begin{aligned} \text{Var}(a_1 y_1 + a_2 y_2) &= \text{Var}(a_1 y_1) + 2 \text{Cov}(a_1 y_1, a_2 y_2) + \text{Var}(a_2 y_2) \\ &= a_1^2 \text{Var}(y_1) + 2a_1 a_2 \text{Cov}(y_1, y_2) + a_2^2 \text{Var}(y_2) \end{aligned}$$

Variance-covariance matrix of the data

When referring to the variance-covariance matrix of the data, it is sometimes emphasized that it is *sample* variance-covariance matrix - but often the correct form is just implied by the context. (If needing to distinguish it from the variance-covariance matrix of a random vector, we will call the latter *stochastic*)

This matrix can be viewed as an “estimator”: obtained by the principle of analogy when the data are rowwise sampled from a common distribution, the distribution of some random vector \mathbf{y} . More important than this motivation is to remember the result: (co)variances $\text{Cov}(\mathbf{y}_k, \mathbf{y}_\ell)$ are replaced by the corresponding sample (co)variances

$$s_{k\ell} = \frac{1}{n-1} \sum_i (\mathbf{y}_{ik} - \bar{\mathbf{y}}_k)(\mathbf{y}_{i\ell} - \bar{\mathbf{y}}_\ell)$$

where $\bar{\mathbf{y}}_j = \frac{1}{n} \sum_i \mathbf{y}_{ij}$ is the average of the j -th column, replacing the mean $E(\mathbf{y}_j)$ from the stochastic version ($j = k, \ell$)

(Note the division by $n-1$: while it is the most common choice, it is not universally accepted; for instance, normal distribution maximum likelihood theory may suggest division by n)

The result

We organize variances and covariances into the **(sample) variance-covariance matrix** of **Y**:

$$\text{var}(\mathbf{Y}) = \mathbf{S}_Y = \begin{pmatrix} s_{11} & s_{12} & \dots & s_{1p} \\ s_{21} & s_{22} & \dots & s_{2p} \\ \dots & \dots & \dots & \dots \\ s_{p1} & s_{p2} & \dots & s_{pp} \end{pmatrix} = \begin{pmatrix} s_1^2 & s_{12} & \dots & s_{1p} \\ s_{21} & s_2^2 & \dots & s_{2p} \\ \dots & \dots & \dots & \dots \\ s_{p1} & s_{p2} & \dots & s_p^2 \end{pmatrix}$$

This matrix is symmetric

(as can be seen directly from its definition)

and also nonnegative definite (some say: positive semidefinite)

- and this can be best seen from its matrix expression

The compact matrix notation

The centered data matrix is $\tilde{\mathbf{Y}} = \mathbf{Y} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top\mathbf{Y}$.

The (sample) **variance-covariance matrix** of \mathbf{Y} is

$$\begin{aligned}\mathbf{S}_{\mathbf{Y}} &= \frac{1}{n-1}\tilde{\mathbf{Y}}^\top\tilde{\mathbf{Y}} = \frac{1}{n-1}\left(\mathbf{Y} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top\mathbf{Y}\right)^\top\left(\mathbf{Y} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top\mathbf{Y}\right) \\ &= \frac{1}{n-1}\mathbf{Y}^\top\left(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top\right)^\top\left(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top\right)\mathbf{Y} \\ &= \frac{1}{n-1}\mathbf{Y}^\top\left(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top\right)\left(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top\right)\mathbf{Y} = \frac{1}{n-1}\mathbf{Y}^\top\left(\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top\right)\mathbf{Y}\end{aligned}$$

The matrix $\mathbf{H} = \mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\top$ is symmetric and idempotent

- which means that $\mathbf{H}\mathbf{H} = \mathbf{H}$

Idempotence immediately implies that the matrix is nonnegative definite - and its rank is equal to its trace: $n - 1$

Correlation matrix

The **(sample) correlation matrix** of \mathbf{Y} is

$$\text{cor}(\mathbf{Y}) = \begin{pmatrix} \rho_{11} & \rho_{12} & \dots & \rho_{1p} \\ \rho_{21} & \rho_{22} & \dots & \rho_{2p} \\ \dots & \dots & \dots & \dots \\ \rho_{p1} & \rho_{p2} & \dots & \rho_{pp} \end{pmatrix} = \begin{pmatrix} 1 & \rho_{12} & \dots & \rho_{1p} \\ \rho_{21} & 1 & \dots & \rho_{2p} \\ \dots & \dots & \dots & \dots \\ \rho_{p1} & \rho_{p2} & \dots & 1 \end{pmatrix}$$

where $\rho_{k\ell}$ is the sample correlation coefficient

$$\rho_{k\ell} = \frac{\sum_{i=1}^n (y_{ik} - \bar{y}_k)(y_{i\ell} - \bar{y}_\ell)}{\sqrt{\sum_{i=1}^n (y_{ik} - \bar{y}_k)^2 \sum_{i=1}^n (y_{i\ell} - \bar{y}_\ell)^2}}$$

The stochastic correlation matrix, the correlation matrix of a random vector \mathbf{y} , is defined analogously, only the $\rho_{k\ell}$'s are replaced by

$$\frac{\text{Cov}(\mathbf{y}_k, \mathbf{y}_\ell)}{\sqrt{\text{Var}(\mathbf{y}_k) \text{Var}(\mathbf{y}_\ell)}}$$

Seeing the data: a word on projections

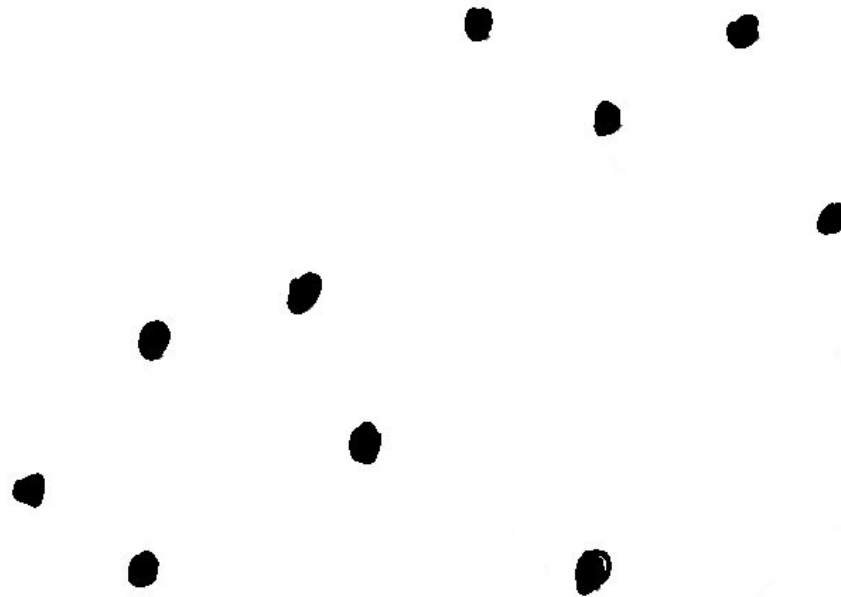
Dimensionality problem

We live in dim 3 and see in dim 2

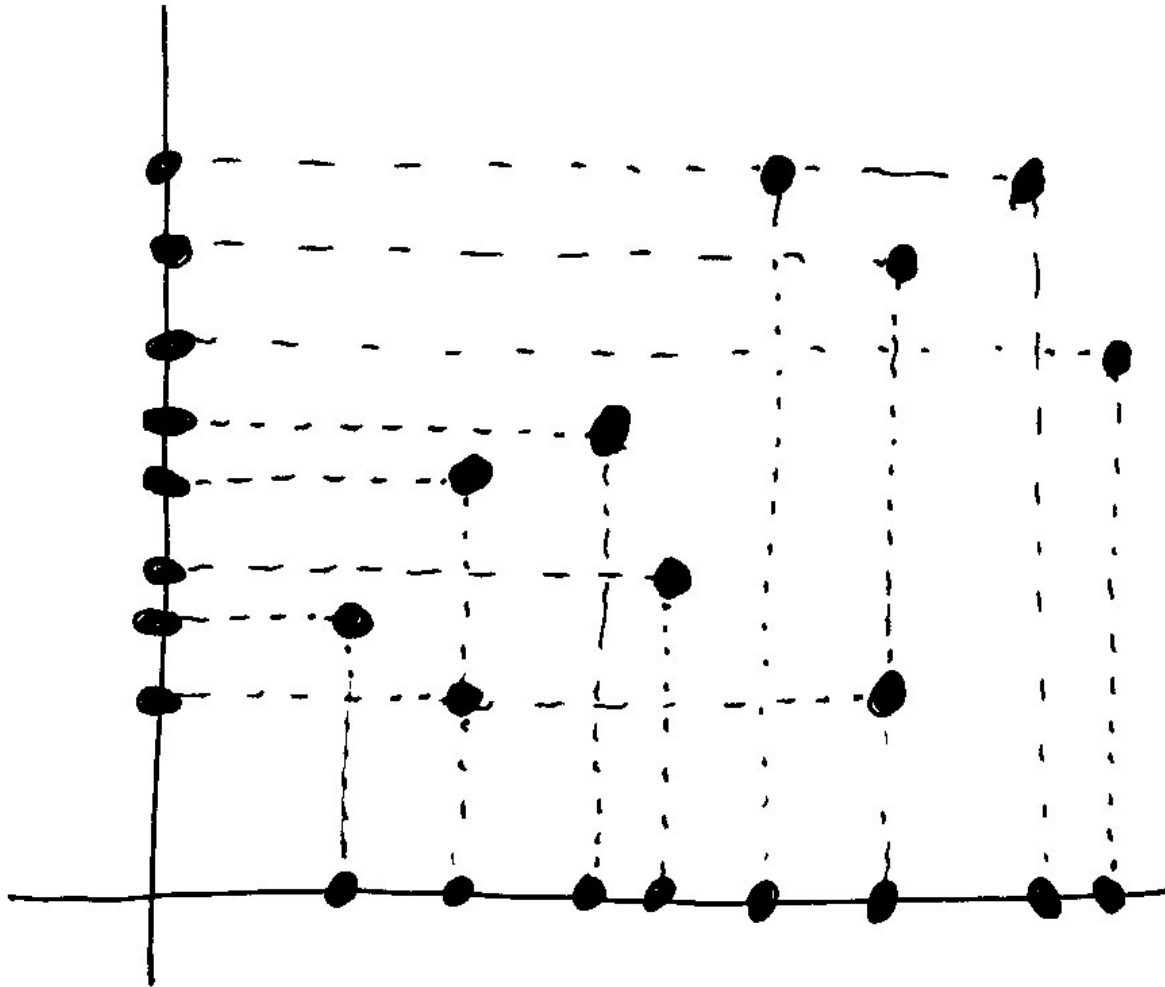
For pedagogical reasons:

we may imagine that we live in dim 2 and see in dim 1

Some few points

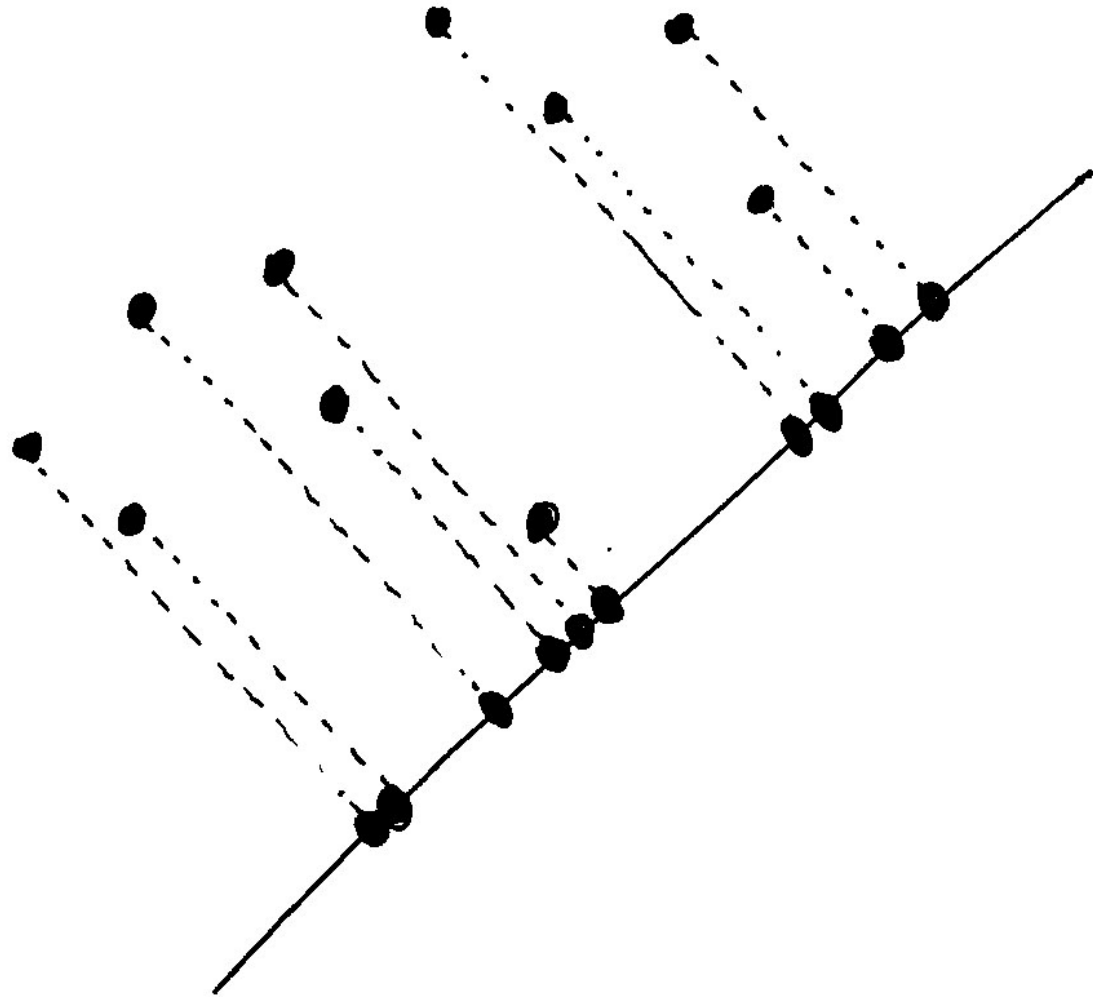


Projections on coordinate axes



Are these views interesting?

Interesting projection



How to find it?

Math in two dimensions: projections

Into the x coordinate - the direction of $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$: $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \mapsto x_1$

Into the y coordinate - the direction of $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$: $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \mapsto x_2$

Into the direction of $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$: $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \mapsto x_1 + x_2$ (???)

... not really! we have to adjust the scale!

Projection into the direction of $\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$ - use inner product:

$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \mapsto a_1 x_1 + a_2 x_2$, provided the length of $\left\| \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \right\| = 1$

$\left\| \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \right\| = 1$ means $\sqrt{a_1^2 + a_2^2} = 1$, equivalent to $a_1^2 + a_2^2 = 1$

Compact matrix notation, general dimension

The projection of \mathbf{x} into the direction of \mathbf{a} such that $\|\mathbf{a}\| = 1$

is $\mathbf{x} \mapsto \mathbf{a}^T \mathbf{x}$

(Note: inner product in the matrix notation is $\mathbf{a}^T \mathbf{x} = \mathbf{x}^T \mathbf{a}$)

What if $\|\mathbf{a}\| \neq 1$?

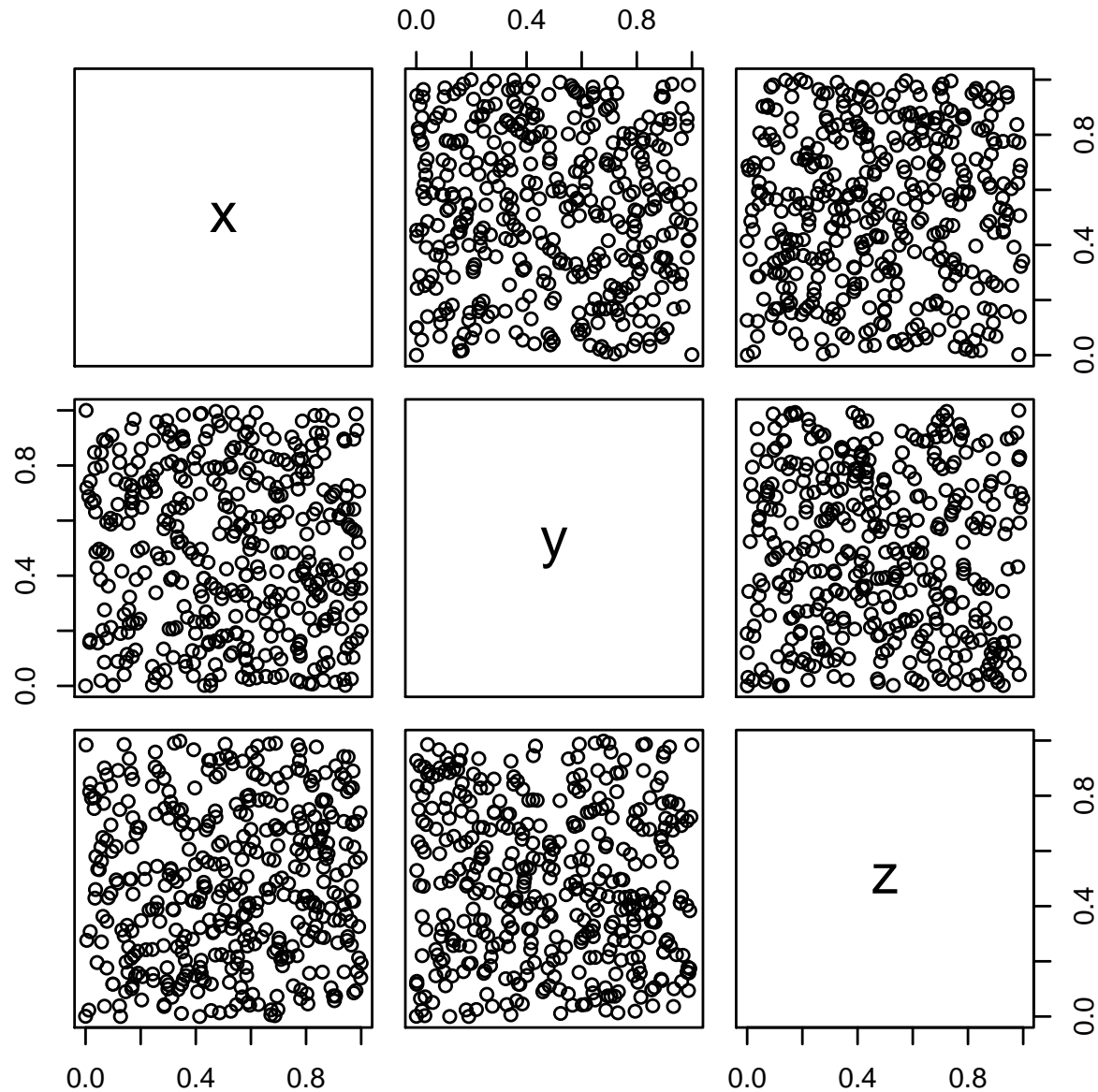
Then we take $\mathbf{a}_0 = \frac{\mathbf{a}}{\|\mathbf{a}\|}$, and $\mathbf{x} \mapsto \mathbf{a}_0^T \mathbf{x} = \left(\frac{\mathbf{a}}{\|\mathbf{a}\|} \right)^T \mathbf{x}$

Try it for the examples above! In particular,

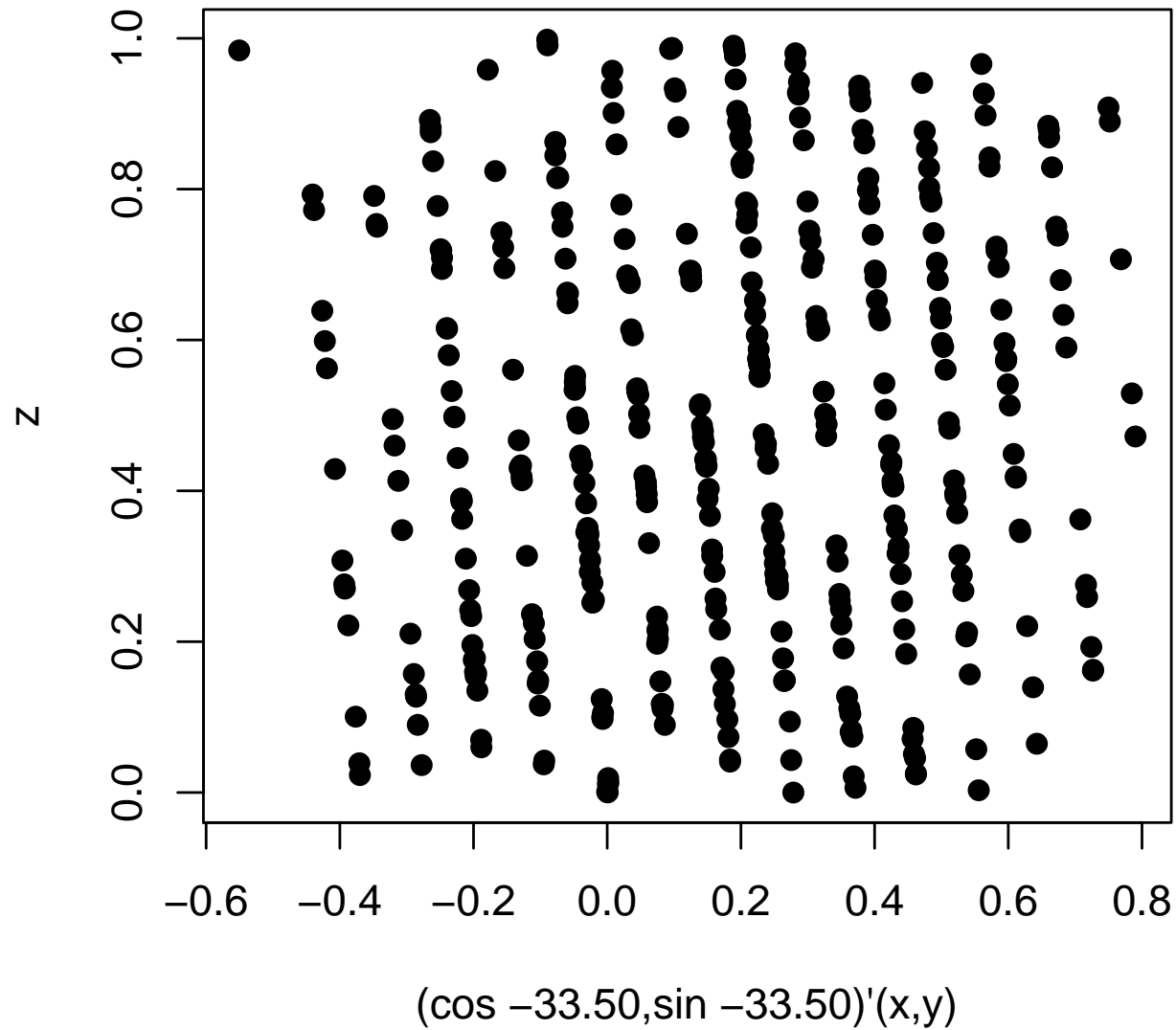
projection into direction of $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ is $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \mapsto \frac{x_1 + x_2}{\sqrt{2}}$

- a linear function $\frac{1}{\sqrt{2}}x_1 + \frac{1}{\sqrt{2}}x_2$

Example: a random generator...



...and a lousy one!



How was it done: the R code

```
> data(randu)
> pairs(randu)
> plot(as.matrix(randu) %*%
+ c(cos(pi*(-33.50)/180),sin(pi*(-33.50)/180),0),
+ as.matrix(randu) %*% c(0,0,1),
+ xlab="(cos -33.50,sin -33.50)'(x,y)", ylab="z", pch=16)
```

Is there an (automatic) way to find interesting projections?

Digression: qualitative (categorical) data

Qualitative - discrete variables

Can arise by themselves, or be created by `cut()` from quantitative. If we have data recorded by items, we can use `table()` to create the cross-tabulated form. Otherwise, data with qualitative variables often come already in a tabular form.

Example: Hair and eye color and sex in 592 statistics students

```
> HairEyeColor
```

```
, , Sex = Male
```

```
Eye
```

```
Hair      Brown Blue Hazel Green
```

```
Black      32   11   10     3
```

```
Brown      53   50   25    15
```

```
Red         10   10    7     7
```

```
Blond        3   30    5     8
```

```
, , Sex = Female
```

```
Eye
```

```
Hair      Brown Blue Hazel Green
```

```
Black      36    9    5     2
```

```
Brown      66   34   29    14
```

```
Red         16    7    7     7
```

```
Blond        4   64    5     8
```

```
> class(HairEyeColor)
```

```
[1] "table"
```

As data frame

The inverse of `table()` is

```
> hair=as.data.frame(HairEyeColor)
```

```
> hair
```

	Hair	Eye	Sex	Freq					
1	Black	Brown	Male	32	17	Black	Brown	Female	36
2	Brown	Brown	Male	53	18	Brown	Brown	Female	66
3	Red	Brown	Male	10	19	Red	Brown	Female	16
4	Blond	Brown	Male	3	20	Blond	Brown	Female	4
5	Black	Blue	Male	11	21	Black	Blue	Female	9
6	Brown	Blue	Male	50	22	Brown	Blue	Female	34
7	Red	Blue	Male	10	23	Red	Blue	Female	7
8	Blond	Blue	Male	30	24	Blond	Blue	Female	64
9	Black	Hazel	Male	10	25	Black	Hazel	Female	5
10	Brown	Hazel	Male	25	26	Brown	Hazel	Female	29
11	Red	Hazel	Male	7	27	Red	Hazel	Female	7
12	Blond	Hazel	Male	5	28	Blond	Hazel	Female	5
13	Black	Green	Male	3	29	Black	Green	Female	2
14	Brown	Green	Male	15	30	Brown	Green	Female	14
15	Red	Green	Male	7	31	Red	Green	Female	7
16	Blond	Green	Male	8	32	Blond	Green	Female	8

Conversion back?

Not `table()`, but `xtabs()`.

```
> xtabs(Freq~Hair+Eye+Sex,data=hair) # xtabs(Freq~.,data=hair)
```

```
, , Sex = Male
```

```
      Eye
```

Hair	Brown	Blue	Hazel	Green
Black	32	11	10	3
Brown	53	50	25	15
Red	10	10	7	7
Blond	3	30	5	8

```
, , Sex = Female
```

```
      Eye
```

Hair	Brown	Blue	Hazel	Green
Black	36	9	5	2
Brown	66	34	29	14
Red	16	7	7	7
Blond	4	64	5	8

We may need (?) to declare the right class: `class(.)="table"`.

But also “something like” the original data

```
> hairdat=hair[rep(row.names(hair),hair$Freq),1:3]
```

```
> hairdat
```

	Hair	Eye	Sex
1	Black	Brown	Male
1.1	Black	Brown	Male
1.2	Black	Brown	Male
...			
32.6	Blond	Green	Female
32.7	Blond	Green	Female

```
> table(hairdat)
```

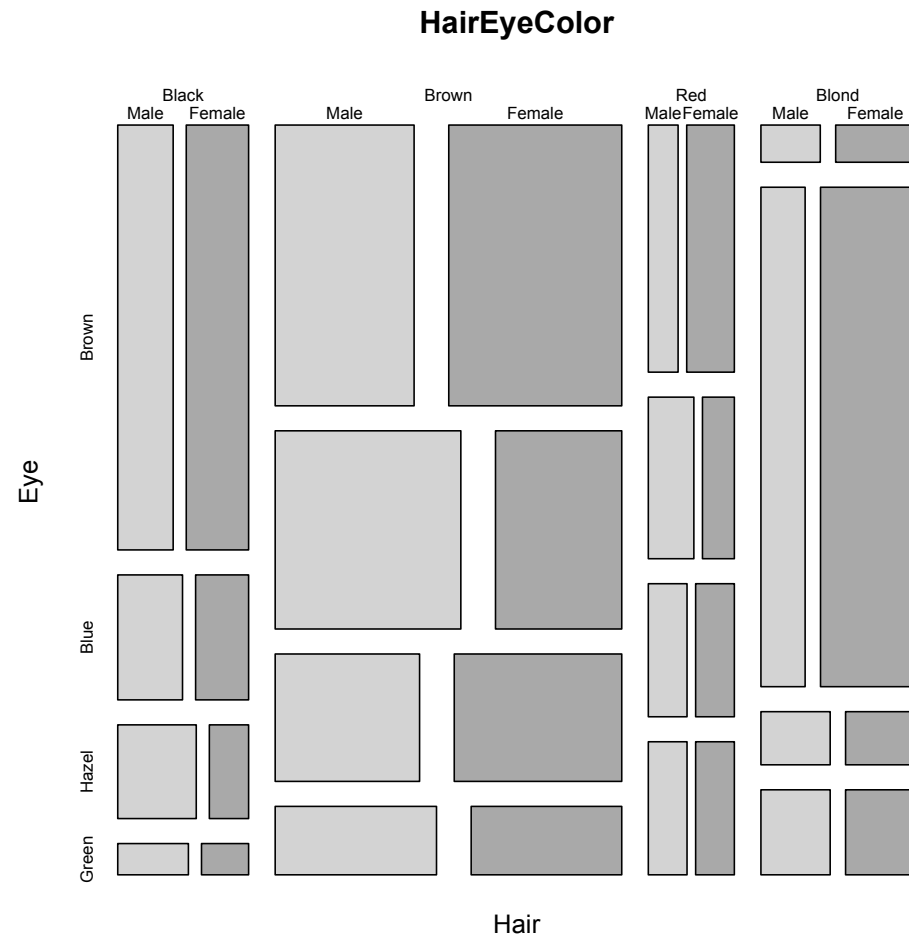
		Sex = Male

		Eye			
Hair		Brown	Blue	Hazel	Green
Black		32	11	10	3
...					
Red		16	7	7	7
Blond		4	64	5	8

Plotting

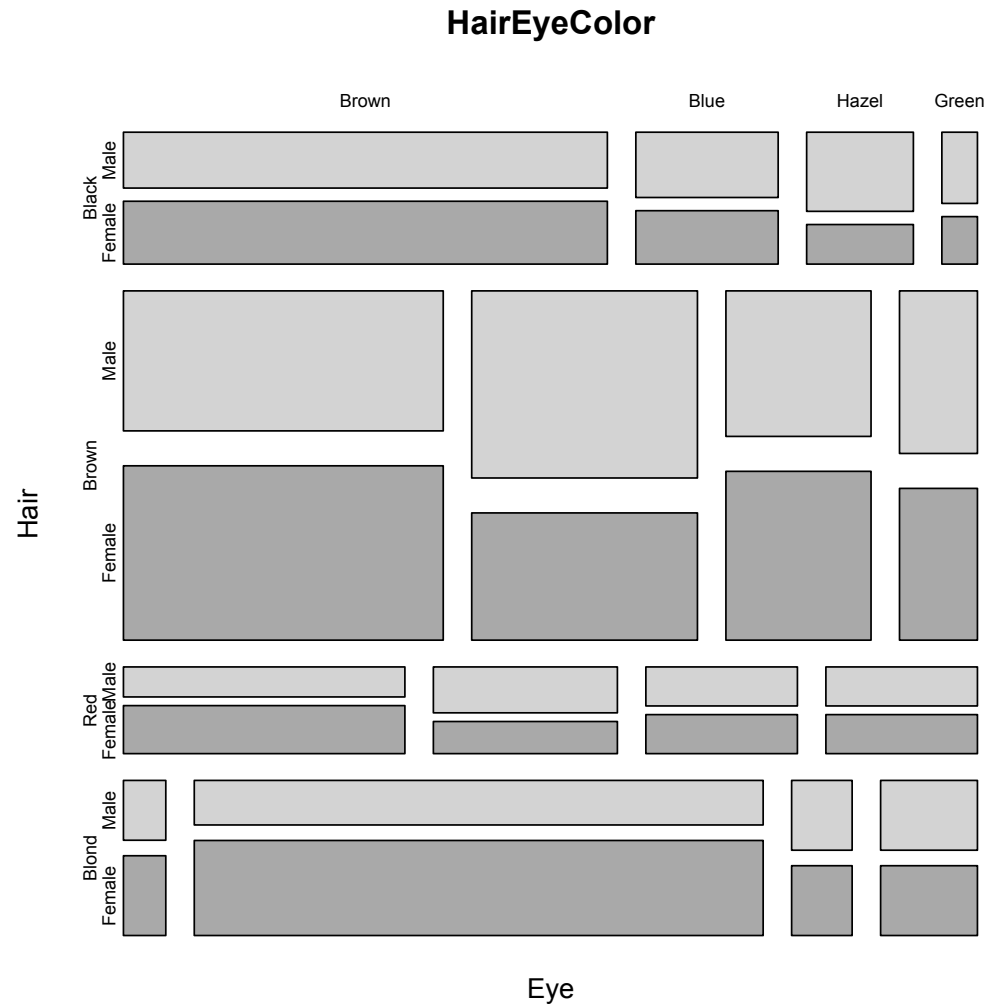
As pie charts, we leave also the “3D histograms” to programs like Excel. A real statistician uses something else: for instance

```
> mosaicplot(HairEyeColor, color=c("lightgray","darkgray"))
```



We can control it

```
> mosaicplot(HairEyeColor,  
+ color=c("lightgray","darkgray"), dir=c("h","v","h"))
```



How about eye and hair color aggregated?

That is, among “statisticiens et statisticiennes” ...

```
> haireye=apply(HairEyeColor,1:2,sum)
```

```
> haireye
```

	Eye			
Hair	Brown	Blue	Hazel	Green
Black	68	20	15	5
Brown	119	84	54	29
Red	26	17	14	14
Blond	7	94	10	16

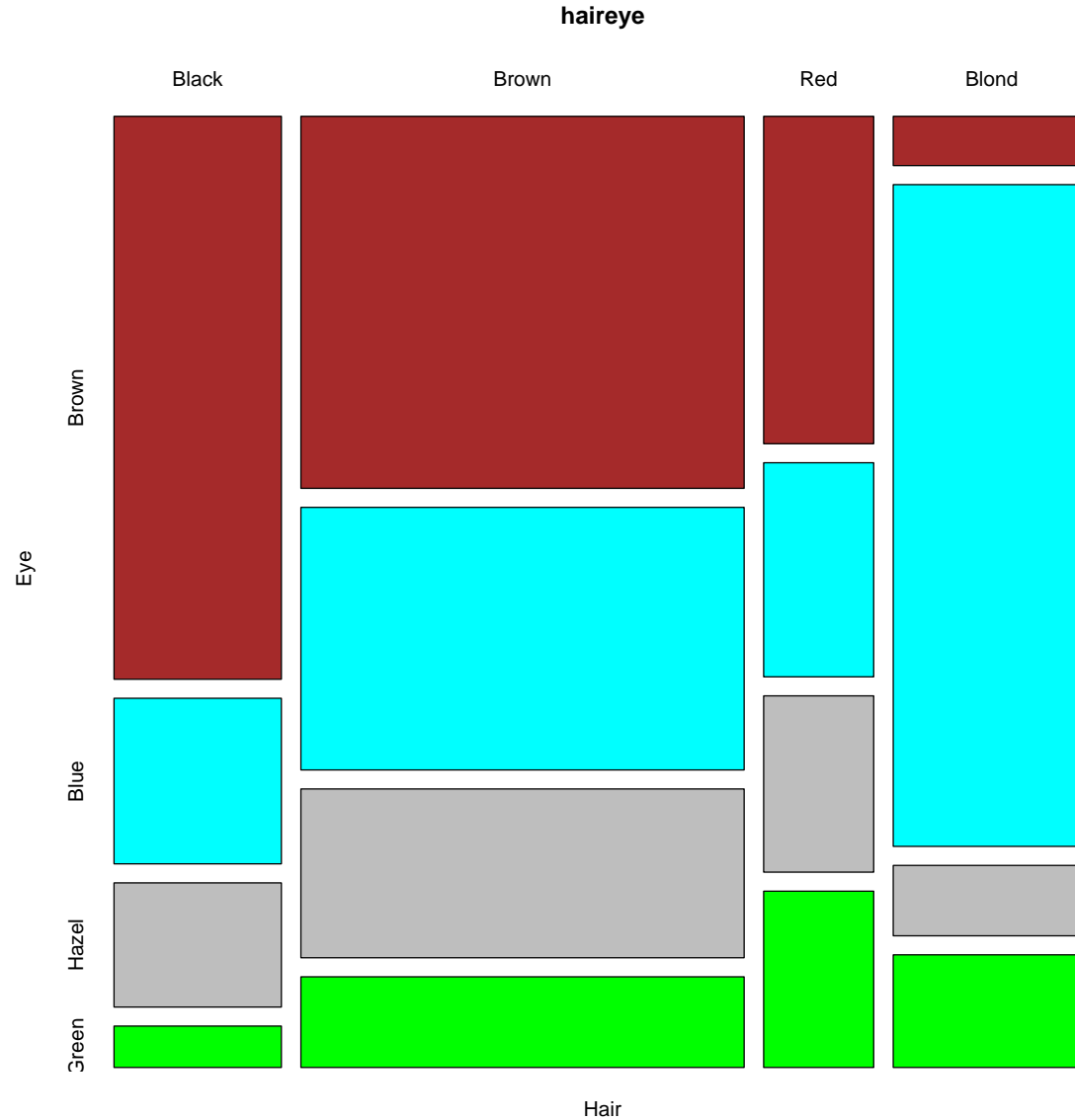
```
> mosaicplot(haireye, color=c("brown","blue","grey","green"))
```

And give it nice colors...

Try also:

```
> mosaicplot(haireye,  
+ color=c("brown","blue","grey","green"),cex=1)
```

In color



What else we can do?

Log-linear models

...as a special case of `glm()`. For frequency data, the distribution is Poisson; the link is the logarithm function. That is, we construct a linear model where the response are logarithms of *expected* frequencies.

We see why we needed to convert the table to the data frame:

```
> hairglm=glm(Freq~Hair*Eye*Sex,family=poisson, data=hair)
> anova(hairglm,test="Chisq")
```

	Df	Deviance	Resid.	Df	Resid.	Dev	Pr(>Chi)
NULL				31		475.12	
Hair	3	165.592		28		309.53	< 2e-16 ***
Eye	3	141.272		25		168.25	< 2e-16 ***
Sex	1	1.954		24		166.30	0.16218
Hair:Eye	9	146.444		15		19.86	< 2e-16 ***
Hair:Sex	3	8.093		12		11.76	0.04413 *
Eye:Sex	3	5.002		9		6.76	0.17162
Hair:Eye:Sex	9	6.761		0		0.00	0.66196

Try also `summary(hairglm)`, to see why we prefer `anova(hairglm)` here. On the other hand, the problem of `anova()` is that the p-values are for incremental composite hypotheses.

Incremental anova

```
> hairtwo=glm(Freq~(Hair+Eye+Sex)^2,data=hair,family=poisson)
> hairsp=glm(Freq~Hair+Eye+Sex+Hair:Eye+Hair:Sex,data=hair,family=poisson)
> anova(hairtwo,hairstwo,test="Chisq")
...
Model 1: Freq ~ (Hair + Eye + Sex)^2
Model 2: Freq ~ Hair * Eye * Sex
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1          9      6.7613
2          0      0.0000  9   6.7613   0.662
> anova(hairsp,hairstwo,test="Chisq")
...
Model 1: Freq ~ Hair + Eye + Sex + Hair:Eye + Hair:Sex
Model 2: Freq ~ Hair * Eye * Sex
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1         12      11.764
2          0       0.000 12   11.764   0.4648
> anova(hairsp,hairtwo,test="Chisq")
...
Model 1: Freq ~ Hair + Eye + Sex + Hair:Eye + Hair:Sex
Model 2: Freq ~ (Hair + Eye + Sex)^2
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1         12      11.7637
2          9       6.7613  3   5.0025   0.1716
```

Also

```
> hairind=glm(Freq~Hair+Eye+Sex,family=poisson, data=hair)
> hairnosex=glm(Freq~Hair*Eye+Sex,family=poisson, data=hair)
> anova(hairnosex,hairstlm,test="Chisq")
...
Model 1: Freq ~ Hair * Eye + Sex
Model 2: Freq ~ Hair * Eye * Sex
  Resid. Df Resid. Dev Df Deviance Pr(>Chi)
1         15      19.857
2          0         0.000 15   19.857  0.1775
> anova(hairind,hairstlm,test="Chisq")
...
Model 1: Freq ~ Hair + Eye + Sex
Model 2: Freq ~ Hair * Eye * Sex
  Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
1         24      166.3
2          0         0.0 24   166.3 < 2.2e-16 ***
> anova(hairind,hairnosex,test="Chisq")
...
Model 1: Freq ~ Hair + Eye + Sex
Model 2: Freq ~ Hair * Eye + Sex
  Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
1         24      166.300
2         15      19.857  9   146.44 < 2.2e-16 ***
```


Predicted frequencies under independence

Let us take predicted values under the additive model—which in the context of qualitative data means independence: all three variables, Sex, Color of Hair, and Color of Eyes, are independent.

```
> hairpr=predict(hairind,type="response")
> xtabs(hairpr~.,cbind(hair[,1:3],hairpr))
, , Sex = Male
```

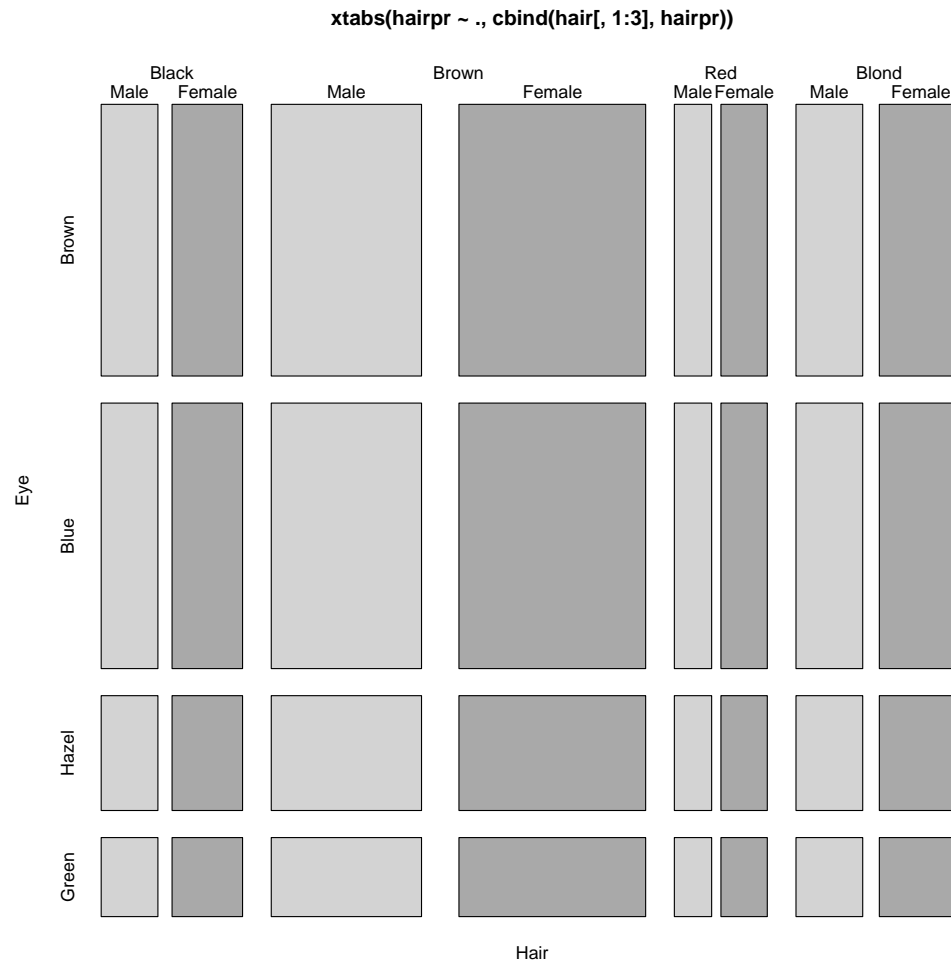
	Eye			
Hair	Brown	Blue	Hazel	Green
Black	18.915038	18.485151	7.995903	5.502557
Brown	50.089824	48.951419	21.174335	14.571585
Red	12.434886	12.152275	5.256566	3.617421
Blond	22.242684	21.737168	9.402589	6.470599

```
, , Sex = Female
```

	Eye			
Hair	Brown	Blue	Hazel	Green
Black	21.220097	20.737822	8.970314	6.173119
Brown	56.193960	54.916825	23.754719	16.347334
Red	13.950249	13.633198	5.897151	4.058254
Blond	24.953262	24.386142	10.548424	7.259131

A picture?

```
> mosaicplot(xtabs(hairpr~., cbind(hair[,1:3], hairpr)),  
+ color=c("lightgray", "darkgray"))
```



Not that interesting...

We would rather like to see residuals

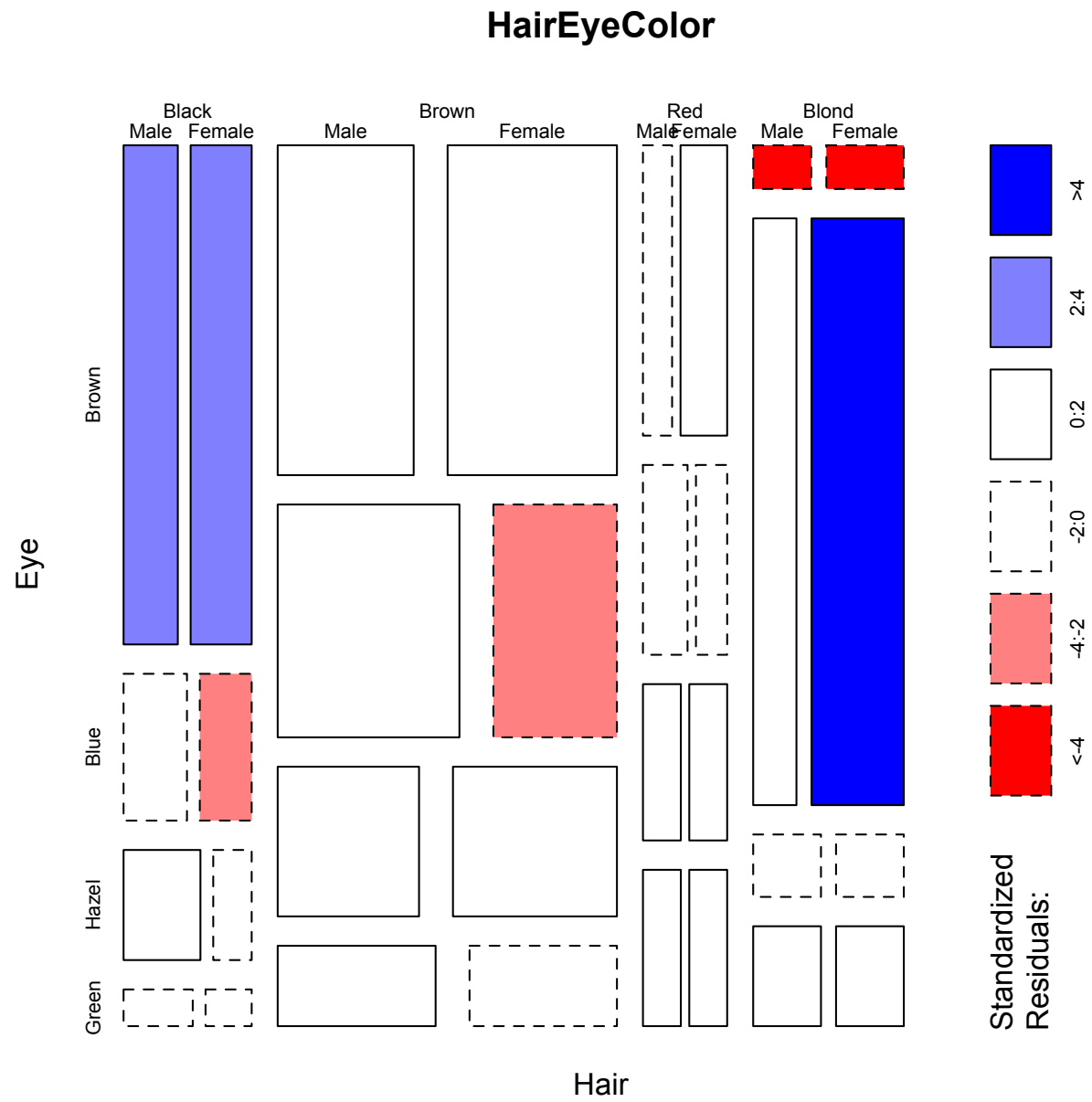
```
> hairr=residuals(hairind,type="response")
> xtabs(hairr~.,cbind(hair[,1:3],hairr))
, , Sex = Male
      Eye
Hair      Brown      Blue      Hazel      Green
  Black  13.0849617  -7.4851511   2.0040974  -2.5025566
  Brown   2.9101762   1.0485813   3.8256654   0.4284149
  Red    -2.4348863  -2.1522753   1.7434344   3.3825785
  Blond -19.2426840   8.2628316  -4.4025891   1.5294010
, , Sex = Female
      Eye
Hair      Brown      Blue      Hazel      Green
  Black  14.7799032 -11.7378219  -3.9703136  -4.1731191
  Brown   9.8060400 -20.9168246   5.2452805  -2.3473338
  Red     2.0497512  -6.6331977   1.1028494   2.9417458
  Blond -20.9532620  39.6138576  -5.5484244   0.7408692
> mosaicplot(HairEyeColor, shade=T, margin=list(1,2,3))
> hairlm=loglin(HairEyeColor, list(1, 2, 3))
2 iterations: deviation 5.684342e-14
> pchisq(hairlm$pearson, hairlm$df, lower.tail = FALSE)
[1] 5.320872e-23
```

Extended mosaic plot - with shading

The *extended mosaic plot* shows also the residuals from the log-linear fit, by shading; the fit is done not by `glm()`, but using function `loglin()`, which is handy when we want to see the result of the χ^2 test for independence. We can check that the predictions are the same:

```
> haipar=loglin(HairEyeColor,margin=list(1,2,3),para=T)$para
2 iterations: deviation 5.684342e-14
> as.vector(exp(outer(outer(outer(haipar[[1]],haipar[[2]],"+"),
+ haipar[[3]],"+"),haipar[[4]],"+"))))
 [1] 18.915038 50.089824 12.434886 22.242684 18.485151 48.951419 12.152275
 [8] 21.737168  7.995903 21.174335  5.256566  9.402589  5.502557 14.571585
[15]  3.617421  6.470599 21.220097 56.193960 13.950249 24.953262 20.737822
[22] 54.916825 13.633198 24.386142  8.970314 23.754719  5.897151 10.548424
[29]  6.173119 16.347334  4.058254  7.259131
```

The plot



What did we achieve?

We can see, among other things, that there are more brown-haired, black-eyed individuals and more blond-haired, blue-eyed individuals (especially women) among statistics students than the independence model would suggest. On the other hand, blue-eyed, black- and brown-haired females are underrepresented. Also blondes with brown eyes are rare.

A technical detail: the shading in the mosaic plot works not with “raw” (`type="response"`) residuals, but “Pearson” residuals (`type="pearson"`)

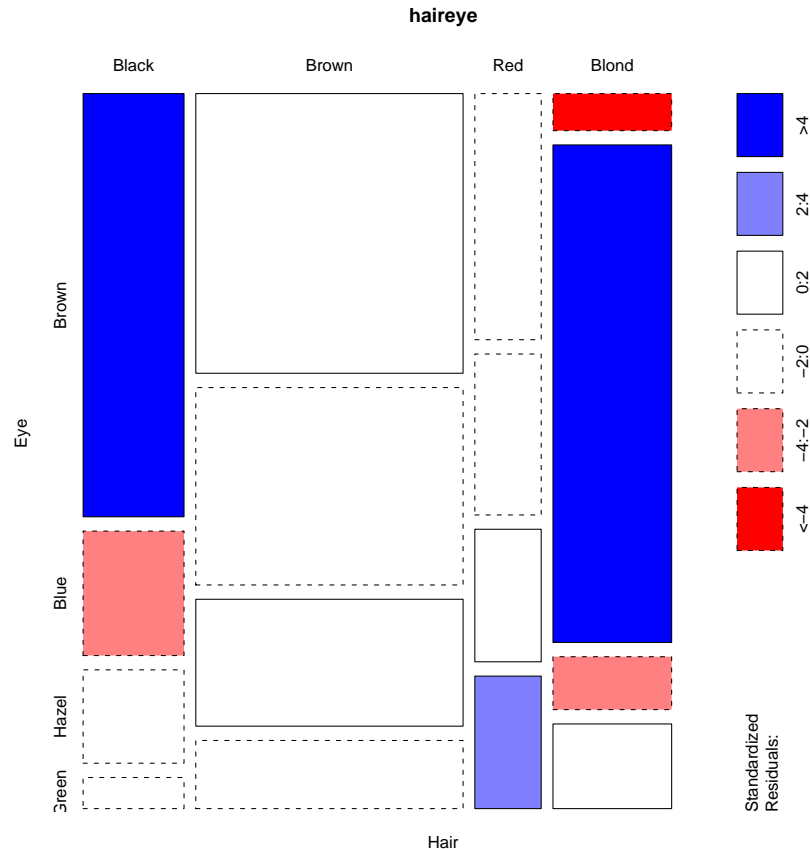
$$\frac{O - P}{\sqrt{P}}$$

O being observed and P predicted frequency

Check it out

```
> hairpea=residuals(hairind,type="pearson")
> as.numeric(hairpea)
 [1]  3.0086304  0.4111919 -0.6904906 -4.0801117 -1.7409611  0.1498716 -0.6174034  1.7722599
 [9]  0.7087370  0.8313848  0.7604218 -1.4357685 -1.0668458  0.1122306  1.7784773  0.6012418
[17]  3.2084695  1.3081238  0.5487950 -4.1945752 -2.5775431 -2.8225591 -1.7964870  8.0218693
[25] -1.3256260  1.0762019  0.4541456 -1.7083462 -1.6796100 -0.5805657  1.4602779  0.2749788
> as.numeric((hair$Freq-hairpr)/sqrt(hairpr))
 [1]  3.0086304  0.4111919 -0.6904906 -4.0801117 -1.7409611  0.1498716 -0.6174034  1.7722599
 [9]  0.7087370  0.8313848  0.7604218 -1.4357685 -1.0668458  0.1122306  1.7784773  0.6012418
[17]  3.2084695  1.3081238  0.5487950 -4.1945752 -2.5775431 -2.8225591 -1.7964870  8.0218693
[25] -1.3256260  1.0762019  0.4541456 -1.7083462 -1.6796100 -0.5805657  1.4602779  0.2749788
> hairq=as.numeric(cut(hairpea,c(-Inf,-4,-2,0,2,4,Inf)))
> xtabs(hairq~.,cbind(hair[,1:3],hairq))
, , Sex = Male
      Eye
Hair   Brown Blue Hazel Green
Black     5     3     4     3
Brown     4     4     4     4
Red       3     3     4     4
Blond     1     4     3     4
, , Sex = Female
      Eye
Hair   Brown Blue Hazel Green
Black     5     2     3     3
Brown     4     2     4     3
Red       4     3     4     4
Blond     1     6     3     4
```

Aggregated data give similar result



```
> haind=loglin(haireye, list(1, 2))  
2 iterations: deviation 0  
> pchisq(haind$pearson, haind$df, lower.tail = FALSE)  
[1] 2.325287e-25
```

For qualitative data, it is quite easy to get the hypothesis of independence rejected... but how to find out more?

How to find out more

Log-linear modeling is a way to go; for instance, we can look at the model that sex is independent conditionally on hair and eye colors. What does that mean? Color of eyes and hair are dependent, but there is no dependence between these two and the sex: the chance of encountering a blue-eye blonde man is given by the proportion of blue-eyed blondes (man or women) and the proportion of men about among statistics students

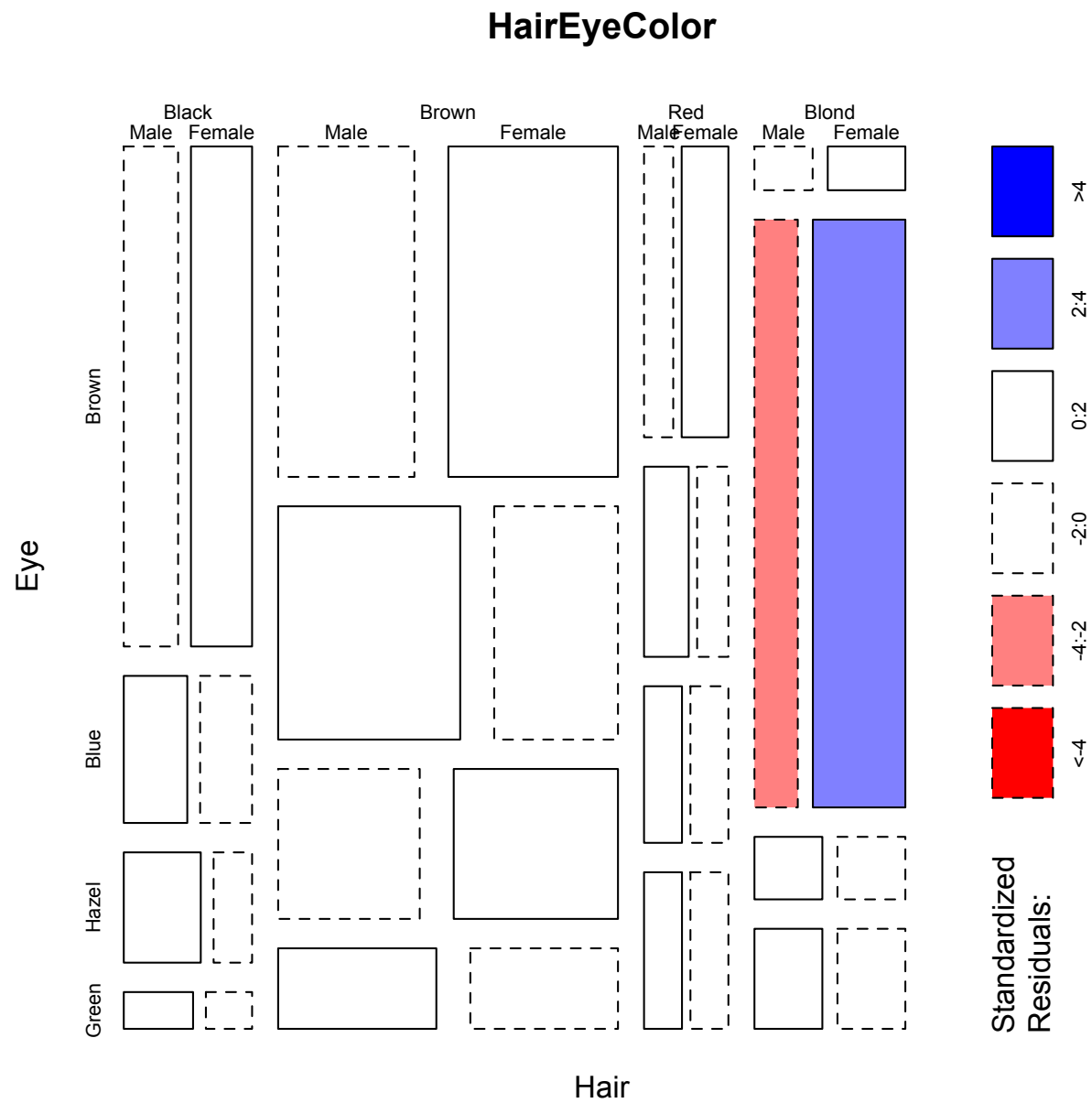
```
> haicind = loglin(HairEyeColor,margin=list(c(1,2),3))
2 iterations: deviation 5.684342e-14
> pchisq(haicind$pearson, haicind$df, lower.tail = FALSE)
[1] 0.1891745
> mosaicplot(HairEyeColor,margin=list(c(1,2),3),shade=T)
```

The plot shows that this fits much better; the most of the discrepancy (pretty much only important from the fitted model) is due to blonde and blue-eyed men and women.

Lack of dependence \equiv lack of (nonzero) interaction

Another way (other than log-linear modeling) to investigate the roots of dependence: correspondence analysis (see later)

Sex vs. hair-eye independence model



What is the corresponding glm model?

```
> haircind=glm(formula = Freq ~ Hair*Eye + Sex, family = poisson, data = hair)
> as.numeric(predict(haircind,type="response"))
[1] 32.047297 56.082770 12.253378 3.298986 9.425676 39.587838 8.011824 44.300676 7.069257
[10] 25.449324 6.597973 4.712838 2.356419 13.667230 6.597973 7.540541 35.952703 62.917230
...
> haicpar=loglin(HairEyeColor,margin=list(c(1,2),3),par=T)$param
> as.vector(exp(outer(outer(outer(haicpar[[1]],haicpar[[2]],"+"),
+ haicpar[[3]],"+"),haicpar[[4]],"+")+rep(as.vector(haicpar[[5]]),2)))
[1] 32.047297 56.082770 12.253378 3.298986 9.425676 39.587838 8.011824 44.300676 7.069257
[10] 25.449324 6.597973 4.712838 2.356419 13.667230 6.597973 7.540541 35.952703 62.917230
...
> haircr=residuals(haircind,type="pearson")
> haircq=as.numeric(cut(haircr,c(-Inf,-4,-2,0,2,4,Inf)))
> xtabs(haircq~.,cbind(hair[,1:3],haircq))
, , Sex = Male
```

	Eye			
Hair	Brown	Blue	Hazel	Green
Black	3	4	4	4
Brown	3	4	3	4
Red	3	4	4	4
Blond	3	2	4	4

, , Sex = Female

	Eye			
Hair	Brown	Blue	Hazel	Green
Black	4	3	3	3
Brown	4	3	4	3
Red	4	3	3	3
Blond	4	5	3	3

Dimension reduction for quantitative data: principal components

Something more sophisticated

Principal components: aim at finding the projections showing the data maximally spread

The measure of spread here is variance: that is, principal components look for directions in which the projected data exhibit maximal variance

The first definition (equivalent to the current one, but not that much used now) given by Pearson (1901): the first principal component is the projection of the datapoints in the direction of the line giving the best orthogonal regression fit to the data points (the sum of squared geometric (orthogonal) distances of points to the line is minimal). In other words, first principal component consists of projections of datapoints giving best orthogonal fit of the data.

The best fit of this type should pass through the mean; hence it is reasonable to consider centered datapoints $\mathbf{y}_i - \bar{\mathbf{y}}$.

Had to wait 50 years to become computationally feasible

The currently used definition of Hotelling

1. **A first principal (component) direction** is a unit vector \mathbf{a}_1 , maximizing the (sample) variance of the projection into its direction: maximizing $s_{\mathbf{Y}\mathbf{a}_1}^2 = \mathbf{a}_1^T \mathbf{S}_Y \mathbf{a}_1$ under $\mathbf{a}_1^T \mathbf{a}_1 = 1$

The first principal component is then that projection, $\mathbf{Y}\mathbf{a}_1$

2. **A second principal (component) direction** is a unit vector \mathbf{a}_2 , orthogonal to \mathbf{a}_1 , maximizing the (sample) variance of the projection into its direction: maximizing $s_{\mathbf{Y}\mathbf{a}_2}^2 = \mathbf{a}_2^T \mathbf{S}_Y \mathbf{a}_2$ under $\mathbf{a}_2^T \mathbf{a}_2 = 1$ and $\mathbf{a}_1^T \mathbf{a}_2 = 0$

The second principal component is then that projection, $\mathbf{Y}\mathbf{a}_2$

3. **A third principal (component) direction** is a unit vector \mathbf{a}_3 , orthogonal to \mathbf{a}_1 and \mathbf{a}_2 , maximizing the (sample) variance of the projection into its direction: maximizing $s_{\mathbf{Y}\mathbf{a}_3}^2 = \mathbf{a}_3^T \mathbf{S}_Y \mathbf{a}_3$ under $\mathbf{a}_3^T \mathbf{a}_3 = 1$ and $\mathbf{a}_1^T \mathbf{a}_3 = 0$, $\mathbf{a}_2^T \mathbf{a}_3 = 0$,

The third principal component is then that projection, $\mathbf{Y}\mathbf{a}_3$

... and so on, up to p principal components

Note: maximizing variance is equivalent to maximizing its square root, standard deviation

Let us try it on the male track data

```
> trackmen.pc <- prcomp(trackmen)
```

```
> summary(trackmen.pc)
```

Importance of components:

	PC1	PC2	PC3	PC4	PC5	PC6
Standard deviation	9.4823	1.1885	0.50975	0.33079	0.1652	0.11284
Proportion of Variance	0.9801	0.0154	0.00283	0.00119	0.0003	0.00014
Cumulative Proportion	0.9801	0.9955	0.99834	0.99953	0.9998	0.99997

```
> trackmen.pc
```

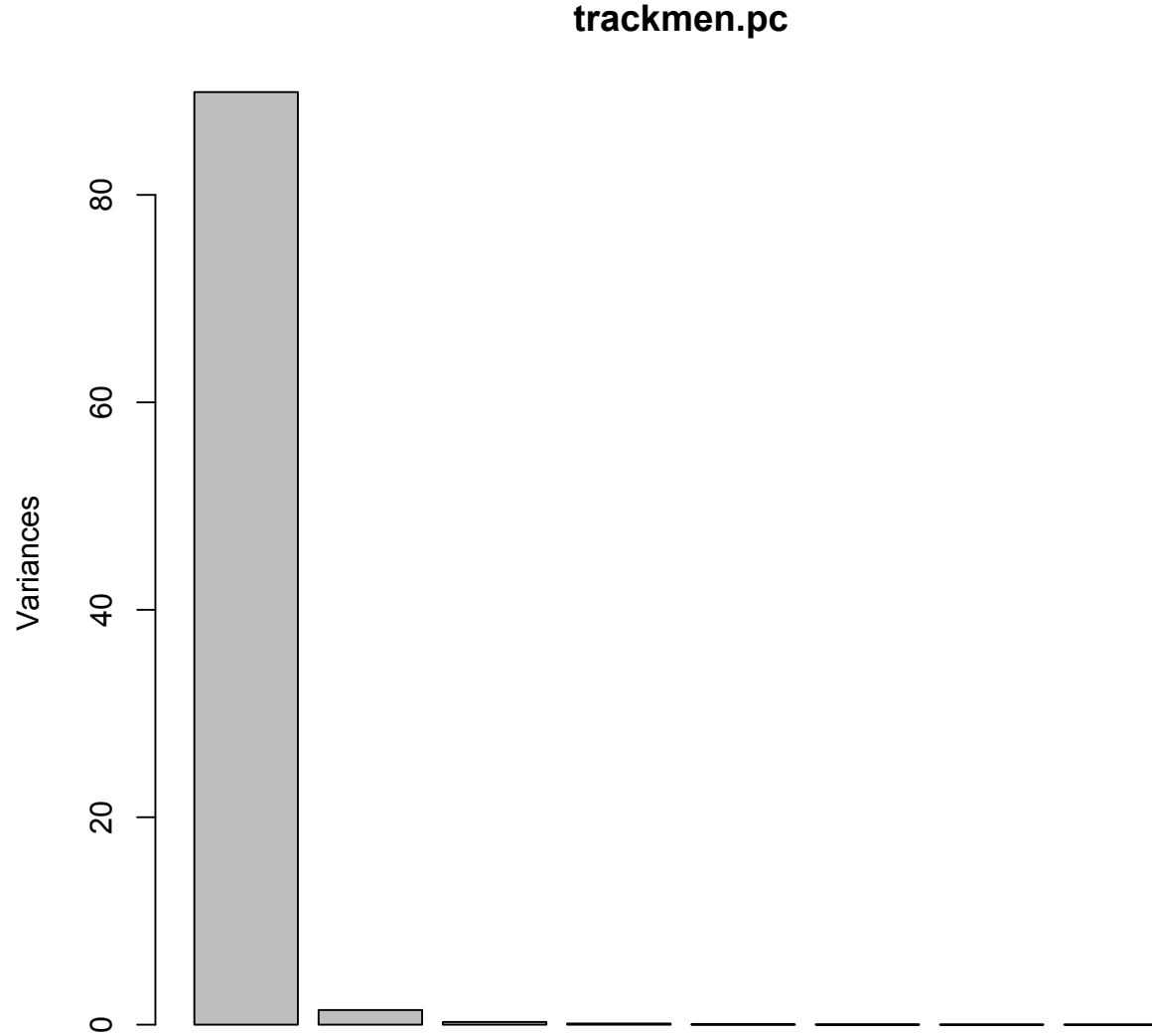
Standard deviations (1, .., p=8):

```
[1] 9.48227935 1.18853948 0.50974911 0.33078740 0.16522894 0.1128397
```

Rotation (n x k) = (8 x 8):

	PC1	PC2	PC3	PC4	PC5
s1	0.019865407	0.21068958	-0.029041979	0.358784470	0.190181784
s2	0.041554499	0.35892579	-0.018390126	0.833534544	-0.048582165
s4	0.110631838	0.82786251	-0.377669011	-0.396041212	-0.012020033
m8	0.005487699	0.02317490	0.005341591	0.009568087	-0.011107487
m15	0.014386822	0.04465255	0.050004337	0.015981502	-0.043222520
m50	0.079308444	0.12996134	0.336448522	-0.018873808	-0.909186992
m100	0.181098994	0.29885393	0.848722695	-0.134662690	0.364239482
m421	0.972787446	-0.18080736	-0.141872114	0.028425488	0.006575083

The screeplot



```
> plot(trackmen.pc)
```


And perhaps also this

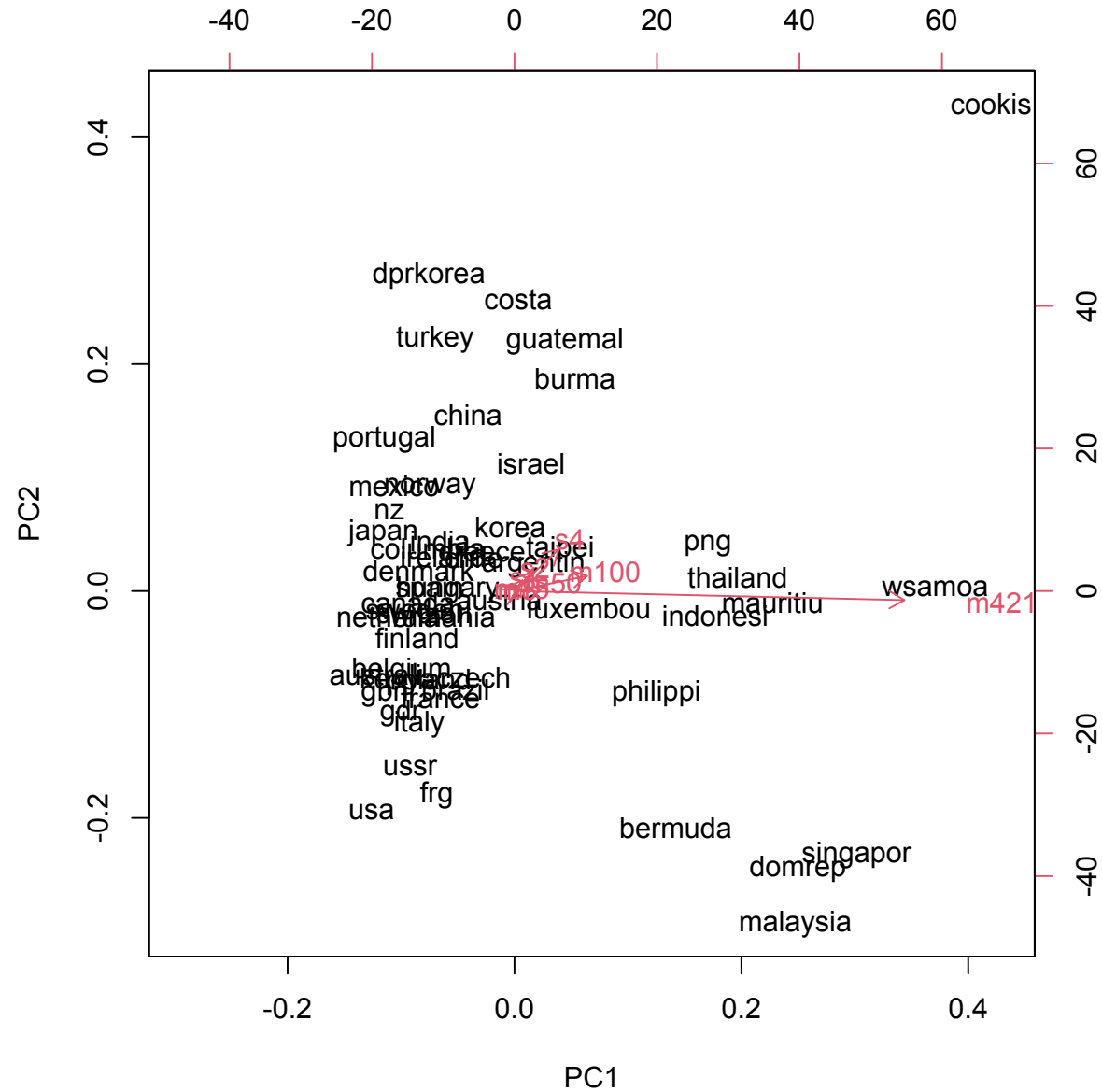
“Loadings” = principal component directions

```
> trackmen.pc2 <- princomp(trackmen)
> trackmen.pc2$loadings
```

Loadings:

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5	Comp.6	Comp.7	Comp.8
s1		0.211		0.359	0.190	0.887		
s2		0.359		0.834		-0.410		
s4	0.111	0.828	0.378	-0.396				
m8							0.261	-0.965
m15							0.959	0.262
m50		0.130	-0.336		-0.909	0.184		
m100	0.181	0.299	-0.849	-0.135	0.364			
m421	0.973	-0.181	0.142					
...								

And possibly also this: the biplot



```
> biplot(trackmen.pc)
```

Uses

Overall, one can use of principal components to condense the information in the data - to reduce the dimension: we retain only certain number of the (initial) principal components, typically guided by the “cumulative proportion of the variance explained” - but also by other criteria

Another use can result in finding interesting projections of the data and subsequently interpreting them

Problem

Note that computing principal components out of the original data (that is: out of the variance-covariance matrix) often results merely in emphasizing the “size factor”

Remember: principal components *do change* after changing the scale of variables

Hence, to mitigate the just mentioned drawback, it may be preferable to compute principal components from the *scaled* data: we subtract the means of the columns of \mathbf{Y} from the corresponding columns (obtaining the centered data matrix $\tilde{\mathbf{Y}}$), and then we also divide those columns by their corresponding standard deviations

Computing principal components out of the variance-covariance matrix of the scaled data is equivalent to computing them directly out of the correlation matrix

Like this

```
> trackmen.pcs = prcomp(trackmen,scale=TRUE)
```

```
> summary(trackmen.pcs)
```

Importance of components:

	PC1	PC2	PC3	PC4	PC5	PC6
Standard deviation	2.5734	0.9368	0.39915	0.35221	0.28263	0.2607
Proportion of Variance	0.8278	0.1097	0.01992	0.01551	0.00999	0.0085
Cumulative Proportion	0.8278	0.9375	0.95739	0.97289	0.98288	0.9914

Same as

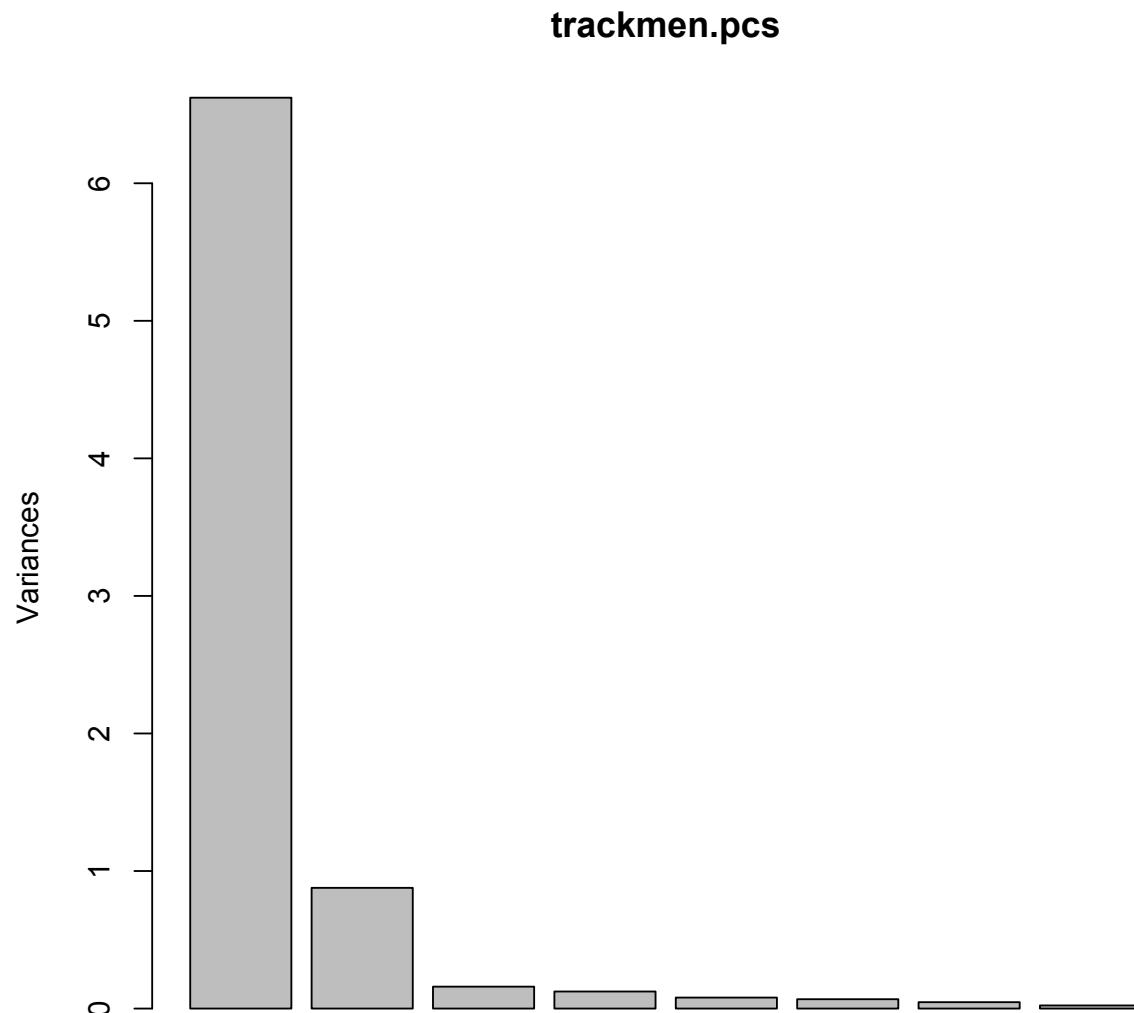
```
> trackmen.pcs = prcomp(scale(trackmen))
```

```
> summary(trackmen.pcs)
```

Importance of components:

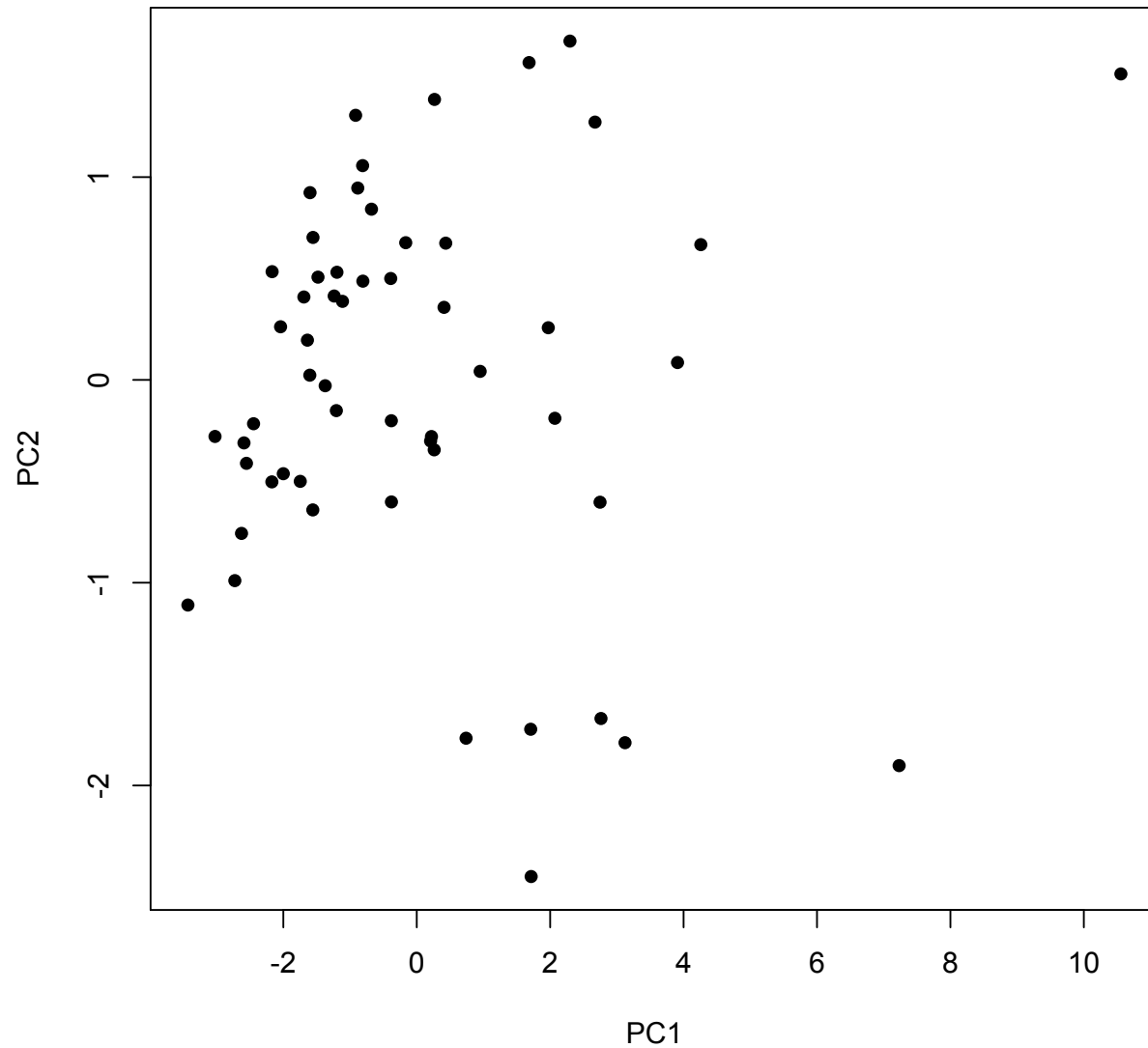
	PC1	PC2	PC3	PC4	PC5	PC6
Standard deviation	2.5734	0.9368	0.39915	0.35221	0.28263	0.2607
Proportion of Variance	0.8278	0.1097	0.01992	0.01551	0.00999	0.0085
Cumulative Proportion	0.8278	0.9375	0.95739	0.97289	0.98288	0.9914

Can you see the difference?



```
> plot(trackmen.pcs)
```

So we may plot the first two components now



```
> plot(predict(trackmen.pcs), pch=16)
```

And look more into them

```
> trackmen.pcs
```

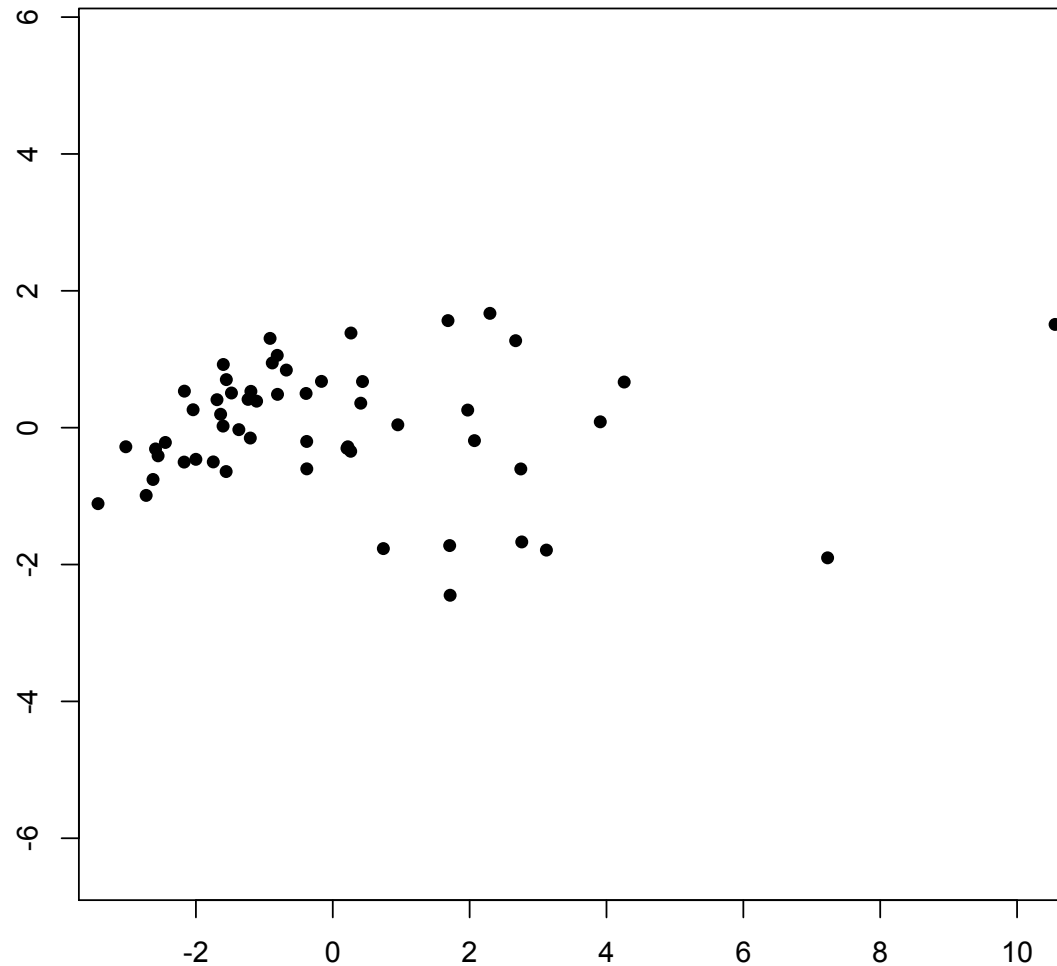
```
Standard deviations (1, ..., p=8):
```

```
[1] 2.5733531 0.9368128 0.3991505 0.3522065 0.2826310 0.2607013 0.21  
[8] 0.1503333
```

```
Rotation (n x k) = (8 x 8):
```

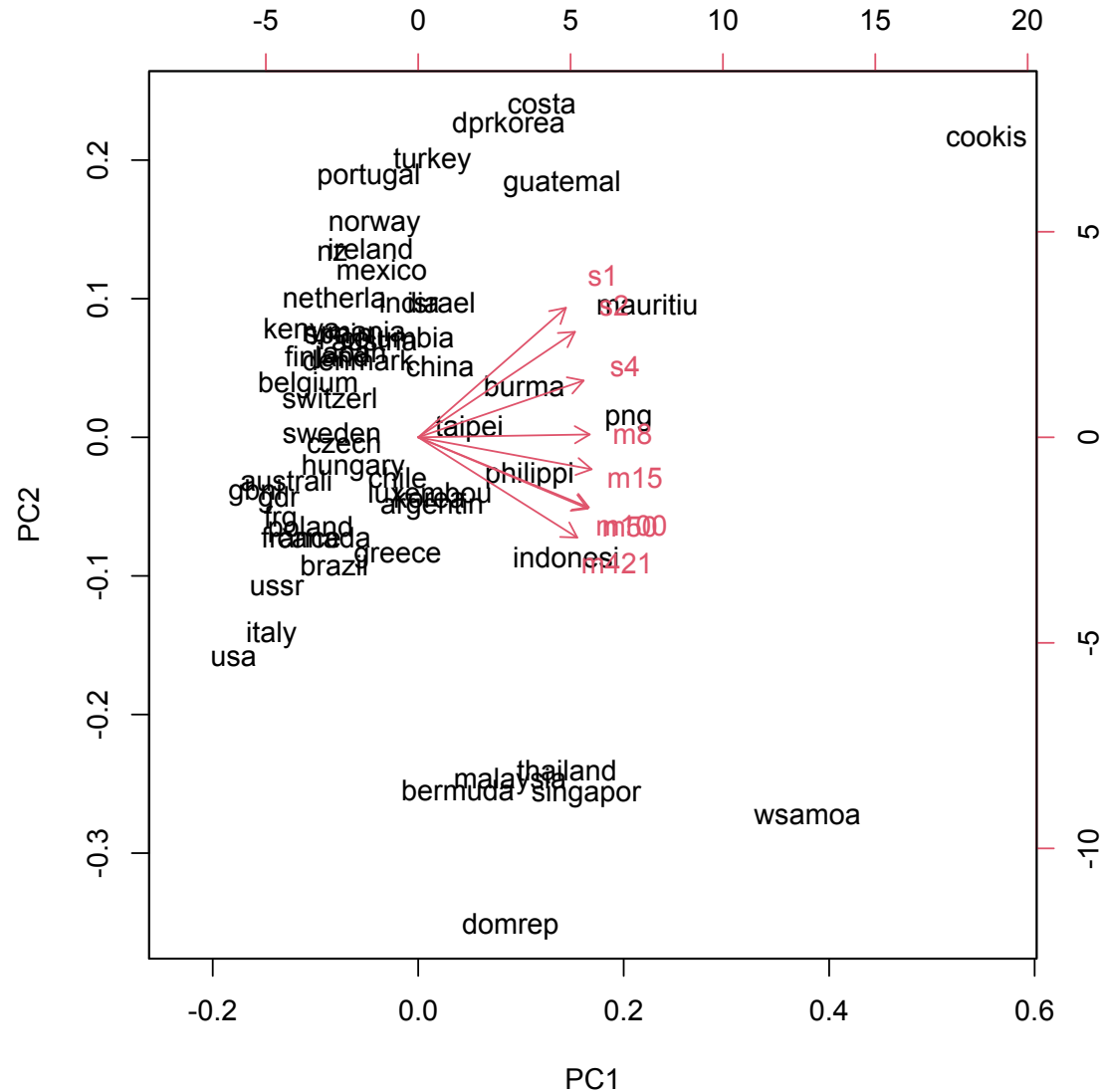
	PC1	PC2	PC3	PC4	PC5	
s1	0.3175565	0.56687750	0.3322620	-0.12762827	0.2625555	-0.5937
s2	0.3369792	0.46162589	0.3606567	0.25911576	-0.1539571	0.6561
s4	0.3556454	0.24827331	-0.5604674	-0.65234077	-0.2183229	0.1566
m8	0.3686841	0.01242993	-0.5324823	0.47999895	0.5400528	-0.0146
m15	0.3728099	-0.13979665	-0.1534427	0.40451039	-0.4877151	-0.1578
m50	0.3643741	-0.31203045	0.1897643	-0.02958755	-0.2539792	-0.1412
m100	0.3667726	-0.30685985	0.1817517	-0.08006862	-0.1331764	-0.2190
m421	0.3419261	-0.43896267	0.2632087	-0.29951213	0.4979283	0.3152

More correct way: an equiscaled plot



```
> library(MASS)
> eqscplot(predict(trackmen.pcs)[,1:2],pch=16)
```

But usually we rather use a biplot



```
> biplot(trackmen.pcs)
> biplot(trackmen.pcs,xlim=c(-0.23,0.57)) # better scaling
```

Biplots of principal components

Biplots handle very well the situation when the first two principal components are plotted (which is often the case)

What is there in “bi”? First, we plot the principal components, the 2-element vectors formed by the corresponding elements of $\mathbf{Y}\mathbf{a}_1$ and $\mathbf{Y}\mathbf{a}_2$. They correspond to the rows of the original data matrix, which implies their possible labels

Then we also plot the 2-element vectors formed by corresponding elements of \mathbf{a}_1 and \mathbf{a}_2 - to distinguish them from the previously plotted points, we use arrows. These arrows correspond to the columns of the original data matrix, the variables

Some rescaling has usually to take place, so that we can see how the first two principal components relate to the original variables

Check it out: first, some look into the R output

```
> attributes(trackmen.pcs)
```

```
$names
```

```
[1] "sdev"      "rotation" "center"    "scale"     "x"
```

```
$class
```

```
[1] "prcomp"
```

```
> trackmen.pcs$rotation
```

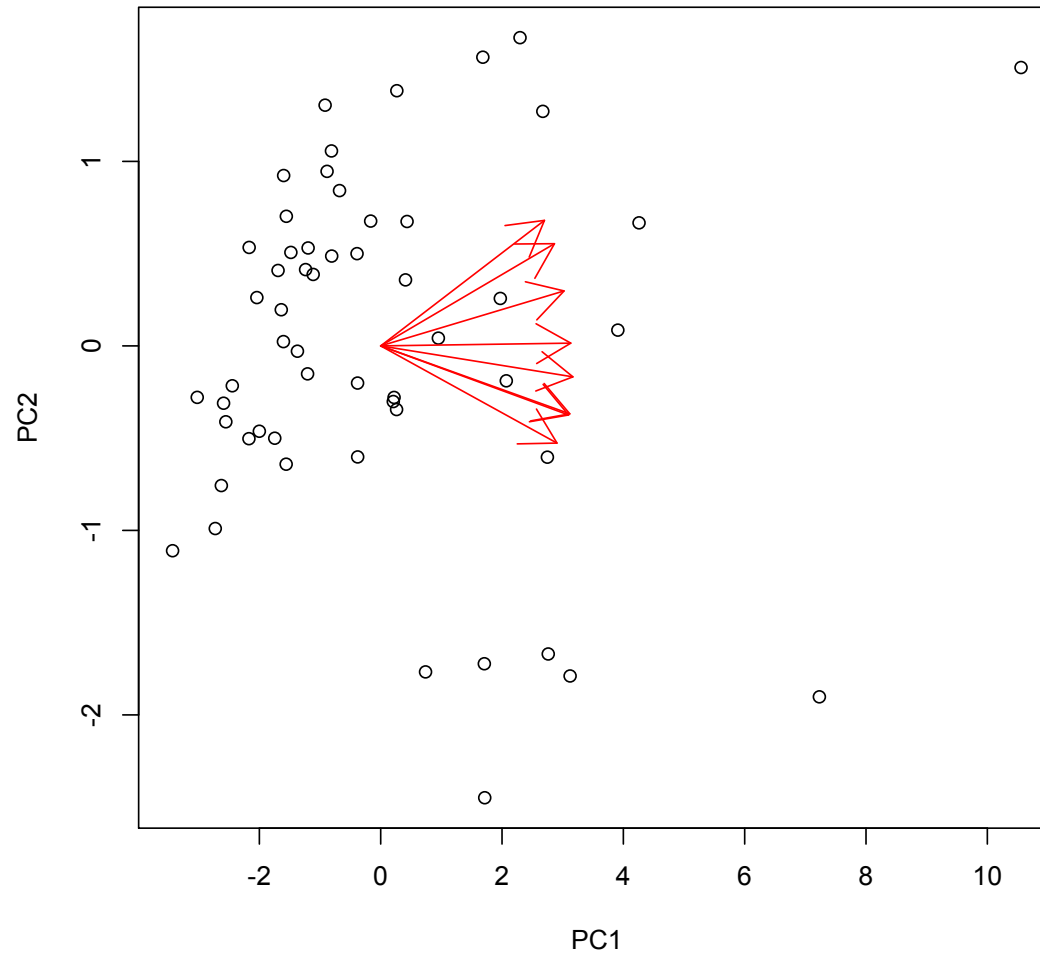
	PC1	PC2	PC3	PC4	PC5	PC6
s1	0.3175565	0.56687750	0.3322620	-0.12762827	0.2625555	-0.5937042
s2	0.3369792	0.46162589	0.3606567	0.25911576	-0.1539571	0.6561367
s4	0.3556454	0.24827331	-0.5604674	-0.65234077	-0.2183229	0.1566252
m8	0.3686841	0.01242993	-0.5324823	0.47999895	0.5400528	-0.0146918
m15	0.3728099	-0.13979665	-0.1534427	0.40451039	-0.4877151	-0.1578430
m50	0.3643741	-0.31203045	0.1897643	-0.02958755	-0.2539792	-0.1412987
m100	0.3667726	-0.30685985	0.1817517	-0.08006862	-0.1331764	-0.2190168
m421	0.3419261	-0.43896267	0.2632087	-0.29951213	0.4979283	0.3152849

```
> plot(predict(trackmen.pcs))
```

```
> arrows(0,0,trackmen.pcs$rotation[,1],trackmen.pcs$rotation[,2])
```

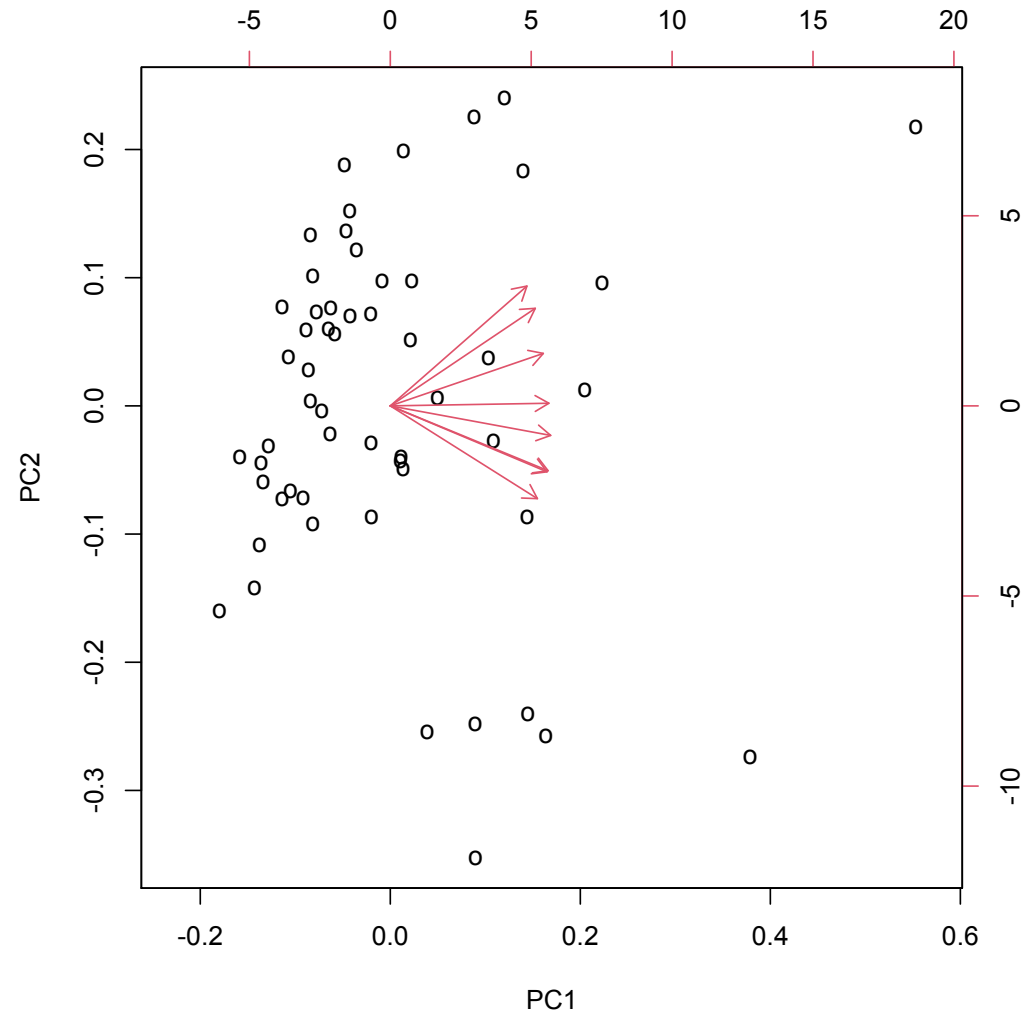
It is not really it yet - but after some rescaling...

Pretty close, right?



```
> plot(predict(trackmen.pcs))  
> arrows(0,0,8.5*trackmen.pcs$rotation[,1],  
+ 1.2*trackmen.pcs$rotation[,2],col="red")
```

Compare to the (somewhat edited) R own



Principal components: computation

Principal components can be obtained via eigenvector-eigenvalue decomposition applied to the variance-covariance matrix (or, in scaled case, correlation matrix). Principal component directions are given by the eigenvectors; eigenvalues give the variance of the principal component

This is done by R function `princomp()` - which can also do the computation without the knowledge of the original data, just out of the variance-covariance or correlation matrix

If `princomp()` uses the original data, it computes the variance-covariance matrix first, and then applies the eigenvector-eigenvalue decomposition to this matrix

Another way is to avoid forming the variance-covariance or correlation matrix and compute principal components by applying singular value decomposition directly to the *centered* data matrix

$$\tilde{\mathbf{Y}} = \mathbf{Y} - \frac{1}{n} \mathbf{1} \mathbf{1}^T \mathbf{Y}$$

This is done by R function `prcomp()`

Principal components: summary

Principal components are projections with maximal spread, the projections that maximize the variance in the given direction - the more precise sense is given above. This may show us interesting projection(s) (although arguably, there may be also more interesting ones)

They can also summarize data in some sense - we retain only a few principal components, with maximal variances. The ratio of a variance to the sum of all variances gives “proportion of the variance explained”. The corresponding plot is called *screeplot*

They are not invariant to the scaling of variables (to the shift and rotation yes, but not to the change of the unit length). Hence the technique is often performed not on covariance matrix, but on the correlation matrix; that is, the covariance matrix of variables scaled to zero sample mean and unit sample variance. One has to watch carefully for this aspect

And also, they are sensitive to outliers (not robust)

Ramifications

It is important to understand principal components, because they are building blocks of other procedures like (among others):

- common principal components
- principal curves and surfaces
(Pearson: the first principal component is the orthogonal regression fit to the data)
- self-organized mappings (Kohonen)
- independent component analysis (ICA)
(note: principal components are uncorrelated)
- partial least squares (PLS)
(“principal components of the regressors with view on a response”)
- projection pursuit

A more about PLS: dimension reduction

We have a linear regression (univariate response)

$$\mathbf{y} \sim \mathbf{X}\boldsymbol{\beta} \quad (\text{or, if you wish, } \hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\beta})$$

This is nice for general theory, but in practice it is useful to separate intercept out of \mathbf{X} (we will abuse the notation and denote the new matrix also by \mathbf{X}).

$$\mathbf{y} \sim \mathbf{1}\alpha + \mathbf{X}\boldsymbol{\beta}$$

We may assume \mathbf{y} , \mathbf{X} centered (otherwise the parameters transform how?) That is, the average of the elements of \mathbf{y} is 0, as well as the averages of the all columns of \mathbf{X} . (Then, if we are doing the least-squares fit, the coefficient α would be 0)

We can also assume the columns of \mathbf{X} scaled (otherwise we may again transform the fitted parameters in the appropriate way)

But \mathbf{X} may have way too many columns; we would like to use fewer of those...

Principal component regression

We compute principal components \mathbf{Z} out of \mathbf{X} and retain only first m of those, \mathbf{Z}_m

$$\mathbf{y} \sim \mathbf{1}\alpha + \mathbf{Z}_m\boldsymbol{\gamma}$$

Now, we know that the columns of \mathbf{Z}_m are orthogonal - when the fitting criterion is least squares, we obtain the solution by solving m univariate regressions

$$\mathbf{y} \sim \mathbf{z}_j\gamma_j$$

Of course, when $M = p$, that is, we use all principal components, we get only the solution of the original regression, nothing new

The just described strategy was and is used, with possible advantages and drawbacks. Rather than going into those, let us mention one fact: principal components do not care about \mathbf{y} ; for every \mathbf{y} they are the same. This led to the following method:

Partial least squares

Partial least squares are “principal components for regression”. This is best seen from the following analogy

Principal component *directions* \mathbf{c}_m are found via maximizing

$$\text{var}(\mathbf{X}\mathbf{c}_m) \quad \text{subject to } \|\mathbf{c}_m\| = 1 \quad \text{and}$$

$$\mathbf{c}_m^T \mathbf{c}_k = 0 \text{ for all } k = 1, 2, \dots, m-1$$

The last condition can be rewritten so that the definition is

$$\text{var}(\mathbf{X}\mathbf{c}_m) \quad \text{subject to } \|\mathbf{c}_m\| = 1 \quad \text{and}$$

$$\mathbf{c}_m^T \mathbf{S}_X \mathbf{c}_k = 0 \text{ for all } k = 1, 2, \dots, m-1$$

where $\mathbf{S}_X = \text{var}(\mathbf{X})$ is the variance-covariance matrix of \mathbf{X}

Partial least squares directions \mathbf{d}_m are found via maximizing

$$(\text{cor}(\mathbf{y}, \mathbf{X}\mathbf{d}_m))^2 \text{var}(\mathbf{X}\mathbf{d}_m) \quad \text{subject to } \|\mathbf{d}_m\| = 1 \quad \text{and}$$

$$\mathbf{d}_m^T \mathbf{S}_X \mathbf{d}_k = 0 \text{ for all } k = 1, 2, \dots, m-1$$

In practical applications, only some small number of directions is used, like in principal components. However, the algorithm for partial least squares is sequential

Partial least squares: the algorithm

We assume the columns, \mathbf{x}_j of \mathbf{X} scaled. However, we do not have to scale \mathbf{y} ; if it is not, we just know that $\alpha = \bar{y}$.

We set $\mathbf{y}^{(0)} = \bar{y}$ and $\mathbf{x}_j^{(0)} = \mathbf{x}_j$

For $m = 1, 2, \dots, p$

$$\mathbf{z}_m = \sum_{j=1}^p \mathbf{d}_{mj} \mathbf{x}_j^{(m-1)} \quad \text{where} \quad \mathbf{d}_{mj} = \mathbf{y}^\top \mathbf{x}_j^{(m-1)}$$

$$\vartheta_m = \frac{\mathbf{y}^\top \mathbf{z}_m}{\mathbf{z}_m^\top \mathbf{z}_m} = (\mathbf{z}_m^\top \mathbf{z}_m)^{-1} (\mathbf{z}_m^\top \mathbf{y})$$

$$\mathbf{y}^m = \mathbf{y}^{m-1} + \vartheta_m \mathbf{z}_m$$

orthogonalize each $\mathbf{x}_j^{(m-1)}$ with respect to \mathbf{z}_m :

$$\mathbf{x}_j^{(m)} = \mathbf{x}_j^{(m-1)} - (\mathbf{z}_m^\top \mathbf{z}_m)^{-1} (\mathbf{z}_m^\top \mathbf{x}_j^{(m-1)}) \mathbf{z}_m \quad \text{for } j = 1, 2, \dots, p$$

The output of the algorithm is the sequence of fitted vectors $\mathbf{y}^{(m)}$ $m = 1, 2, \dots, p$. As \mathbf{z}_ℓ , $\ell = 1, 2, \dots, m$ are linear in the original \mathbf{x}_j , so is

$$\mathbf{y}_m = \mathbf{X} \boldsymbol{\beta}^{\text{PLS}}(m)$$

Projection pursuit

Named by Friedman and Tukey (Kruskal considered earlier under different name). Evolved from “Grand Tour” - a technique that “traveled all” directions to find those yielding interesting projections.

The objective is to find the directions giving most interesting projections of the data. Deemed to be those maximizing some *projection index*.

While principal components are also a kind of projection pursuit, this kind of projection is not considered that interesting here. Hence the datapoints are first scaled so that their covariance matrix is identity: *sphering*. This is equivalent to transforming to principal components (the original ones, computed from the covariance matrix, after subtracting the mean) and then scaling to unit variance (dividing by square root of eigenvalues).

The projections of interest are one- and two-dimensional. There are several indices, mostly quantifying a degree of deviation from normality as a measure of interestingness. Thus, the computation of the index *often involves the estimation of the density of projected points*.

Examples of projection indices

Indices assessing “non-uniformity” (uniform = uninteresting)

$$\text{entropy } \int f \log f$$

Indices assessing “non-normality” (normal = uninteresting)

skewness and kurtosis

variations of L^2 deviation from normality

$$\int (f - \varphi)^2 / 2\varphi \quad \int (f - \varphi)^2 \quad \int (f - \varphi)^2 \varphi$$

Indices finding “holes” in the data

Indices finding clusters in the data

(the above rather superimpose them)

Technical details

Computing involves some kind of numerical minimization.

Once an interesting projection is found, there is a need to perform a *structure removal* before finding another one. The structural removal can be accomplished, for instance, by transforming to normality in the selected projection

Limitations:

Still somewhat in development (that is, was 20 years ago)

The opinions on various indices differ

Computationally demanding, needs sophisticated optimization methods (many local maxima)

Practical impact?

**Reducing dimension of hidden causes:
factor analysis**

Preamble

Attempts of interpreting principal components

may lead to the entities with their own lives: factors

And consequently to the technique, or bundle of techniques,
dealing with those: factor analysis

Which in turn may be approached from other viewpoints

one of them being: reading from the variance-covariance matrix

(And one can see it also as an attempt to make principal
components invariant with respect to rescaling)

Motivation: principal components

Recall: we have the data matrix \mathbf{Y} , and we decompose its variance-covariance matrix $\mathbf{S_Y} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$.

The principal component directions are columns of \mathbf{U} :

$$(\mathbf{a}_1 \quad \mathbf{a}_2 \quad \dots \quad \mathbf{a}_p) = (\mathbf{u}_1 \quad \mathbf{u}_2 \quad \dots \quad \mathbf{u}_p) = \mathbf{U}$$

Principal components are the projections into those directions:

$$\mathbf{C} = (\mathbf{c}_1 \quad \mathbf{c}_2 \quad \dots \quad \mathbf{c}_p) = (\mathbf{Y}\mathbf{u}_1 \quad \mathbf{Y}\mathbf{u}_2 \quad \dots \quad \mathbf{Y}\mathbf{u}_p) = \mathbf{Y}\mathbf{U}.$$

That is, principal components are expressed as linear combinations of the original variables - the columns of \mathbf{Y} :

$$\begin{pmatrix} c_{11} & \dots & c_{1p} \\ c_{21} & \dots & c_{2p} \\ \dots & \dots & \dots \\ c_{n1} & \dots & c_{np} \end{pmatrix} = \begin{pmatrix} y_{11} & \dots & y_{1p} \\ y_{21} & \dots & y_{2p} \\ \dots & \dots & \dots \\ y_{n1} & \dots & y_{np} \end{pmatrix} \begin{pmatrix} u_{11} & \dots & u_{1p} \\ u_{21} & \dots & u_{2p} \\ \dots & \dots & \dots \\ u_{p1} & \dots & u_{pp} \end{pmatrix}$$

This is all standard, nothing new here.

Principal components inverted

We may invert the relationship $\mathbf{YU} = \mathbf{C}$: express the original variables as linear combinations of principal components. It should not be a problem, because $\mathbf{U}^{-1} = \mathbf{U}^T$.

$$\mathbf{Y} = \mathbf{CU}^T = (\mathbf{c}_1 \quad \dots \quad \mathbf{c}_p) \begin{pmatrix} \mathbf{u}_1^T \\ \vdots \\ \mathbf{u}_p^T \end{pmatrix} = \mathbf{c}_1 \mathbf{u}_1^T + \dots + \mathbf{c}_p \mathbf{u}_p^T$$

However, we usually want only few first principal components (reduction of the information)

$$\begin{aligned} \mathbf{Y} &= \mathbf{c}_1 \mathbf{u}_1^T + \dots + \mathbf{c}_m \mathbf{u}_m^T + \mathbf{c}_{m+1} \mathbf{u}_{m+1}^T + \dots + \mathbf{c}_p \mathbf{u}_p^T \\ &= \mathbf{c}_1 \mathbf{u}_1^T + \dots + \mathbf{c}_m \mathbf{u}_m^T + \mathbf{E} = \mathbf{C}_m \mathbf{U}_m^T + \mathbf{E} \end{aligned}$$

This is the motivation of the factor analysis model, but before that, we have to address a technicality: centering

Centering

Return to the equation

$$\begin{pmatrix} \mathbf{c}_{11} & \dots & \mathbf{c}_{1p} \\ \mathbf{c}_{21} & \dots & \mathbf{c}_{2p} \\ \dots & \dots & \dots \\ \mathbf{c}_{n1} & \dots & \mathbf{c}_{np} \end{pmatrix} = \begin{pmatrix} \mathbf{y}_{11} & \dots & \mathbf{y}_{1p} \\ \mathbf{y}_{21} & \dots & \mathbf{y}_{2p} \\ \dots & \dots & \dots \\ \mathbf{y}_{n1} & \dots & \mathbf{y}_{np} \end{pmatrix} \begin{pmatrix} \mathbf{u}_{11} & \dots & \mathbf{u}_{1p} \\ \mathbf{u}_{21} & \dots & \mathbf{u}_{2p} \\ \dots & \dots & \dots \\ \mathbf{u}_{p1} & \dots & \mathbf{u}_{pp} \end{pmatrix}$$

Taking means columnwise shows that

$$(\bar{\mathbf{c}}_1 \quad \dots \quad \bar{\mathbf{c}}_p) = (\bar{\mathbf{y}}_1 \quad \dots \quad \bar{\mathbf{y}}_p) \mathbf{U}, \text{ that is, } \bar{\mathbf{c}}^\top = \bar{\mathbf{y}}^\top \mathbf{U}.$$

In plain language: means projects onto means. Hence, if we take \mathbf{Y} centered - instead of \mathbf{Y} we consider $\tilde{\mathbf{Y}} = \mathbf{Y} - \mathbf{1}\bar{\mathbf{y}}^\top$, obtained by subtracting the column means from \mathbf{Y} , then the column means of \mathbf{C} are zeros - as are those of $\tilde{\mathbf{Y}}$ (and everything is all right).

Instead of

$$\mathbf{Y} = \mathbf{C}_m \mathbf{U}_m^\top + \mathbf{D}$$

we may assume that \mathbf{C}_m is centered and write instead

$$\tilde{\mathbf{Y}} = \mathbf{C}_m \mathbf{U}_m^\top + \mathbf{D}$$

Factor model - an attempt in the sample form

All the above could lead to a hypothetic factor model

$$\tilde{\mathbf{Y}} = \mathbf{C}_m \mathbf{U}_m^T + \mathbf{D} \quad \text{where} \quad \tilde{\mathbf{Y}} = \mathbf{Y} - \mathbf{1}\bar{\mathbf{y}}^T,$$

and $\mathbf{1}$ is the $n \times 1$ column of ones; we could call the $n \times m$ matrix \mathbf{C}_m the matrix of (common) factors (columns of \mathbf{C}_m), and \mathbf{D} would be the $n \times p$ matrix of specific factors.

We may also write

$$\mathbf{Y} - \mathbf{1}\bar{\mathbf{y}}^T = \mathbf{C}_m \mathbf{U}_m^T + \mathbf{D}$$

and it may be instructive to write it in components; if, say, $m = 2$, then the i -th variable, the i -th column of \mathbf{Y} , is

$$\begin{pmatrix} y_{1i} \\ y_{2i} \\ \dots \\ y_{ni} \end{pmatrix} = \begin{pmatrix} \bar{y}_i \\ \bar{y}_i \\ \dots \\ \bar{y}_i \end{pmatrix} + \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \\ \dots & \dots \\ c_{n1} & c_{n2} \end{pmatrix} \begin{pmatrix} u_{i1} \\ u_{i2} \end{pmatrix} + \begin{pmatrix} d_{1i} \\ d_{2i} \\ \dots \\ d_{ni} \end{pmatrix}$$

that is, $\mathbf{y}_i - \bar{y}_i \mathbf{1} = \mathbf{C}_m \mathbf{u}_i + \mathbf{d}_i$ (\mathbf{d}_i being the columns of \mathbf{D})

and together all $i = 1, 2, \dots, p$ give the matrix form above.

An attempt at assumptions

Note that although it looks like a regression model, the difference is that *both* \mathbf{C}_m and \mathbf{U}_m are unobserved. Having that many unobserved quantities brings a lot of ambiguity (nonuniqueness of solutions); to alleviate at least some of that, we require

the *columns* of \mathbf{C}_m to have

- zero mean and unit standard deviation

- are uncorrelated with the columns of \mathbf{D}

- are uncorrelated among themselves (however: *sometimes* not)

and the *columns* of \mathbf{D} to have zero mean...

...but when we would like to postulate that the columns of \mathbf{E} to be uncorrelated, then in general this will neither be true nor feasible - and thus: we have to switch to the corresponding *stochastic*, “population” model instead (that is, introduce underlying random variables and their variance-covariance matrices)

We need to go stochastic

Note: we did not need any underlying stochastic model for principal components - but we do now; so “forget” the above, and start to think from scratch in terms of random variables (vectors)

From now on, we view lines of the data matrix \mathbf{Y} as arising from independent sampling, from a certain distribution - which will be the distribution of some vector \mathbf{y} (this vector is introduced solely for notational convenience)

Let $\boldsymbol{\mu} = E(\mathbf{y})$ be its componentwise mean.

Factor model: regression form

This model, to emphasize the fact that factors are assumed uncorrelated, is often called **orthogonal factor form**

It is assumed that $\mathbf{y} - \boldsymbol{\mu} = \mathbf{L}\mathbf{f} + \mathbf{e}$ where

\mathbf{y} is a $p \times 1$ random vector

\mathbf{L} is $p \times m$ matrix of fixed, but unknown **loadings**

\mathbf{f} is an $m \times 1$ random vector of **common factors**

and \mathbf{e} is a $p \times 1$ random vector \mathbf{e} of **specific factors**

The components of both \mathbf{f} and \mathbf{e} are all assumed to have **zero expectation**, $E(\mathbf{f}) = \mathbf{0}$, $E(\mathbf{e}) = \mathbf{0}$

The components of \mathbf{f} are assumed to be **uncorrelated with the components of \mathbf{e}** , $\text{Cov}(f_i, e_j) = 0$ for all i and j

The components of \mathbf{f} are assumed to have unit variance, and also be **uncorrelated among themselves**: $\text{Var}(\mathbf{f}) = \mathbf{I}$

The components of \mathbf{e} are also assumed to be **uncorrelated among themselves**, but their variance is not restricted: $\text{Var}(\mathbf{e})$ is a diagonal matrix $\boldsymbol{\Psi}$ (not necessarily equal to \mathbf{I})

Rotations

Despite all the moment restrictions in the assumptions, the factor model

$$\mathbf{y} = \boldsymbol{\mu} + \mathbf{L}\mathbf{f} + \mathbf{e}$$

is not unique; putting in $\mathbf{I} = \mathbf{A}\mathbf{A}^\top$, where \mathbf{A} is any orthogonal matrix, we obtain

$$\mathbf{y} = \boldsymbol{\mu} + \mathbf{L}\mathbf{f} + \mathbf{e} = \boldsymbol{\mu} + \mathbf{L}\mathbf{I}\mathbf{f} + \mathbf{e} = \boldsymbol{\mu} + (\mathbf{L}\mathbf{A})(\mathbf{A}^\top\mathbf{f}) + \mathbf{e}$$

which is a new, equivalent - as good as the first one, and satisfying all the assumptions - model, with new factors $\mathbf{A}^\top\mathbf{f}$ and new loadings $\mathbf{L}\mathbf{A}$

Any such transformation represented by an orthogonal matrix \mathbf{A} is called **rotation**. In factor analysis, a fortuitous choice of \mathbf{A} may improve the interpretability of the resulting factor model (“the art of rotations”)

Varimax

Good rotations are often considered to be those giving as much zeros as possible in the loadings. A popular one, the rotation known to behave favorably in this respect is called **varimax**

(*varimax* = *variance maximal*)

It maximizes, over all *orthogonal* \mathbf{A} , the criterion expressed in terms of the elements ℓ_{ij} of the matrix of *rotated* loadings

$$\sum_{j=1}^m \left(\sum_{i=1}^p (\ell_{ij}^2 - \frac{1}{p} \sum_{i=1}^p \ell_{ij}^2)^2 \right) = \sum_{j=1}^m \left(\sum_{i=1}^p \ell_{ij}^4 - \frac{1}{p} (\sum_{i=1}^p \ell_{ij}^2)^2 \right)$$

(Iterative solution required)

There are many other types: entropy, quartimax, equamax, parsimax, varimin, mccammon,... (R package `GPArotation`)

Consumer preference data: chocolate bars

In a consumer preference study, a random sample of consumers were asked to rate several attributes of a new product. The responses, on a 7-point semantic differential scale, were tabulated and the attribute correlation matrix constructed.

```
> cons
```

	Taste	Money	Flavor	Snack	Energy
Taste	1.00	0.02	0.96	0.42	0.01
Good buy for money	0.02	1.00	0.13	0.71	0.85
Flavor	0.96	0.13	1.00	0.50	0.11
Suitable for snack	0.42	0.71	0.50	1.00	0.79
Provides lots of energy	0.01	0.85	0.11	0.79	1.00

```
> princomp(covmat=cons)
```

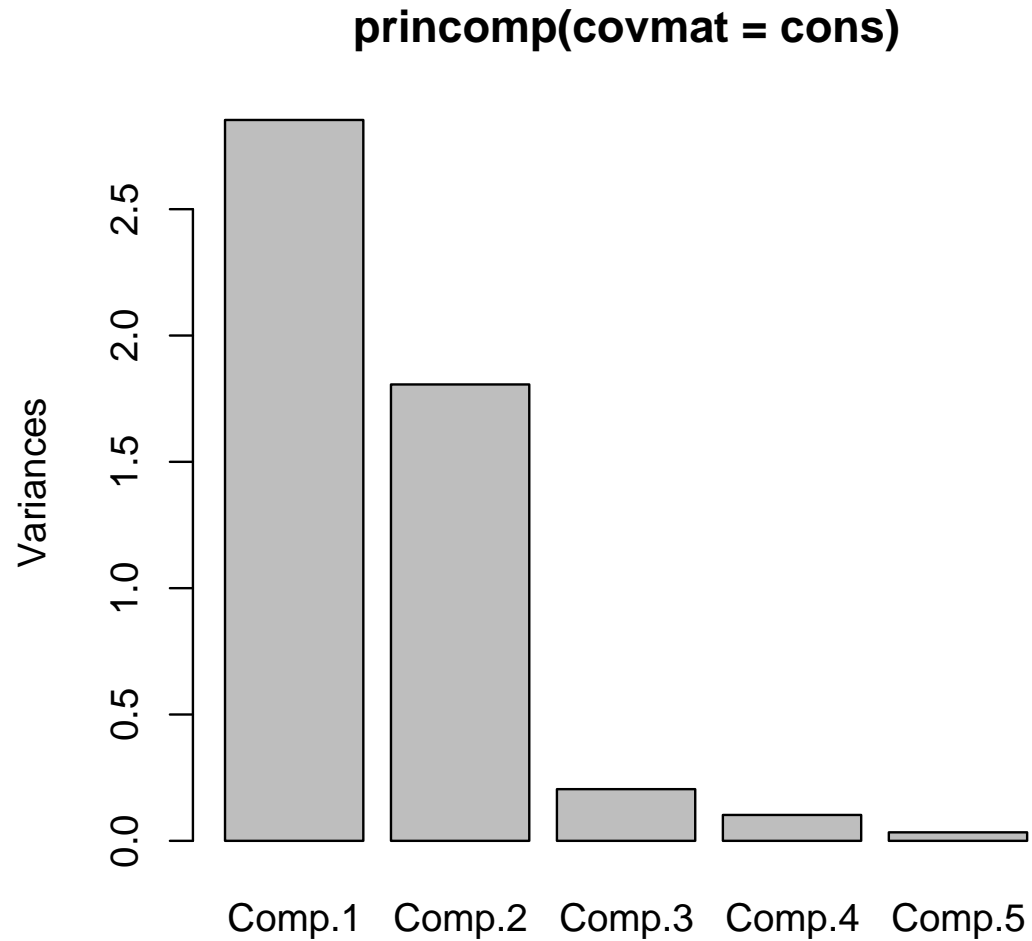
Standard deviations:

Comp.1	Comp.2	Comp.3	Comp.4	Comp.5
1.6891094	1.3439987	0.4522060	0.3200148	0.1835141

```
> plot(princomp(covmat=cons))
```

Consumer preference data: chocolate bars

First two components summarize data quite well:



Principal components of chocolate bars

We know only the correlation matrix; the correct ways are:

```
> eigen(cons)$values
```

```
[1] 2.85309042 1.80633245 0.20449022 0.10240947 0.03367744
```

```
> princomp(covmat=cons)$sdev^2
```

```
      Comp.1      Comp.2      Comp.3      Comp.4      Comp.5  
2.85309042 1.80633245 0.20449022 0.10240947 0.03367744
```

Other ways may give various dubious (and wrong!) results:

```
> prcomp(cons)$sdev^2
```

```
[1] 8.371054e-01 3.307840e-02 5.509727e-03 5.964502e-04 6.841399e-34
```

```
> prcomp(cons,scale=T)$sdev^2
```

```
[1] 4.533917e+00 4.345533e-01 2.799983e-02 3.530248e-03 6.059843e-33
```

```
> princomp(cons,cor=T)$sdev^2
```

```
      Comp.1      Comp.2      Comp.3      Comp.4      Comp.5  
4.533916642 0.434553284 0.027999826 0.003530248 0.000000000
```

```
> eigen(cor(cons))$values
```

```
[1] 4.533917e+00 4.345533e-01 2.799983e-02 3.530248e-03 1.201875e-16
```

```
> eigen(var(cons))$values
```

```
[1] 8.371054e-01 3.307840e-02 5.509727e-03 5.964502e-04 -1.594915e-17
```

```
> eigen(var(cons)*4/5)$values
```

```
[1] 6.696843e-01 2.646272e-02 4.407781e-03 4.771602e-04 9.421876e-17
```

```
> princomp(cons)$sdev^2
```

```
      Comp.1      Comp.2      Comp.3      Comp.4      Comp.5  
0.6696843389 0.0264627197 0.0044077813 0.0004771602 0.0000000000
```

Factor analysis of consumer preferences

```
> factanal(cov=cons,factors=2,rotation="none")
```

Uniquenesses:

```
[1] 0.028 0.237 0.040 0.168 0.052
```

Loadings:

	Factor1	Factor2
[1,]	0.976	-0.139
[2,]	0.150	0.860
[3,]	0.979	
[4,]	0.535	0.738
[5,]	0.146	0.963

Now, let us try some rotation, to see whether we can transform the result by a suitable rotation to obtain better interpretation

Varimax rotation

```
> fcp = factanal(cov=cons,factors=2,rotation="varimax")
```

Uniquenesses:

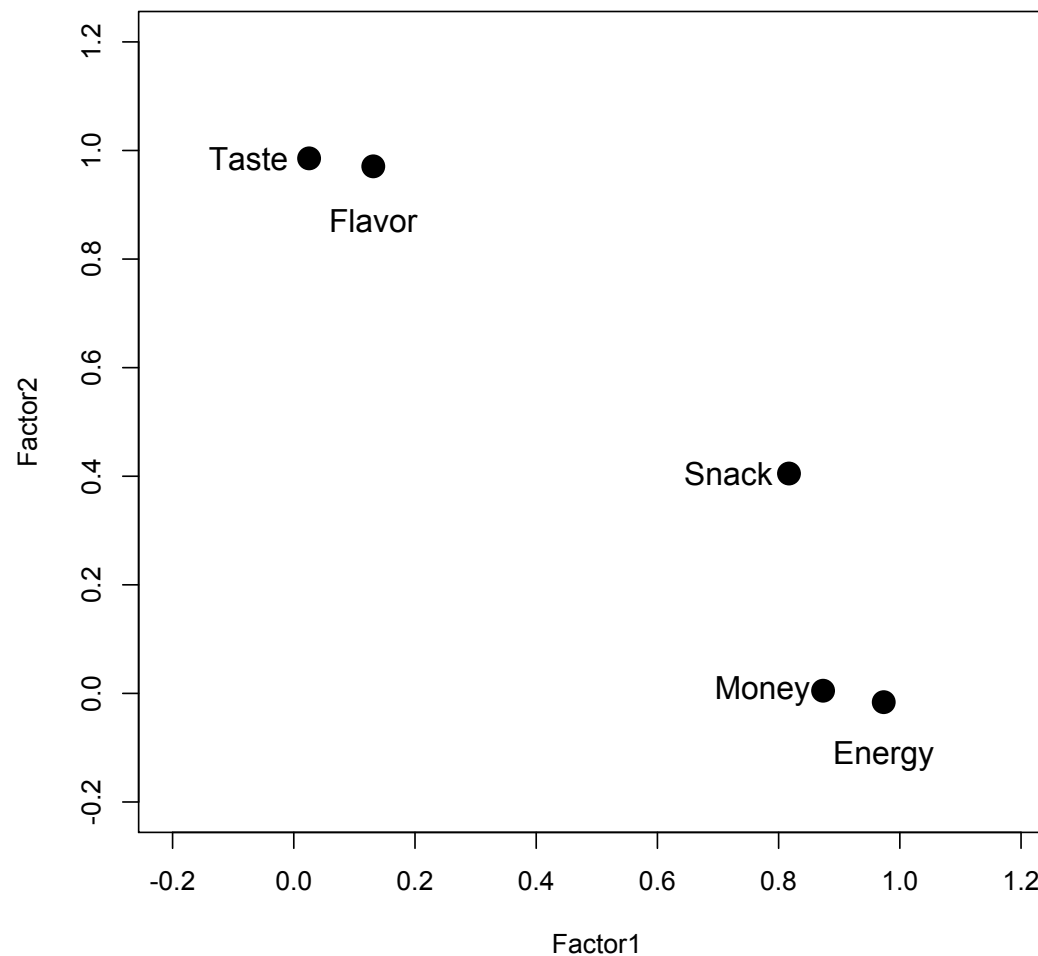
```
[1] 0.028 0.237 0.040 0.168 0.052
```

Loadings:

	Factor1	Factor2
[1,]		0.985
[2,]	0.873	
[3,]	0.131	0.971
[4,]	0.817	0.405
[5,]	0.973	

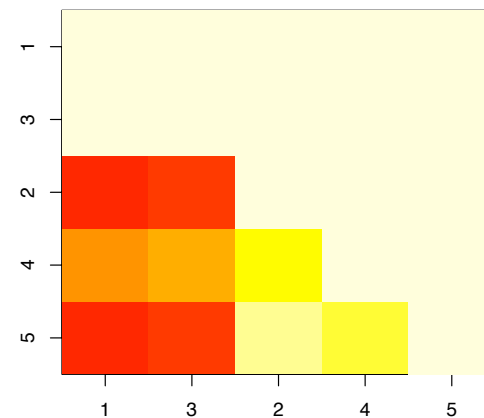
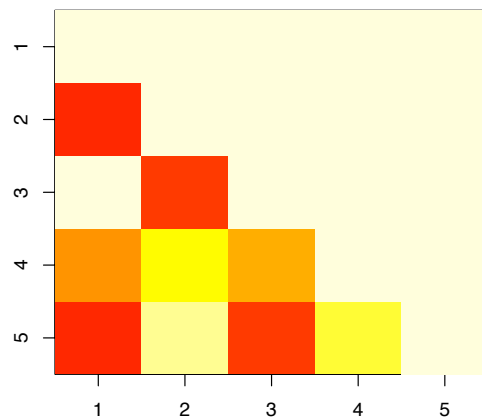
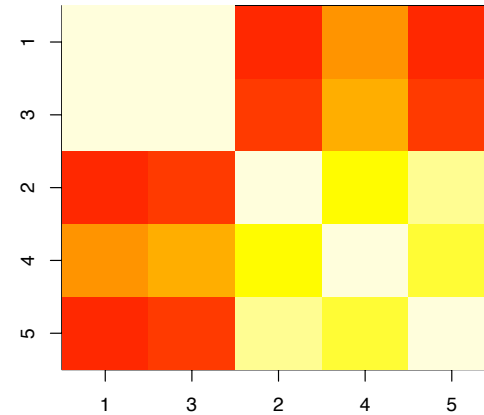
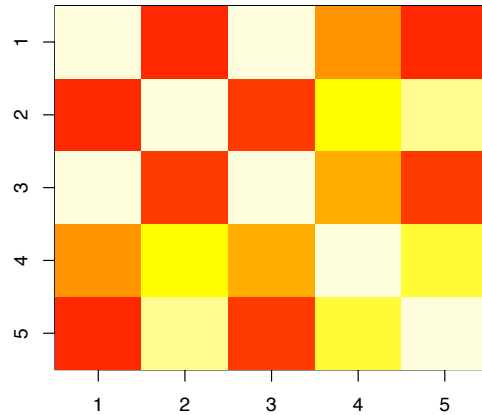
How about a plot?

```
> plot(loadings(fcp),xlim=c(-0.2,1.2),ylim=c(-0.2,1.2),cex=2,pch=16)  
> text(loadings(fcp)-c(0.1,0.1,0,0.1,0,0,0,0.1,0,0.1),  
+ labels=dimnames(cons)[[2]],cex=1.2)
```



Plotting of variance-covariance matrices

We may plot also original and permuted (1,3,2,4,5) correlation matrix: (hint: use `image()`)



In fact, it is all about variance-covariance matrix

The orthogonal factor analysis model in the regression form has consequences for the variance-covariance matrix of the random vector with underlying distribution. Recall the formula

$$\text{Var}(\mathbf{y}) = E[(\mathbf{y} - \boldsymbol{\mu})(\mathbf{y} - \boldsymbol{\mu})^T]$$

The factor model says that $\mathbf{y} - \boldsymbol{\mu} = \mathbf{L}\mathbf{f} + \mathbf{e}$. This yields

$$\begin{aligned}\text{Var}(\mathbf{y}) &= E[(\mathbf{L}\mathbf{f} + \mathbf{e})(\mathbf{f}^T\mathbf{L}^T + \mathbf{e}^T)] \\ &= \mathbf{L} E(\mathbf{f}\mathbf{f}^T) \mathbf{L}^T + \mathbf{L} E(\mathbf{f}\mathbf{e}^T) + E(\mathbf{e}\mathbf{f}^T) \mathbf{L}^T + E(\mathbf{e}\mathbf{e}^T)\end{aligned}$$

and, because $E(\mathbf{f}) = 0$, $E(\mathbf{e}) = 0$

$$\begin{aligned}&= \mathbf{L} \text{Var}(\mathbf{f}) \mathbf{L}^T + \mathbf{L} \text{Cov}(\mathbf{f}, \mathbf{e}) + \text{Cov}(\mathbf{e}, \mathbf{f}) \mathbf{L}^T + \text{Var}(\mathbf{e}) \\ &= \mathbf{L} \text{Var}(\mathbf{f}) \mathbf{L}^T + \boldsymbol{\Psi} = \mathbf{L}\mathbf{L}^T + \boldsymbol{\Psi}\end{aligned}$$

using that $\text{Var}(\mathbf{f}) = \mathbf{I}$ and $\text{Cov}(\mathbf{f}, \mathbf{e})$ is a zero matrix

In a similar way, we obtain that $\text{Cov}(\mathbf{y}, \mathbf{f}) = \mathbf{L}$

Factor model for the variance-covariance matrix

Thus, the orthogonal factor model in the regression form implies the following (orthogonal) factor model for the variance-covariance matrix:

$$\text{Var}(\mathbf{y}) = \mathbf{L}\mathbf{L}^T + \mathbf{\Psi} \quad \text{with} \quad \text{Cov}(\mathbf{y}, \mathbf{f}) = \mathbf{L}$$

Also this model remains unchanged under the rotation of factors, when \mathbf{L} is replaced by $\mathbf{L}\mathbf{A}$, where \mathbf{A} is an orthogonal $m \times m$ matrix

In terms of the elements ℓ_{ij} of \mathbf{L} , we have

$$\text{Var}(\mathbf{y}_i) = \ell_{i1}^2 + \cdots + \ell_{im}^2 + \psi_i,$$

$$\text{Cov}(\mathbf{y}_i, \mathbf{y}_j) = \ell_{i1}\ell_{j1} + \cdots + \ell_{im}\ell_{jm}, \quad \text{Cov}(\mathbf{y}_i, \mathbf{f}_j) = \ell_{ij}.$$

Diagonal components of $\mathbf{L}\mathbf{L}^T$, equal to the sum of ℓ_{ij}^2 , $j = 1, 2, \dots, m$ are called **communalities**; note that they are independent of rotations. Diagonal elements ψ_i of $\mathbf{\Psi}$ are called **uniquenesses**, or *specific variances*. Loadings and uniquenesses are estimated as parameters, that is, for the whole sample; this estimation requires only knowledge of $\text{var}(\mathbf{Y})$. Factors may be then estimated from \mathbf{Y} as unobserved quantities specific for the i -th item.

Oblique rotations

By the analogy with principal components - which are uncorrelated - it is also natural to assume that common factors are uncorrelated. This assumption, generally considered standard, blends well with the orthogonal modeling of factor analysis, with equivalence classes induced by orthogonal rotations (orthogonal transformations of common factors)

At times, the assumption of uncorrelatedness of factors is relaxed in a hope of possibly more unequivocal (“clear-cut”) interpretation of factors. This is accomplished by relaxing the requirement on a rotation transformation/matrix **A**: it does not have to be orthogonal, but merely invertible - **oblique rotation**

Such a move is somewhat controversial, as it typically does not reflect itself in the corresponding factor models; but it is occasionally used in practice anyway. Note that after general oblique rotation, the resulting common factors may be correlated

Promax

Once again, oblique factor loadings are estimated in the same way as the orthogonal factors; it is non-orthogonal rotation that makes them oblique. The “rotation” matrix **A** has to be only invertible now

A prominent (and often preferred) method in this case is so-called **promax**. The method (depends on s , typical values of s are $s = 1, 2, 3, 4$) proceeds in the following steps:

1. **L** (orthogonally) rotated by varimax (by an orthogonal matrix **T**); the rotated **LT** becomes new **L**.
2. **Q** with the same dimension as **L**, $q_{ij} = |\ell_{ij}^{s-1}| \ell_{ij}$; the nonzero elements are increased or decreased depending on whether they are > 1 or < 1 .
3. **LT** is sought (**T** not necessarily orthogonal now) that best approximates **Q** in the Hilbert-Schmidt metric. The expected effect is to decrease small and increase large loadings.

Other “oblique rotations”: oblimin, quartimin, oblimax, simplimax, ... (R package `GPArotation` again)

Oblique rotation for chocolate bars

```
> factanal(cov=cons,factors=2,rotation="promax")
```

Loadings:

	Factor1	Factor2
[1,]		1.004
[2,]	0.892	-0.103
[3,]		0.975
[4,]	0.786	0.313
[5,]	0.997	-0.137

Estimation: loadings from principal components

In this method, estimates of loadings are obtained through *low-rank approximation* $\hat{\mathbf{L}}\hat{\mathbf{L}}^T$ of the variance-covariance matrix \mathbf{S}_Y (or, in practice, rather of the correlation matrix \mathbf{R}_Y)

The estimates of uniqueness, diagonal elements of Ψ are then obtained as the *diagonal elements* of $\mathbf{S}_Y - \hat{\mathbf{L}}\hat{\mathbf{L}}^T$ (non-diagonal elements are dismissed)

If estimates are obtained in this way, they are all nonnegative

A modification of the above scheme is possible too: uniquenesses are estimated first, then the diagonal matrix formed by them is subtracted from \mathbf{S}_Y ; the resulting matrix is then low-rank approximated as above. New estimates of uniquenesses can be obtained in this way and the whole process can be iterated

Low-rank approximation

The problem is defined as follows: given a matrix \mathbf{A} , we are looking for a matrix \mathbf{B} , with rank not greater than m , which minimizes the Hilbert-Schmidt distance of \mathbf{A} and \mathbf{B} .

By its definition, the square of the Hilbert-Schmidt distance, $d^2(\mathbf{A}, \mathbf{B})$, is just the sum of squares of all element-wise differences. In matrix notation, it can be expressed as

$$\text{tr}(\mathbf{A} - \mathbf{B})(\mathbf{A} - \mathbf{B})^\top = \text{tr}(\mathbf{A} - \mathbf{B})^\top(\mathbf{A} - \mathbf{B})$$

(if both matrices are symmetric, as is our case, then the transposition sign can be dropped)

For symmetric, nonnegative definite matrices, the approximation is easily found via the eigenvalue decomposition. If $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^\top$, with \mathbf{U} orthogonal, $\mathbf{\Lambda}$ diagonal, and m is the desired approximation rank, then we put $\mathbf{B} = \mathbf{U}\mathbf{\Lambda}_m\mathbf{U}^\top$, where $\mathbf{\Lambda}_m$ is the matrix obtained from $\mathbf{\Lambda}$ by taking its m largest diagonal elements, m largest eigenvalues (all eigenvalues should be ≥ 0), and replacing the rest of them by 0. As

$$\mathbf{A} = \mathbf{U}\mathbf{\Lambda}_m^{1/2}\mathbf{\Lambda}_m^{1/2}\mathbf{U}^\top = \mathbf{U}\mathbf{\Lambda}_m^{1/2}(\mathbf{U}\mathbf{\Lambda}_m^{1/2})^\top$$

we can also see that how \mathbf{A} can be written as $\hat{\mathbf{L}}\hat{\mathbf{L}}^\top$.

Estimation: maximum likelihood

The method(s) based on low-rank approximation are considered somewhat historic - the predominantly used method these days is maximum likelihood. It is based on the factor model and normality assumption on \mathbf{y} . Its advantage is yielding the same loadings even from rescaled data, consistently with the stochastic factor model; but, on the other hand, it may introduce so-called **Heywood cases**, estimates of uniquenesses that are 0 or negative.

The latter are then usually adjusted: either directly to 0, or in some other way: some implementations constrain uniquenesses to be \geq than some preselected small number

Once loadings are estimated, then they are usually also rotated, to facilitate their interpretation.

Maximum likelihood and testing for m

Maximum likelihood estimates are particularly suitable testing with the aim to assess m , the number of factors.

The null hypothesis H_0 that the variance-covariance matrix has the form $\text{Var}(\mathbf{y}) = \mathbf{L}\mathbf{L}^\top + \mathbf{\Psi}$ is tested against a general $\text{Var}(\mathbf{y})$ alternative using likelihood ratio test, using the ratio of the maximized likelihood under m factors and the maximized likelihood in general, that is, under p factors. The $-2\log$ of this ratio is

$$n \log \left(\frac{\det(\hat{\mathbf{L}}\hat{\mathbf{L}}^\top + \hat{\mathbf{\Psi}})}{\det(\frac{n-1}{n}\mathbf{S}_\mathbf{Y})} \right)$$

where $\hat{\mathbf{L}}$ and $\hat{\mathbf{\Psi}}$ are maximum likelihood estimates under the factor model, and $\frac{n-1}{n}\mathbf{S}_\mathbf{Y}$ is the maximum likelihood estimate of unrestricted variance-covariance matrix $\text{Var}(\mathbf{y})$ - all under normality assumption

The test statistic has approximately $\chi^2_{\frac{1}{2}[(p-m)^2-p-m]}$ distribution; the approximation is improved (Bartlett) by replacing n by $(n-1-(2p+4m+5)/6)$. The null hypothesis that m factors are sufficient is rejected when the statistic is large.

Estimation of scores

As mentioned above, loadings and uniqueness can be estimated from the variance-covariance (or correlation) matrix alone. Once the $p \times m$ matrix \mathbf{L} of loadings is estimated, the estimates become “known” regressors in the regression form of the factor model. *If full data are available*, we can also estimate factor scores for each given i : that is, estimate \mathbf{f}_i under the assumption that it is sampled with the same distribution as \mathbf{f} .

There are two ways to do it:

Bartlett scores

For fixed i , the sample version for i -th observation given by the factor model is

$$\mathbf{y}_i - \boldsymbol{\mu} = \mathbf{L}\mathbf{f}_i + \mathbf{e}_i$$

Once we “know” \mathbf{L} - that is, we plug in its estimate $\hat{\mathbf{L}}$ - the estimation of \mathbf{f}_i can be done by the least squares method, as in any standard linear model. Given, however, that the variances of the “errors” are not equal - the matrix $\boldsymbol{\Psi}$ is not diagonal - the usually used estimate is that by the weighted least squares

$$\hat{\mathbf{f}}_i = (\hat{\mathbf{L}}\hat{\boldsymbol{\Psi}}^{-1}\hat{\mathbf{L}})^{-1}\hat{\mathbf{L}}^T\hat{\boldsymbol{\Psi}}^{-1}(\mathbf{y}_i - \bar{\mathbf{y}})$$

where $\hat{\boldsymbol{\Psi}}$ is the estimate of $\boldsymbol{\Psi}$ obtained by one of the methods described above

The formula is the standard regression estimate, except for the fact that $\boldsymbol{\mu}$ is estimated by

$$\bar{\mathbf{y}} = \frac{1}{n} \sum_{i=1}^n \mathbf{y}_i.$$

Thomson (regression) scores

As both \mathbf{y}_i and \mathbf{f}_i are stochastic, we may also regress \mathbf{f}_i on \mathbf{y}_i in a stochastic way (recall that the mean of \mathbf{f}_i is zero). That is, we first find \mathbf{U}_i minimizing

$$E(\|\mathbf{f}_i - \mathbf{U}_i \mathbf{y}_i\|^2)$$

which is

$$\mathbf{U}_i = \text{Cov}(\mathbf{f}_i, \mathbf{y}_i) [\text{Var}(\mathbf{y}_i)]^{-1}$$

and then construct a prediction

$$\hat{\mathbf{f}}_i = \mathbf{U}_i (\mathbf{y}_i - \boldsymbol{\mu}) = \text{Cov}(\mathbf{f}_i, \mathbf{x}_i) [\text{Var}(\mathbf{x}_i)]^{-1} (\mathbf{y}_i - \boldsymbol{\mu})$$

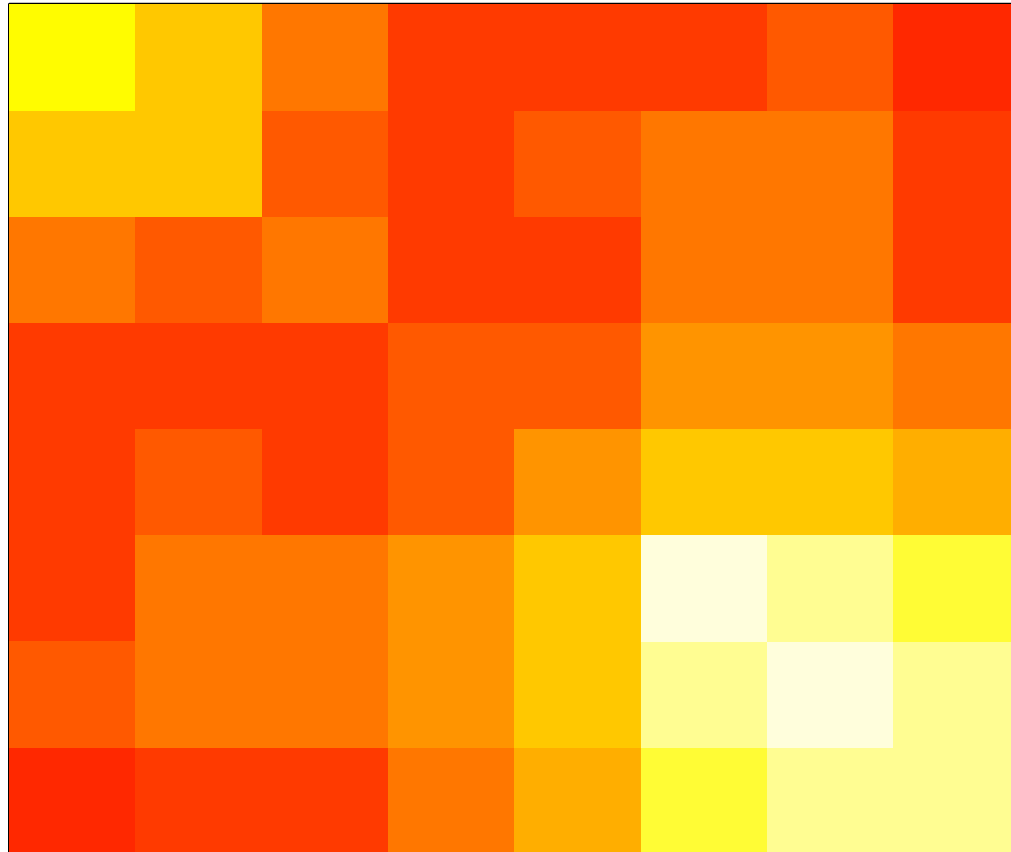
The Thomson scores are then obtained by replacing $\text{Cov}(\mathbf{f}_i, \mathbf{y}_i)$, $\text{Var}(\mathbf{y}_i)$, and $\boldsymbol{\mu}$ by their corresponding estimates $\hat{\mathbf{L}}^\top$, $\mathbf{S} = \text{var}(\mathbf{Y})$, and $\bar{\mathbf{y}}$. For fixed i , this yields the formula

$$\hat{\mathbf{f}}_i = \hat{\mathbf{L}}^\top \mathbf{S}^{-1} (\mathbf{y}_i - \bar{\mathbf{y}})$$

Track velocity records - men: variance matrix

	X1	X2	X4	X8	X15	X50	X100	M
X1	0.090	0.080	0.064	0.056	0.056	0.058	0.061	0.048
X2	0.080	0.083	0.063	0.058	0.060	0.064	0.065	0.054
X4	0.064	0.063	0.067	0.057	0.058	0.064	0.066	0.058
X8	0.056	0.058	0.057	0.063	0.061	0.069	0.071	0.064
X15	0.056	0.060	0.058	0.061	0.072	0.080	0.082	0.074
X50	0.058	0.064	0.064	0.069	0.080	0.100	0.100	0.096
X100	0.061	0.065	0.066	0.071	0.082	0.100	0.110	0.099
M	0.048	0.054	0.058	0.064	0.074	0.096	0.099	0.100

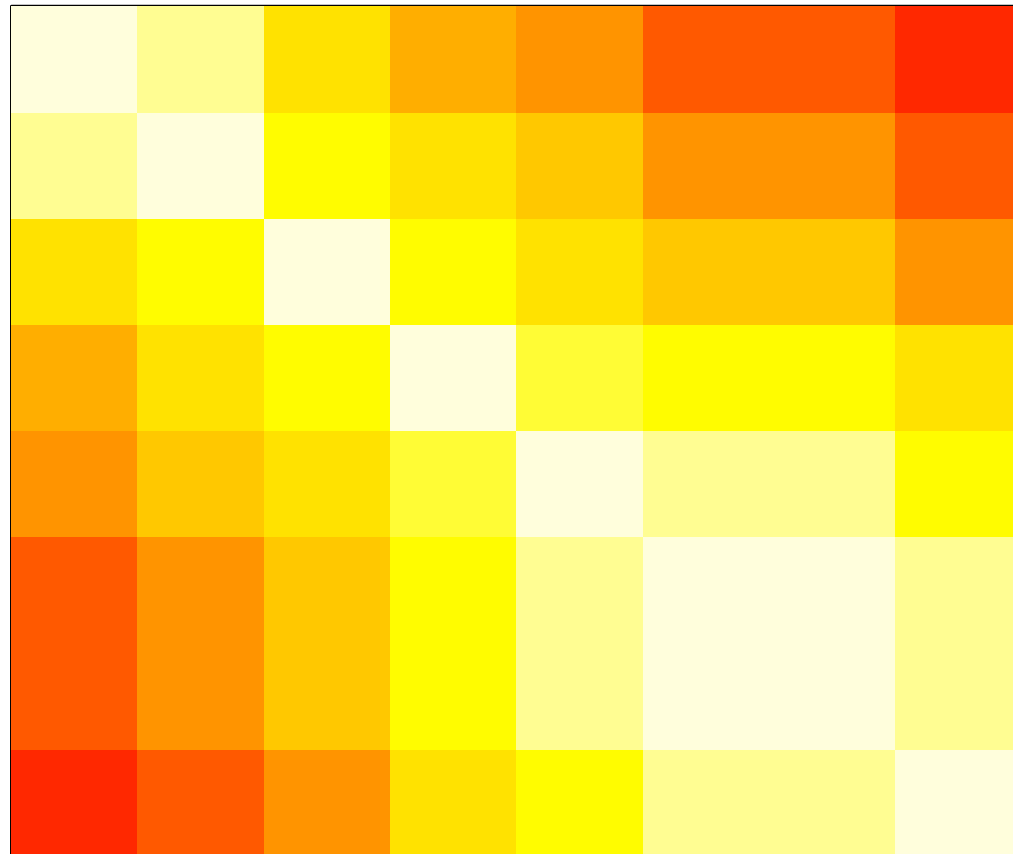
In colors



Track velocity records - men: correlation matrix

	X1	X2	X4	X8	X15	X50	X100	M
X1	1.00	0.92	0.83	0.75	0.69	0.60	0.61	0.50
X2	0.92	1.00	0.85	0.80	0.77	0.69	0.69	0.59
X4	0.83	0.85	1.00	0.87	0.83	0.77	0.78	0.70
X8	0.75	0.80	0.87	1.00	0.91	0.85	0.86	0.80
X15	0.69	0.77	0.83	0.91	1.00	0.93	0.93	0.86
X50	0.60	0.69	0.77	0.85	0.93	1.00	0.97	0.93
X100	0.61	0.69	0.78	0.86	0.93	0.97	1.00	0.94
M	0.50	0.59	0.70	0.80	0.86	0.93	0.94	1.00

Again in colors



Track records velocity - men: factor analysis

```
> factanal(trackmen,factors=2,rotation="varimax")
```

```
...
```

Uniquenesses:

	s1	s2	s4	m8	m15	m50	m100	m421
	0.081	0.076	0.151	0.135	0.082	0.034	0.018	0.086

Loadings:

	Factor1	Factor2
s1	0.291	0.914
s2	0.382	0.882
s4	0.543	0.744
m8	0.691	0.622
m15	0.799	0.530
m50	0.901	0.394
m100	0.907	0.399
m421	0.915	0.278

```
...
```

Test of the hypothesis that 2 factors are sufficient.

The chi square statistic is 16.36 on 13 degrees of freedom.

The p-value is 0.23

Note: the p-value indicates that two factors are enough

For comparison: 1 factor

```
> factanal(trackmen,factors=1,rotation="varimax")
```

```
...
```

Uniquenesses:

s1	s2	s4	m8	m15	m50	m100	m421
0.556	0.461	0.332	0.196	0.094	0.036	0.025	0.118

Loadings:

	Factor1
s1	0.666
s2	0.734
s4	0.817
m8	0.897
m15	0.952
m50	0.982
m100	0.988
m421	0.939

```
...
```

Test of the hypothesis that 1 factor is sufficient.

The chi square statistic is 156.37 on 20 degrees of freedom.

The p-value is 3.77e-23

Track records velocity - men: oblique factors

```
> factanal(trackmen,factors=2,rotation="promax")
```

```
...
```

Uniquenesses:

	s1	s2	s4	m8	m15	m50	m100	m421
	0.081	0.076	0.151	0.135	0.082	0.034	0.018	0.086

```
...
```

	Factor1	Factor2
s1	-0.153	1.066
s2		0.970
s4	0.288	0.689
m8	0.560	0.437
m15	0.760	0.249
m50	0.979	
m100	0.985	
m421	1.067	-0.160

Factor Correlations:

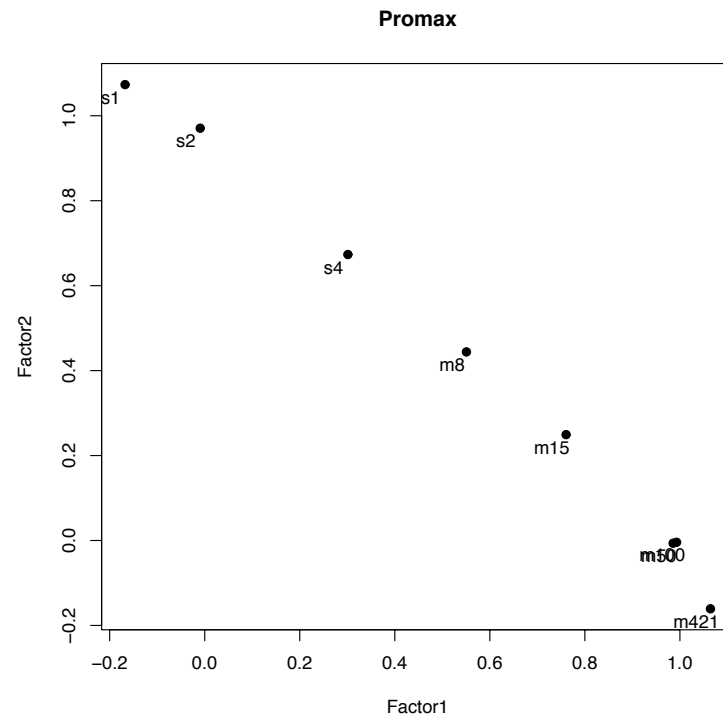
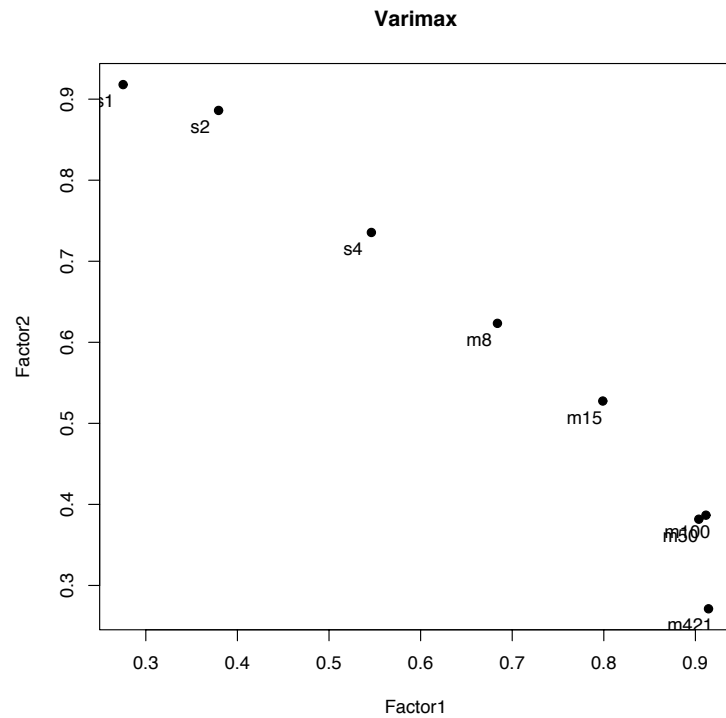
	Factor1	Factor2
Factor1	1.000	0.735
Factor2	0.735	1.000

Test of the hypothesis that 2 factors are sufficient.

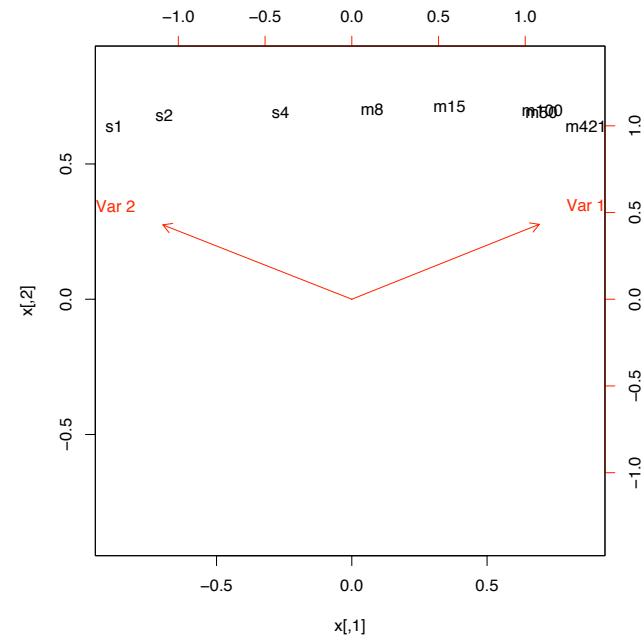
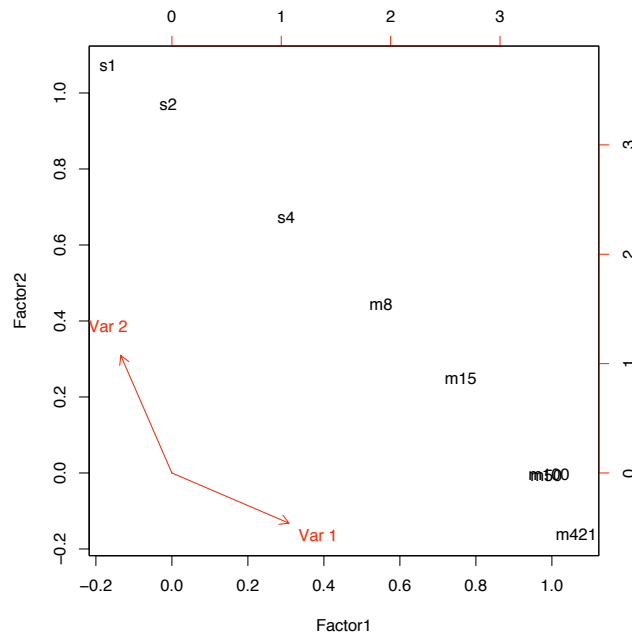
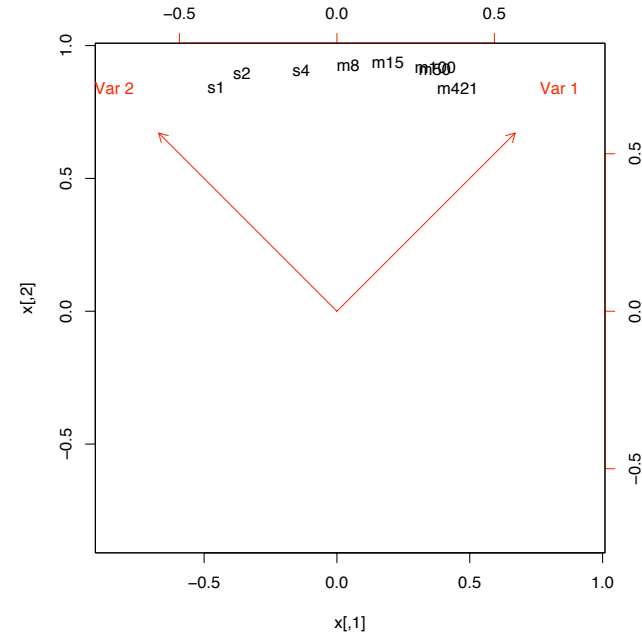
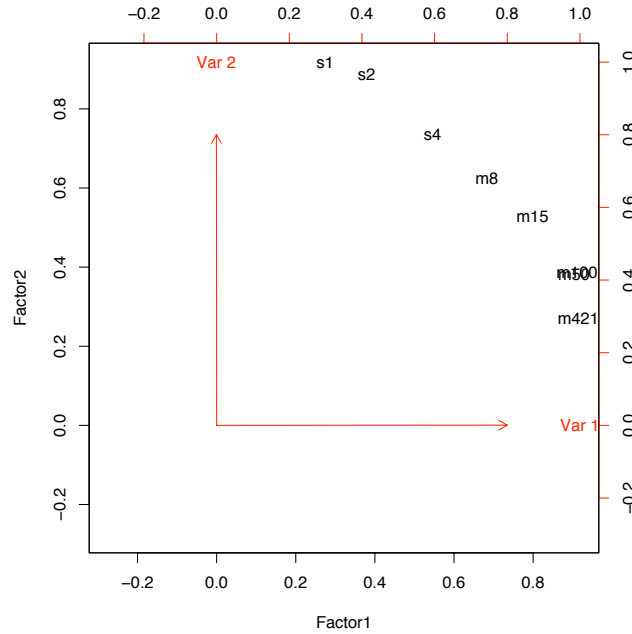
The chi square statistic is 16.36 on 13 degrees of freedom.

The p-value is 0.23

Track records velocity - men



Track records velocity men - more rotations



Track records velocity - women: factor analysis

```
factanal(x = welo, factors = 2, rotation = "varimax")
```

Uniquenesses:

s1	s2	s4	m8	m15	m30	m421
0.078	0.005	0.182	0.142	0.014	0.058	0.228

Loadings:

	Factor1	Factor2
s1	0.449	0.849
s2	0.395	0.916
s4	0.591	0.685
m8	0.812	0.447
m15	0.912	0.394
m30	0.881	0.407
m421	0.753	0.453

Test of the hypothesis that 2 factors are sufficient.

The chi square statistic is 50.17 on 8 degrees of freedom.

The p-value is 3.78e-08

Track records velocity - women: oblique factors

```
factanal(x = welo, factors = 2, rotation = "promax")
```

Uniquenesses:

	s1	s2	s4	m8	m15	m30	m421
	0.078	0.005	0.182	0.142	0.014	0.058	0.228

Loadings:

	Factor1	Factor2
s1		0.918
s2		1.052
s4	0.371	0.585
m8	0.855	
m15	1.035	
m30	0.982	
m421	0.766	0.139

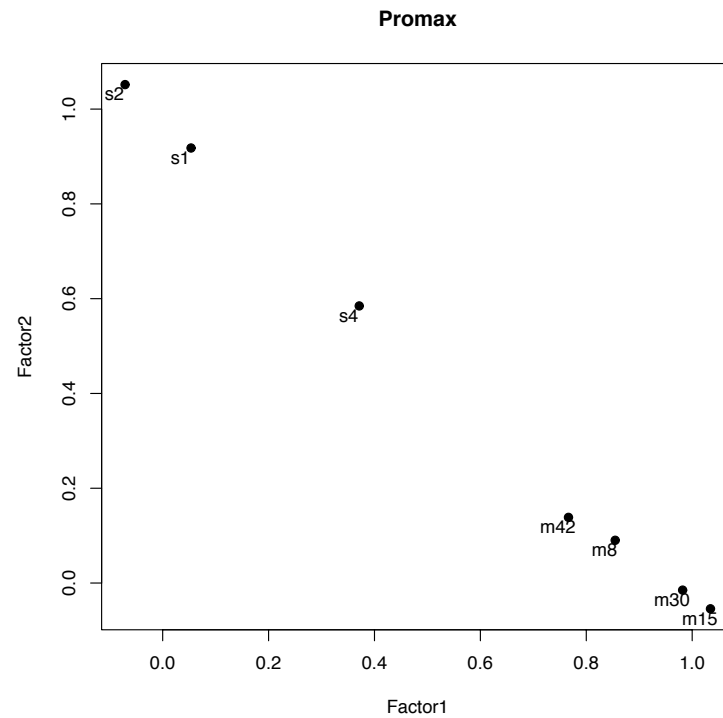
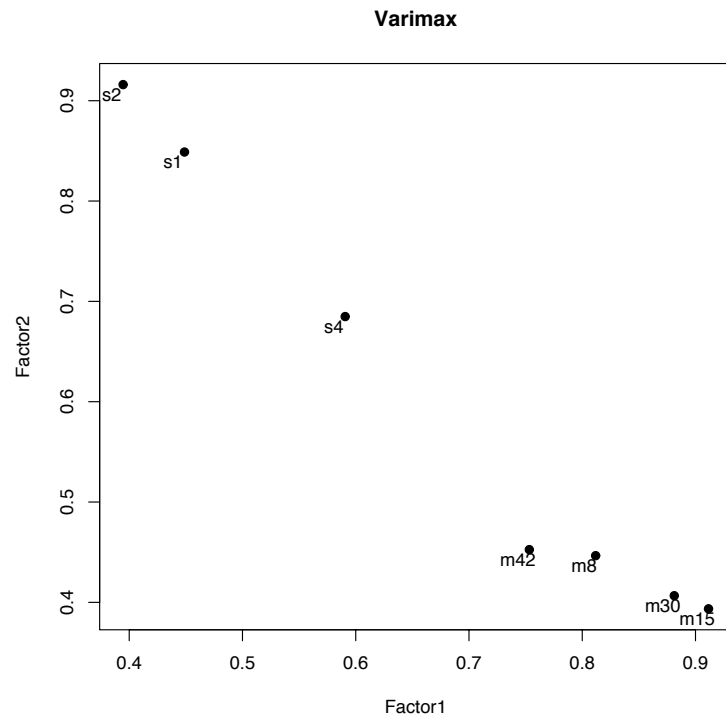
Test of the hypothesis that 2 factors are sufficient.

The chi square statistic is 50.17 on 8 degrees of freedom.

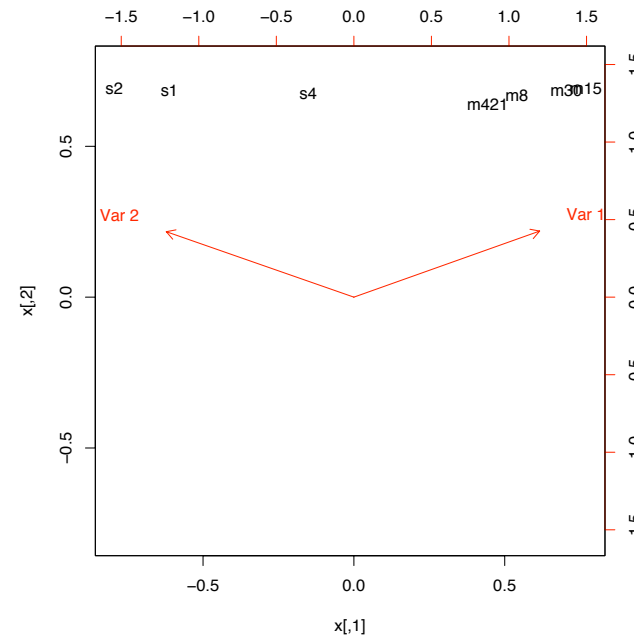
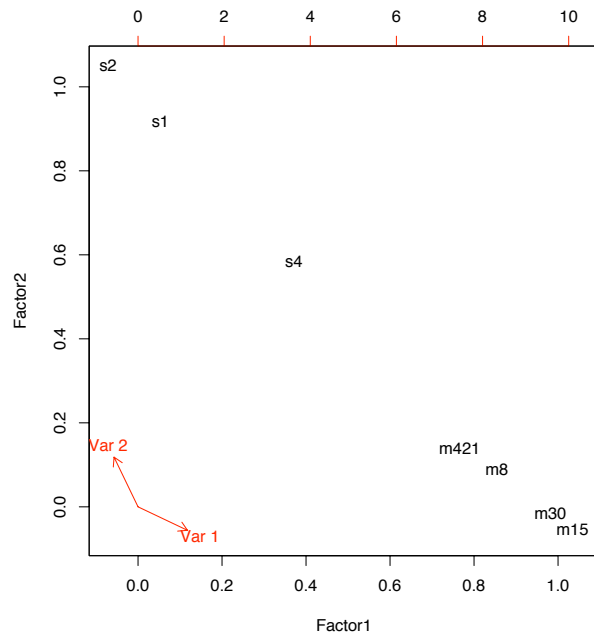
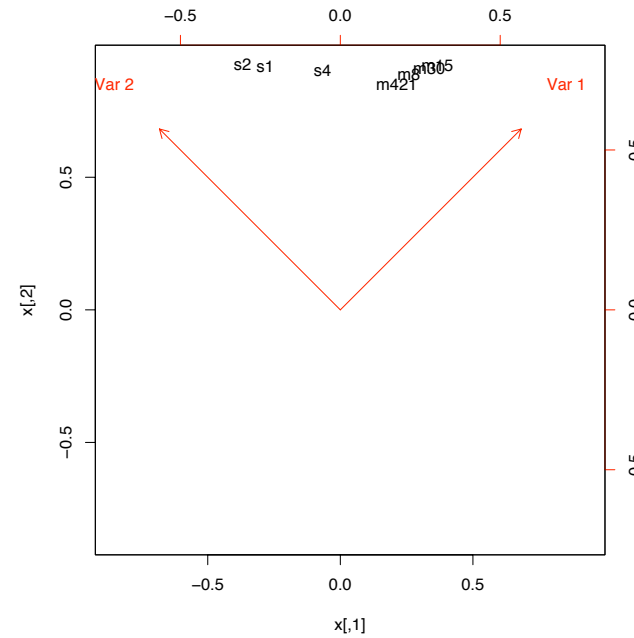
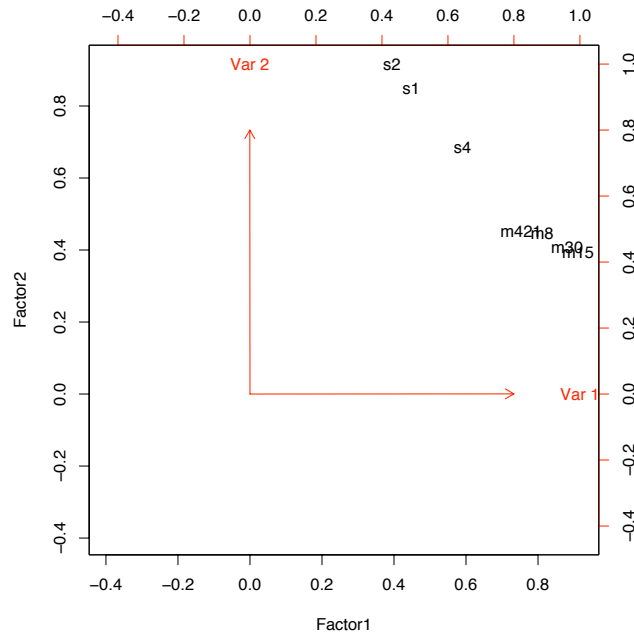
The p-value is 3.78e-08

Note: p-values indicate that two factors are *not* enough.

Track records velocity - women



Track records velocity women - more rotations



Track records velocity women - 3 factors

```
factanal(x = welo, factors = 3, rotation = "varimax")
```

Uniquenesses:

s1	s2	s4	m8	m15	m30	m421
0.076	0.005	0.088	0.005	0.037	0.018	0.192

Loadings:

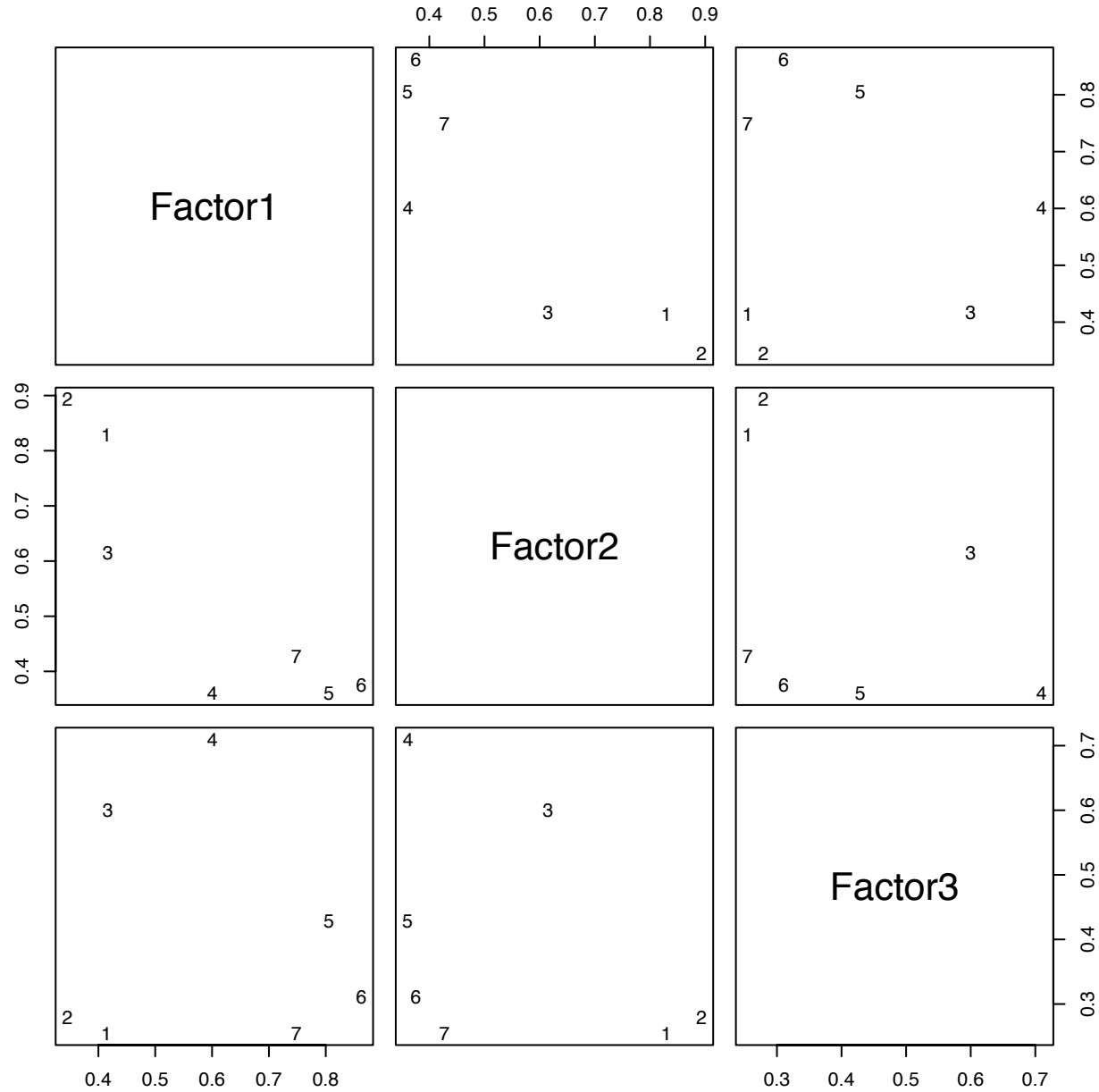
	Factor1	Factor2	Factor3
s1	0.414	0.829	0.255
s2	0.345	0.893	0.279
s4	0.417	0.615	0.600
m8	0.600	0.362	0.710
m15	0.806	0.360	0.429
m30	0.863	0.376	0.311
m421	0.749	0.428	0.255

Test of the hypothesis that 3 factors are sufficient.

The chi square statistic is 4.65 on 3 degrees of freedom.

The p-value is 0.199

Plotting those 3 factors



Track records velocity women - 3 oblique factors

```
factanal(x = welo, factors = 3, rotation = "promax")
```

Uniquenesses:

s1	s2	s4	m8	m15	m30	m421
0.076	0.005	0.088	0.005	0.037	0.018	0.192

Loadings:

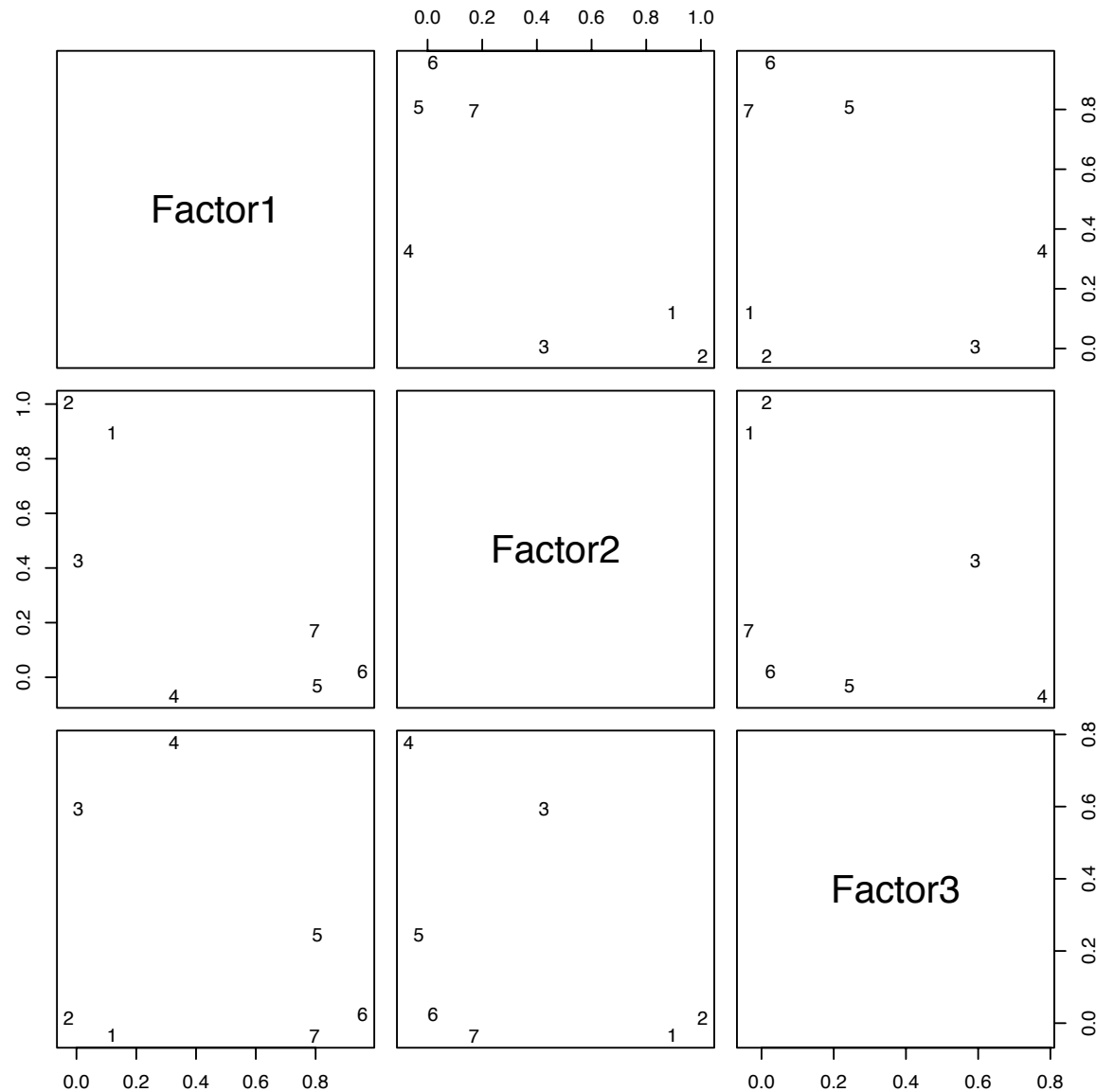
	Factor1	Factor2	Factor3
s1	0.120	0.895	
s2		1.006	
s4		0.427	0.593
m8	0.326		0.778
m15	0.806		0.244
m30	0.957		
m421	0.796	0.170	

Test of the hypothesis that 3 factors are sufficient.

The chi square statistic is 4.65 on 3 degrees of freedom.

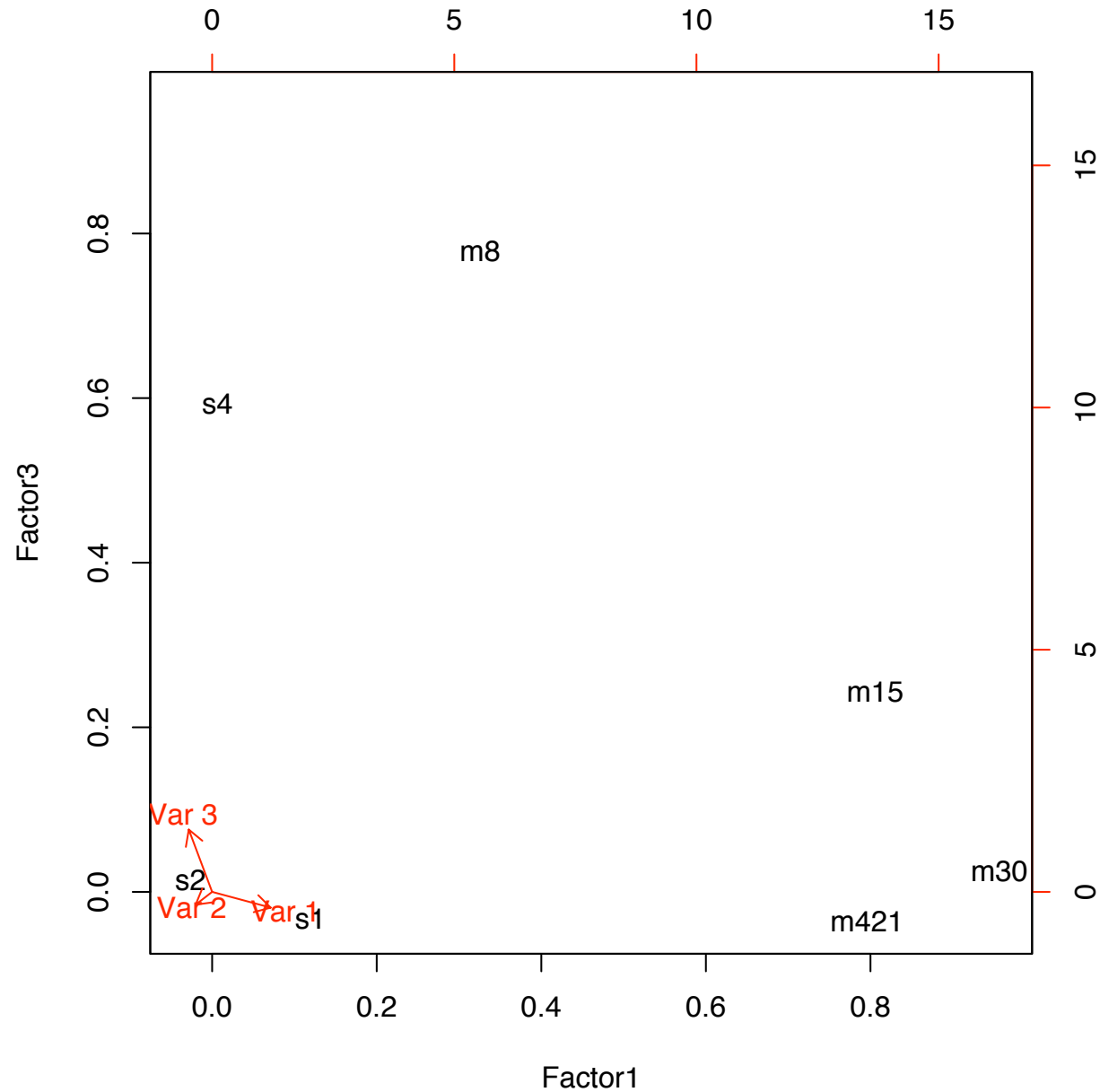
The p-value is 0.199

Plotting those 3 oblique factors

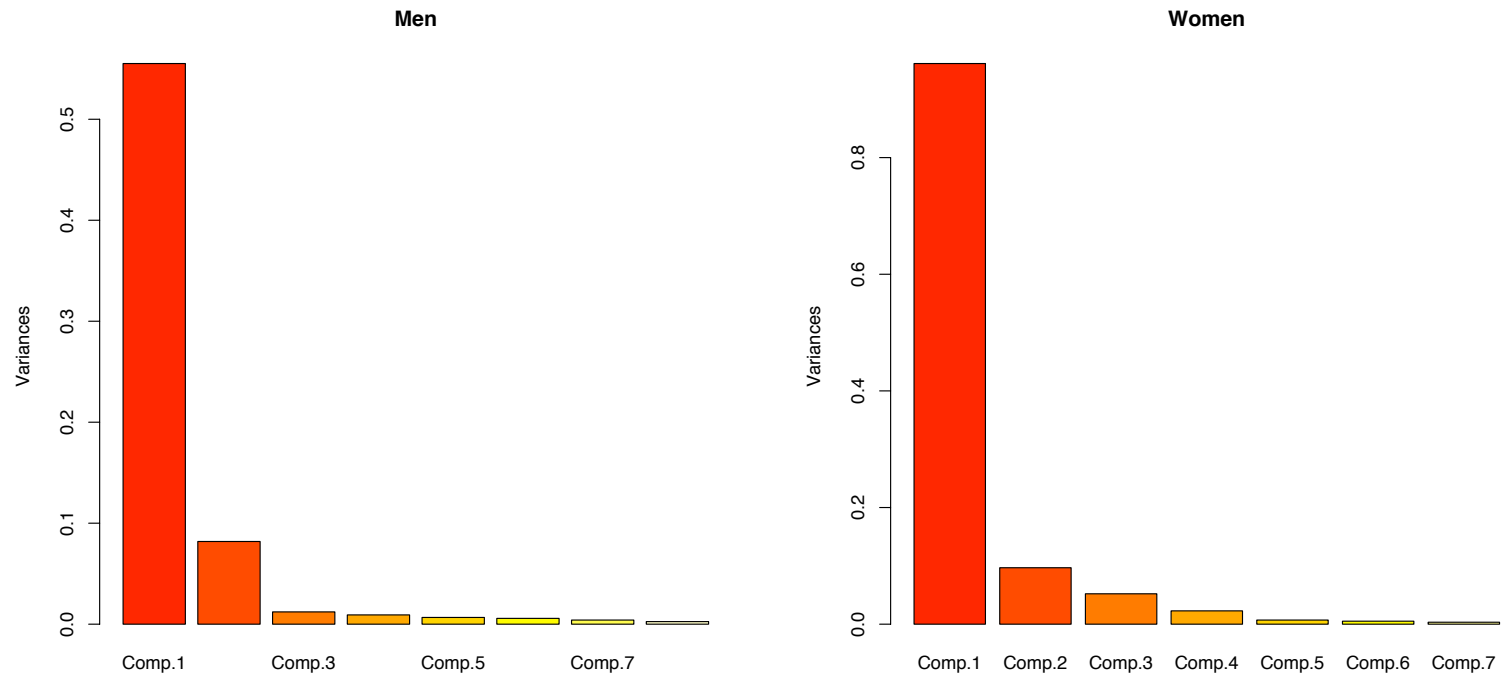


Note: p-values indicate that three factors are enough.

Perhaps this way... but aren't there outliers?



Not really... but there is something in women...



But who really knows... correlation matrices

The difference between sample and fitted correlation matrix

2 factors

	s1	s2	s4	m8	m15	m30	m421
s1	0.16	0.00	-0.01	-0.01	0.00	0.01	0.00
s2	0.00	0.01	0.00	0.00	0.00	0.00	0.00
s4	-0.01	0.00	0.36	0.11	0.00	-0.02	-0.04
m8	-0.01	0.00	0.11	0.28	0.00	-0.02	-0.03
m15	0.00	0.00	0.00	0.00	0.03	0.00	-0.01
m30	0.01	0.00	-0.02	-0.02	0.00	0.12	0.04
m421	0.00	0.00	-0.04	-0.03	-0.01	0.04	0.46

3 factors

	s1	s2	s4	m8	m15	m30	m421
s1	0.15	0.00	0.00	0.00	0.00	0.00	-0.01
s2	0.00	0.01	0.00	0.00	0.00	0.00	0.00
s4	0.00	0.00	0.18	0.00	-0.01	0.01	-0.01
m8	0.00	0.00	0.00	0.01	0.00	0.00	0.00
m15	0.00	0.00	-0.01	0.00	0.07	0.00	-0.01
m30	0.00	0.00	0.01	0.00	0.00	0.04	0.00
m421	-0.01	0.00	-0.01	0.00	-0.01	0.00	0.38

And variance-covariance matrices

The difference between sample and fitted variance matrix

2 factors

	s1	s2	s4	m8	m15	m30	m421
s1	0.002	0.002	0.001	0.000	0.002	0.003	0.002
s2	0.002	0.003	0.002	0.002	0.002	0.002	0.003
s4	0.001	0.002	0.003	0.016	0.002	0.000	-0.006
m8	0.000	0.002	0.016	0.002	0.003	-0.001	-0.002
m15	0.002	0.002	0.002	0.003	0.003	0.003	0.002
m30	0.003	0.002	0.000	-0.001	0.003	0.003	0.013
m421	0.002	0.003	-0.006	-0.002	0.002	0.013	0.006

3 factors

	s1	s2	s4	m8	m15	m30	m421
s1	0.002	0.002	0.002	0.001	0.002	0.002	0.000
s2	0.002	0.003	0.002	0.002	0.002	0.002	0.003
s4	0.002	0.002	0.003	0.002	0.001	0.003	0.000
m8	0.001	0.002	0.002	0.002	0.002	0.002	0.003
m15	0.002	0.002	0.001	0.002	0.003	0.003	0.002
m30	0.002	0.002	0.003	0.002	0.003	0.003	0.004
m421	0.000	0.003	0.000	0.003	0.002	0.004	0.006

Finally, scores

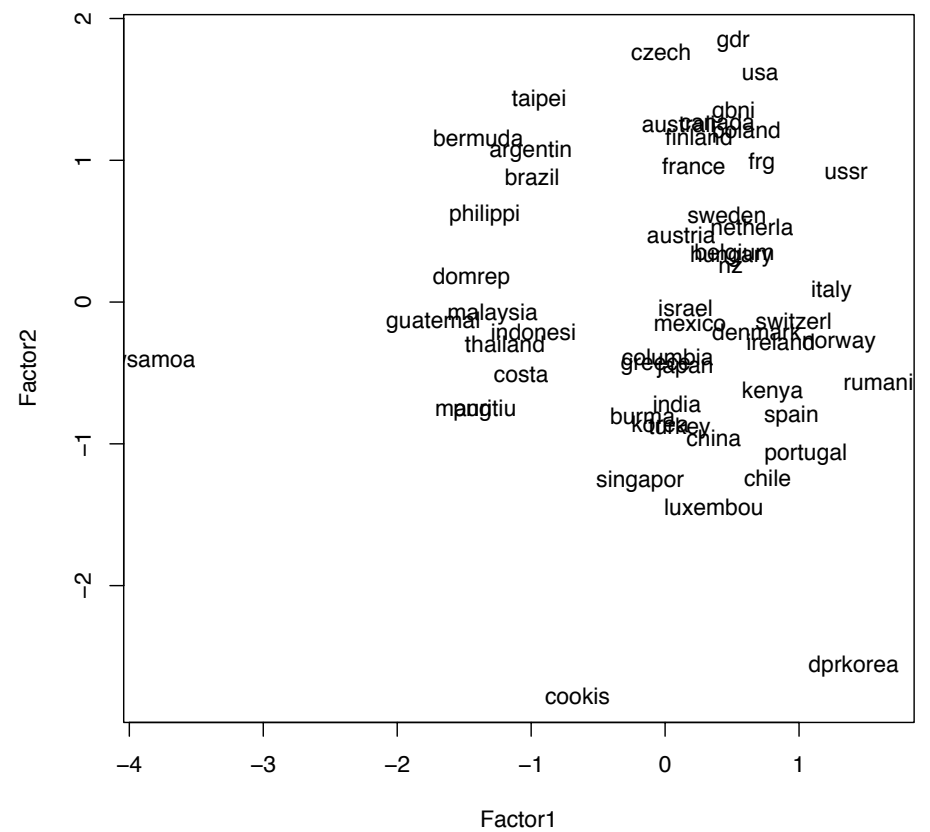
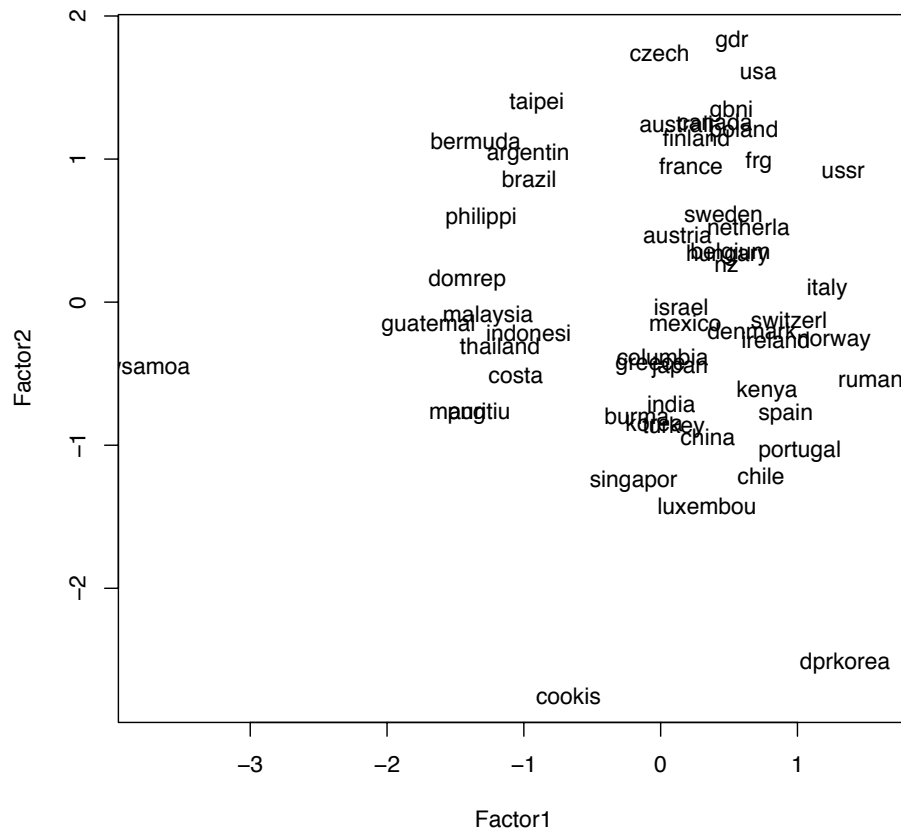
	Thomson		Bartlett	
	Factor1	Factor2	Factor1	Factor2
1	-0.9685	1.0361	-1.0018	1.0610
2	0.1143	1.2442	0.1013	1.2583
3	0.1241	0.4665	0.1209	0.4708
4	0.5114	0.3397	0.5180	0.3376
5	-1.3524	1.1252	-1.3950	1.1560
6	-0.9612	0.8619	-0.9923	0.8846
7	-0.1739	-0.7955	-0.1677	-0.8032
8	0.3970	1.2592	0.3898	1.2699
9	0.7348	-1.2138	0.7654	-1.2380
10	0.3453	-0.9417	0.3644	-0.9577
11	0.0148	-0.3813	0.0198	-0.3862
12	-0.6737	-2.7544	-0.6537	-2.7802
13	-1.0572	-0.5152	-1.0732	-0.5085
14	-0.0072	1.7394	-0.0289	1.7611
15	0.6685	-0.1988	0.6852	-0.2096
16	-1.4133	0.1522	-1.4451	0.1716
17	0.2623	1.1515	0.2535	1.1625
18	0.2222	0.9521	0.2150	0.9611
19	0.5213	1.8263	0.5097	1.8424
20	0.7190	0.9759	0.7221	0.9791
21	0.5180	1.3311	0.5124	1.3412
22	-0.0732	-0.4504	-0.0692	-0.4550
23	-1.6964	-0.1641	-1.7303	-0.1451
24	0.4889	0.3275	0.4952	0.3255
25	0.0781	-0.7086	0.0886	-0.7184
26	-0.9647	-0.2176	-0.9824	-0.2083
27	0.8428	-0.2668	0.8640	-0.2806
28	0.1501	-0.0359	0.1537	-0.0382
29	1.2172	0.0875	1.2419	0.0735

Country
argentin
australiali
austria
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bermuda
brazil
burma
canada
chile
china
columbia
cookis
costa
czech
denmark
domrep
finland
france
gdr
frg
gbni
greece
guatemal
hungary
india
indonesi
ireland
israel
italy

	Thomson		Bartlett	
	Factor1	Factor2	Factor1	Factor2
30	0.1438	-0.4528	0.1525	-0.4602
31	0.7781	-0.6194	0.8023	-0.6368
32	-0.0466	-0.8468	-0.0371	-0.8568
33	1.3485	-2.5211	1.4084	-2.5692
34	0.3394	-1.4243	0.3643	-1.4462
35	-1.2613	-0.1018	-1.2868	-0.0874
36	-1.3936	-0.7575	-1.4137	-0.7496
37	0.1802	-0.1426	0.1858	-0.1467
38	0.6421	0.5287	0.6491	0.5272
39	0.4826	0.2514	0.4897	0.2486
40	1.2676	-0.2807	1.2979	-0.2999
41	-1.4162	-0.7880	-1.4364	-0.7802
42	-1.3113	0.5868	-1.3464	0.6104
43	0.6095	1.1938	0.6076	1.2011
44	1.0166	-1.0459	1.0511	-1.0715
45	1.6000	-0.5378	1.6406	-0.5644
46	-0.1974	-1.2508	-0.1861	-1.2638
47	0.9142	-0.7825	0.9433	-0.8036
48	0.4597	0.6143	0.4618	0.6162
49	0.9392	-0.1212	0.9606	-0.1343
50	-0.9043	1.3934	-0.9407	1.4219
51	-1.1739	-0.3031	-1.1950	-0.2923
52	0.0950	-0.8768	0.1079	-0.8888
53	0.7142	1.5986	0.7094	1.6095
54	1.3350	0.9125	1.3519	0.9072
55	-3.7497	-0.4584	-3.8234	-0.4175

Country
japan
kenya
korea
dprkorea
luxembou
malaysia
mauritiu
mexico
netherla
nz
norway
png
philippi
poland
portugal
rumania
singapor
spain
sweden
switzerl
taipei
thailand
turkey
usa
ussr
wsamoa

And their plots



Summary: what is done

In factor analysis,

1. we need to (pre)determine the number of factors - either from the principal component analysis, or via testing methods
2. then estimate the loadings of the specified number of factors (nowadays mostly by the method of maximum likelihood)
3. and then we typically want to find a suitable rotation of the solution; if we want to keep common factors uncorrelated, we use only *orthogonal rotations* (like “varimax”); if we do not care about this particular aspect, we may also use *oblique rotations* (like “promax”)
4. and finally, we may want to estimate the individual scores

Summary: why it is done

A possible objective is to arrive to some plausible interpretation of the mechanism generating the data. This was the motivation of factor analysis in its classical era - and is still vital in certain areas of application. In this context, factor analysis was frequently confused with principal component analysis, so it is important to be aware of differences: the latter is not, but the former is invariant (more precisely, equivariant) with respect to the change of scale (at least in its stochastic model, but then also in the maximum likelihood estimates)

This classical objective has been a subject of criticism: from the scientific point of view, factor interpretation has to be confirmed by other sources - otherwise, from the statistical viewpoint, factor analysis as presented here is merely a sophisticated *exploratory method*.

We can, however, also use the individual scores (which implicitly involve some dimensional reduction) for prediction. This objective received new impetus in so-called recommender systems; as such application is focused on prediction, interpretability is not an issue there

Empiricist relationships: canonical correlations

Outline

Find directions in the first and second sample, respectively, that exhibit maximal correlation

And then second maximal, third maximal...

To summarize correlations between two samples

Alternative name: canonical variates

Sample correlation coefficient

Recall:

$$\rho_{xy} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (y_i - \bar{y})^2}}$$

Properties?

The prescription

Consider two data matrices:

X composed of lines \mathbf{x}_i^\top , and

Y composed of lines \mathbf{y}_i^\top , $i = 1, \dots, n$

Note: the numbers p and q of variables, the number of columns of **X** and **Y** respectively, may be different; but the number of their rows, the number of datapoints, has to be the same

We seek (nonzero) vectors \mathbf{a}_1 and \mathbf{b}_1 such that the (sample) correlation coefficient of $\mathbf{X}\mathbf{a}_1$ and $\mathbf{Y}\mathbf{b}_1$ is maximal

Once found, we may continue: seek nonzero vectors \mathbf{a}_2 and \mathbf{b}_2 such that \mathbf{a}_2 is orthogonal to \mathbf{a}_1 and \mathbf{b}_2 to \mathbf{b}_1 , again maximizing correlation of $\mathbf{X}\mathbf{a}_2$ and $\mathbf{Y}\mathbf{b}_2$ now

Continuing this, we may seek nonzero vector \mathbf{a}_j orthogonal to all previous \mathbf{a}_i , and nonzero \mathbf{b}_j orthogonal to all previous \mathbf{b}_i such that the correlation of $\mathbf{X}\mathbf{a}_j$ and $\mathbf{Y}\mathbf{b}_j$ is maximal. Of course, this is possible only if $j \leq p$ and $j \leq q$; hence we can repeat the above only $\min\{p, q\}$ times

Remarks

Note that the correlation coefficient changes only by the sign of c if either \mathbf{a}_i or \mathbf{b}_i is replaced by $c\mathbf{a}_i$ or $c\mathbf{b}_i$, respectively

Thus, we do not have to worry about negative correlations - just take the opposite \mathbf{a}_i or \mathbf{b}_i and they become positive. Then, when we are multiplying either \mathbf{a}_i or \mathbf{b}_i by positive constants, the correlations remain the same. Therefore, the only side condition on \mathbf{a}_i and \mathbf{b}_i is that they are nonzero - from the mathematical point of view, everything else is well-posed

From the numerical point of view, however, it may be practical to scale \mathbf{a}_i and \mathbf{b}_i in some convenient way; *it is usually done that the variances of resulting linear combinations of the data - canonical variates - are 1*

Canonical variates come in pairs, and given what was specified above, there are $\min\{p, q\}$ of these pairs. In a special case when p or q is equal to one, there is only one pair; the maximized correlation coefficient is the **multiple correlation coefficient**

Solution: variance matrices again

Notation: $\text{var}(\mathbf{X}) = \mathbf{S}_X$ is now denoted as \mathbf{S}_{XX} , and analogously $\text{var}(\mathbf{Y}) = \mathbf{S}_Y$ as \mathbf{S}_{YY} . Symbols $\mathbf{S}_{XY} = \text{cov}(\mathbf{X}, \mathbf{Y})$ and $\mathbf{S}_{YX} = \text{cov}(\mathbf{Y}, \mathbf{X})$ denote now the matrices of (sample) cross-covariances between \mathbf{X} and \mathbf{Y} , with $\mathbf{S}_{XY} = \mathbf{S}_{YX}^\top$. Then

$$\text{var}(\mathbf{X} \ \mathbf{Y}) = \begin{pmatrix} \mathbf{S}_{XX} & \mathbf{S}_{XY} \\ \mathbf{S}_{YX} & \mathbf{S}_{YY} \end{pmatrix}$$

is the variance-covariance matrix of the joint data matrix $(\mathbf{X} \ \mathbf{Y})$.

The correlation between $\mathbf{X}\mathbf{a}$ and $\mathbf{Y}\mathbf{b}$ is

$$\frac{\mathbf{a}^\top \mathbf{S}_{XY} \mathbf{b}}{\sqrt{(\mathbf{a}^\top \mathbf{S}_{XX} \mathbf{a})(\mathbf{b}^\top \mathbf{S}_{YY} \mathbf{b})}}$$

Solution continued

Then, the maximal correlation between \mathbf{Xa} and \mathbf{Yb} ,
maximized over $\mathbf{a} \neq 0$ and $\mathbf{b} \neq 0$,

is $\sqrt{\lambda}$, where λ is the largest eigenvalue of both

$$\begin{matrix} \mathbf{S}_{\mathbf{XX}}^{-1}\mathbf{S}_{\mathbf{XY}}\mathbf{S}_{\mathbf{YY}}^{-1}\mathbf{S}_{\mathbf{YX}} \\ \mathbf{S}_{\mathbf{YY}}^{-1}\mathbf{S}_{\mathbf{YX}}\mathbf{S}_{\mathbf{XX}}^{-1}\mathbf{S}_{\mathbf{XY}} \end{matrix} \quad \text{and} \quad \begin{matrix} \mathbf{a} \\ \mathbf{b} \end{matrix} \text{ are the corresponding eigenvectors}$$

More generally, if \mathbf{X} has p and \mathbf{Y} has q columns, then the number of canonical correlations is $m = \min\{p, q\}$ and they are the square roots of the first m maximal eigenvalues of the matrices above, with coefficients being the corresponding eigenvectors

Yes, and if this $m = 1$, that is, when either p or q is equal to 1, then the only canonical correlation is called **multiple correlation coefficient**, of one variable against the reminding ones

Example: sons

Length and breadth, respectively, of the head of the first and second son

	L1	B1	L2	B2
1	191	155	179	145
2	195	149	201	152
3	181	148	185	149
4	183	153	188	149
5	176	144	171	142
6	208	157	192	152
7	189	150	190	149
8	197	159	189	152
9	188	152	197	159
10	192	150	187	151
11	179	158	186	148
12	183	147	174	147
13	174	150	185	152

	L1	B1	L2	B2
14	190	159	195	157
15	188	151	187	158
16	163	137	161	130
17	195	155	183	158
18	186	153	173	148
19	181	145	182	146
20	175	140	165	137
21	192	154	185	152
22	174	143	178	147
23	176	139	176	143
24	197	167	200	158
25	190	163	187	150

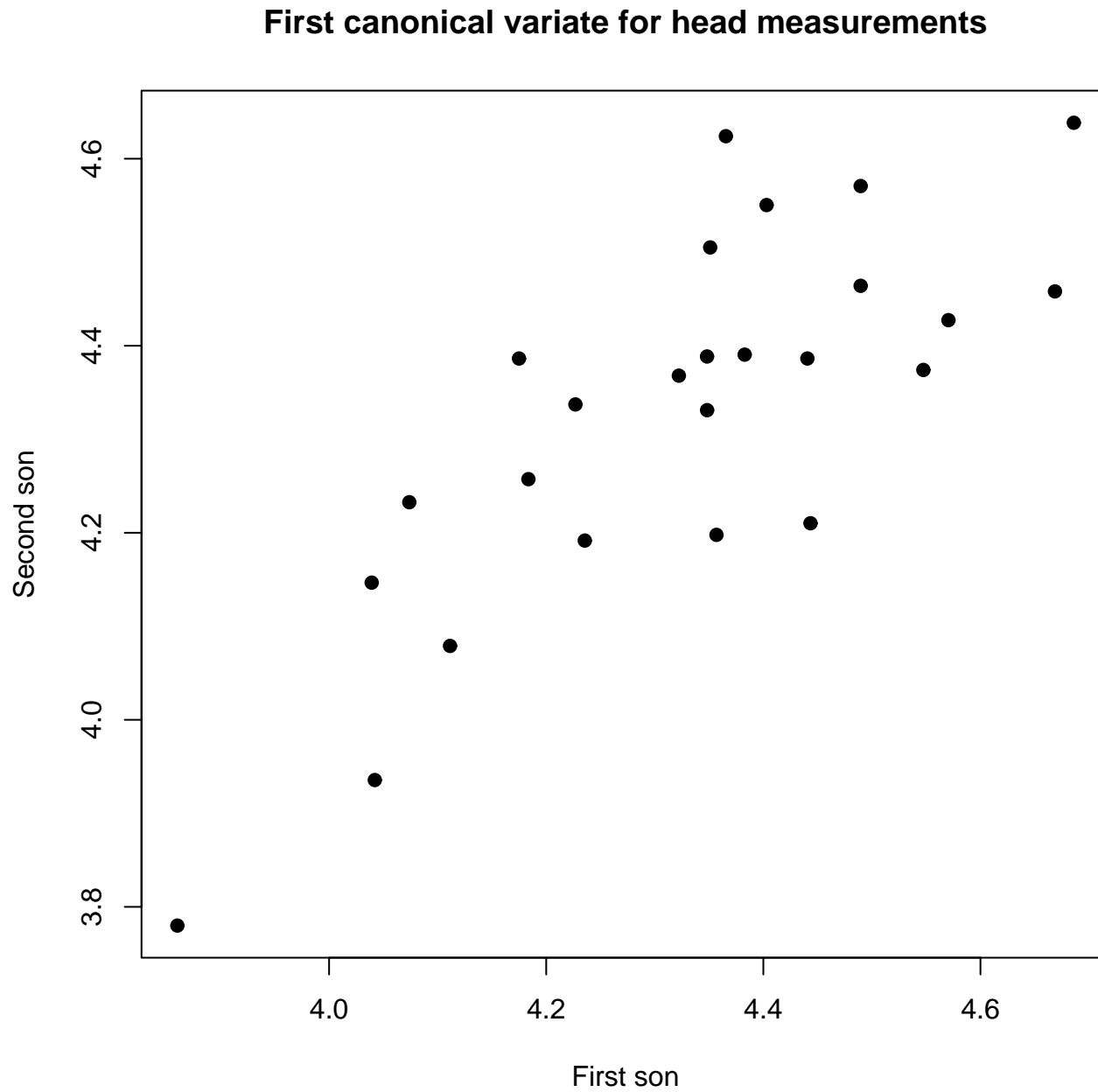
The result

```
> sons <- read.table("sons.d")
> cancor(sons[,1:2],sons[,3:4])
$cor
[1] 0.7885079 0.0537397
$xcoef
      [,1]      [,2]
L1 0.01154653 -0.02857148
B1 0.01443910  0.03816093
$ycoef
      [,1]      [,2]
L2 0.01025573 -0.03595605
B2 0.01637533  0.05349758
$xcenter
      L1      B1
185.72 151.12
$ycenter
      L2      B2
183.84 149.24
```


Canonical variates?

```
> sons.cc <- cancel(sons[,1:2],sons[,3:4])  
> canvarx <- as.matrix(sons[,1:2]) %*% sons.cc$xcoef[,1]  
> canvary <- as.matrix(sons[,3:4]) %*% sons.cc$ycoef[,1]  
> plot(canvarx, canvary, pch=16,  
+ xlab='First son',ylab='Second son')
```

And the plot



What else?

```
> var(sons)
```

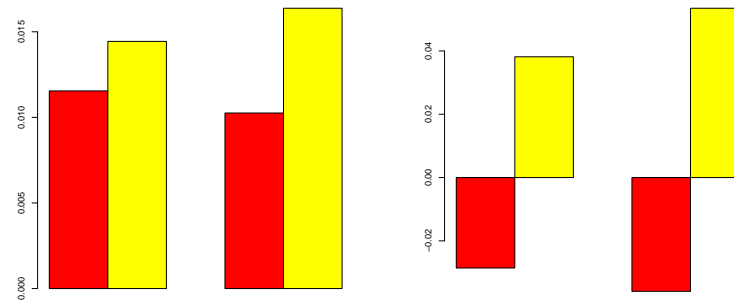
	L1	B1	L2	B2
L1	95.29333	52.86833	69.66167	46.11167
B1	52.86833	54.36000	51.31167	35.05333
L2	69.66167	51.31167	100.80667	56.54000
B2	46.11167	35.05333	56.54000	45.02333

```
$xcoef
```

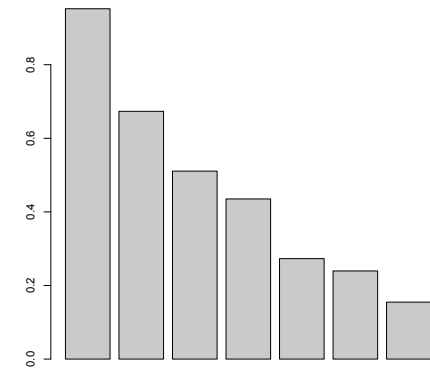
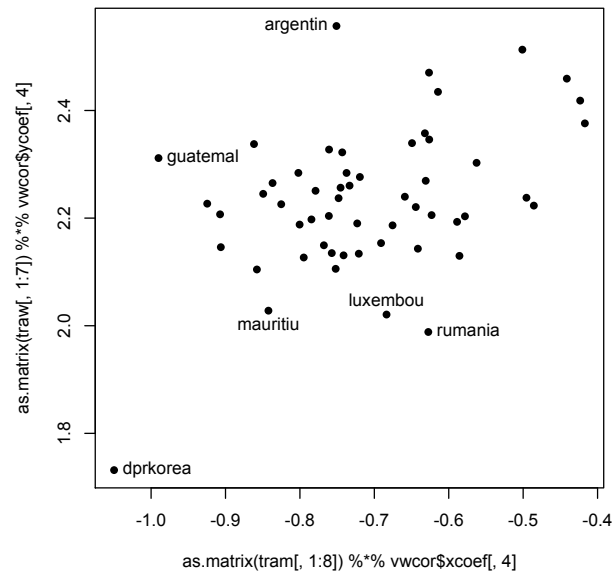
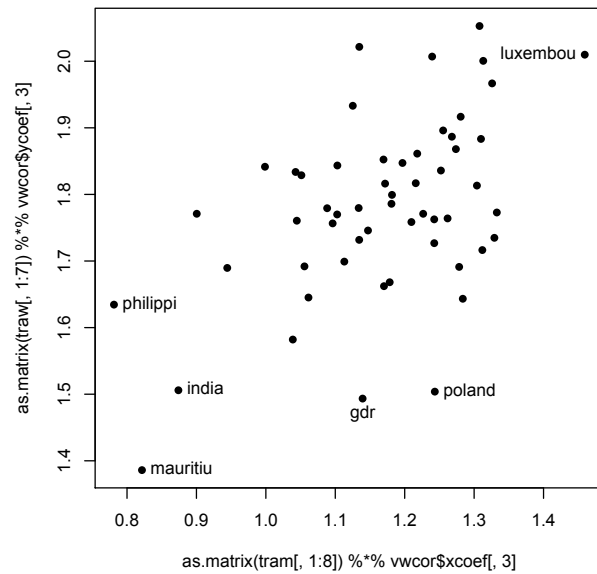
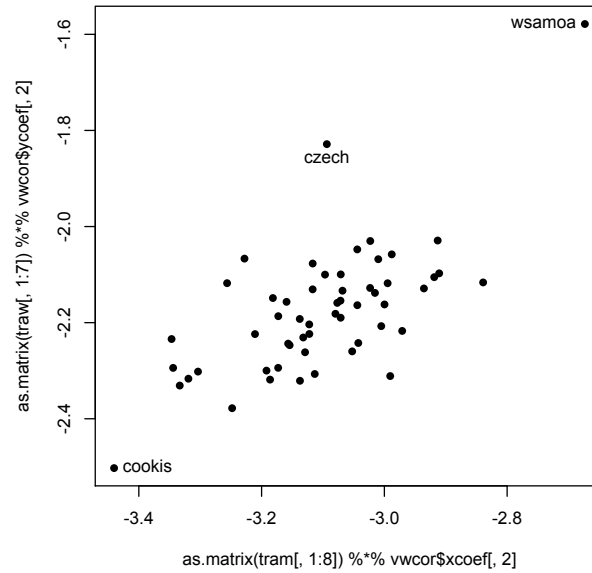
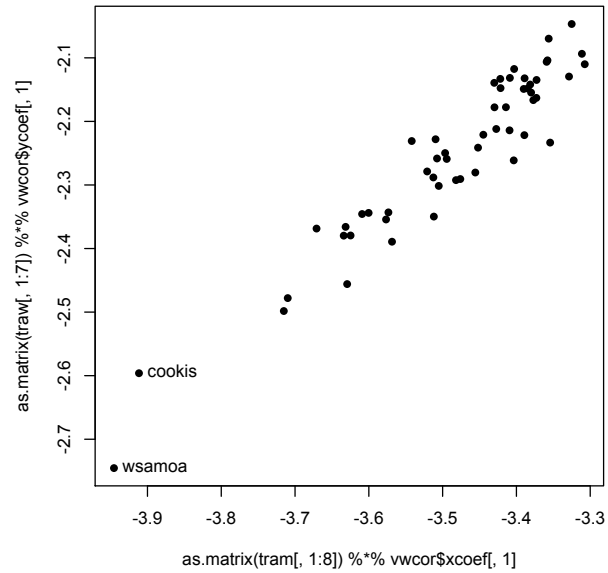
	[,1]	[,2]
L1	0.01154653	-0.02857148
B1	0.01443910	0.03816093

```
$ycoef
```

	[,1]	[,2]
L2	0.01025573	-0.03595605
B2	0.01637533	0.05349758



Example: running data

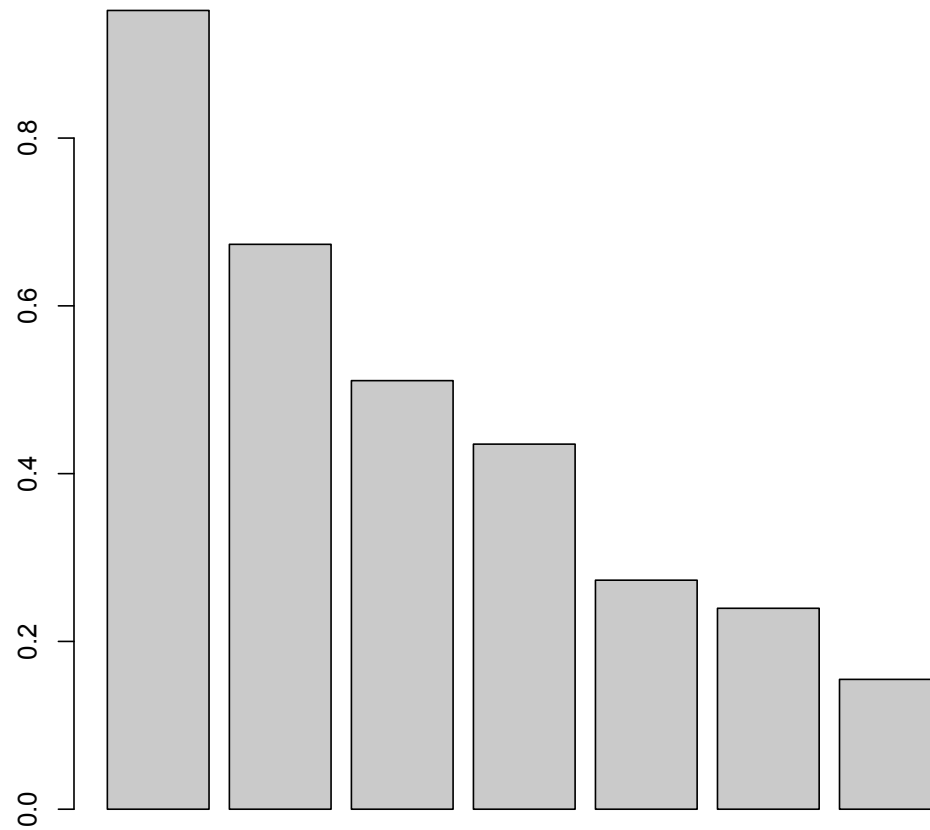


Running data transcript

```
> vwcov=cancor(tram[,1:8],traw[,1:7])
> par(mfrow=c(2,2))
> plot(as.matrix(tram[,1:8]) %*% vwcov$xcoef[,1],
+ as.matrix(traw[,1:7]) %*% vwcov$ycoef[,1],pch=16)
> identify(as.matrix(tram[,1:8]) %*% vwcov$xcoef[,1],
+ as.matrix(traw[,1:7]) %*% vwcov$ycoef[,1],labels=traw[,8])
[1] 12 55
> plot(as.matrix(tram[,1:8]) %*% vwcov$xcoef[,2],
...
[1] 12 14 55
> plot(as.matrix(tram[,1:8]) %*% vwcov$xcoef[,3],
...
[1] 19 25 34 36 42 43
> plot(as.matrix(tram[,1:8]) %*% vwcov$xcoef[,4],
...
[1] 1 23 33 34 36 45
```

How canonical correlations fare here?

```
> barplot{vwcor}
```



Running data transcript continued

```
> vwcov
```

```
$cor
```

```
[1] 0.9521159 0.6733411 0.5108601 0.4351771 0.2730063 0.2395034 0.1547629
```

```
$xcoef
```

	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]
s1	0.104094168	-0.107380162	-0.515664832	-0.25908559	-0.6883280074	0.376619624
s2	-0.108737342	-0.106936978	-0.109330683	0.06559543	0.4299810105	-0.217250889
s4	0.013809246	-0.124909061	0.174467768	0.08240273	0.0093848913	0.041841603
m8	-0.846947526	2.292211283	2.128900905	-4.67774851	-0.5470794211	-0.441871257
m15	-0.206532529	0.277130648	-0.415851876	1.31836018	-0.0001939217	-1.524535704
m50	-0.008423944	-0.080300588	-0.030690671	0.01810175	-0.5673227355	-0.309327155
m100	-0.024762400	0.087875854	-0.007190537	-0.10191559	0.2682108659	0.241688938
m421	0.001308979	-0.003716701	-0.006534732	0.02209632	-0.0084966587	0.006218362

```
...
```

```
$ycoef
```

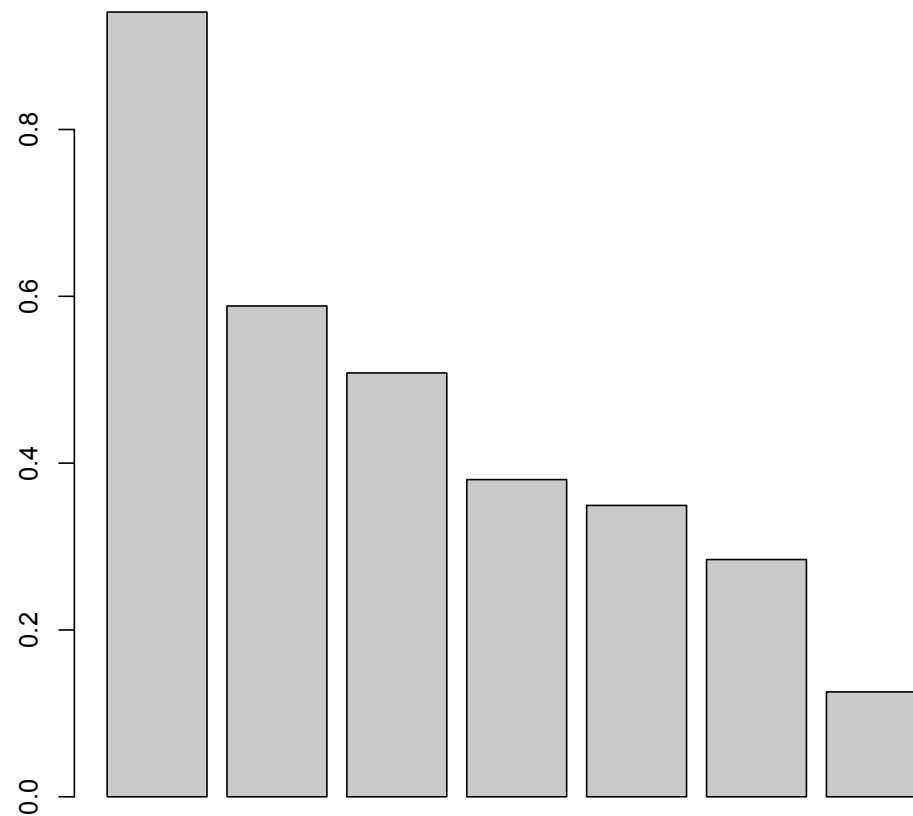
	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]
s1	-0.0130055307	0.0176386680	0.061917582	0.5792507543	0.216963524	-0.64954132
s2	-0.0605052422	-0.0957820269	-0.015752815	-0.3076449771	0.097987108	0.13392170
s4	0.0209834118	-0.0064488138	0.073967723	-0.0029267579	-0.112539112	0.04433569
m8	-0.5073336300	-1.6614889659	-2.314920945	2.2016538222	1.758300290	0.07128654
m15	0.0094233762	1.0338571845	1.374913004	-0.2205103685	0.701931326	0.69584361
m30	-0.0694585560	-0.0872183745	-0.281419643	-0.0572468827	-0.469592348	-0.36565080
m421	-0.0007024018	0.0001743919	-0.005775172	-0.0008261367	0.001848462	0.00326083

```
...
```

How about omitting very small countries?

(Cook Island, Luxembourg, Western Samoa omitted)

```
> vwnew=cancor(tram[-c(12,34,55),1:8],traw[-c(12,34,55),1:7])  
> barplot(vwnew$cor)
```



The result

```
> vwnew
```

```
$cor
```

```
[1] 0.9407974 0.5884286 0.5081459 0.3802782 0.3493206 0.2844400 0.1257613
```

```
$xcoef
```

	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]
s1	-0.0592844998	0.42333578	-0.092313052	0.36266317	1.21069000	0.2341572681
s2	-0.0586454028	-0.23234027	-0.316222887	-0.32816777	-0.39066849	-0.1487345454
s4	0.0081157972	-0.10537898	0.213525556	-0.03270155	0.06395563	-0.0241539365
m8	-0.6341725899	-0.58367704	-0.768746039	4.99394224	-2.81142541	0.0256325079
m15	-0.2088342032	-0.06469008	0.085591407	-1.70388403	-0.50357199	0.4721261302
m50	-0.0603341980	-0.01619295	-0.031304150	0.14973689	0.15662788	0.7664245903
m100	-0.0225362139	0.05796283	-0.021212688	0.14387843	-0.07560743	-0.3486315644
m421	0.0007541957	0.01502310	0.006513154	-0.02803850	0.01260490	0.0005577576

```
...
```

```
$ycoef
```

	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]
s1	-0.0003540832	0.050271374	0.178529200	-0.817049127	-0.375775582	0.077606779
s2	-0.0593500609	-0.203584049	-0.148173170	0.308869741	-0.006811645	-0.139683776
s4	0.0158728665	0.009585147	0.060670314	0.040390516	0.097630689	0.094526166
m8	-0.3105236092	-1.532243337	-0.262419707	-3.163682685	-0.185052036	-2.292433786
m15	-0.1714313947	1.075555404	1.094736369	1.344590415	-0.446258250	-0.552282755
m30	-0.0500201340	-0.116154880	-0.351132266	-0.093779920	-0.098462780	0.545947847
m421	-0.0011833621	0.003367182	-0.004573076	-0.002911054	0.005610899	-0.004093673

```
...
```

Canonical correlations via SVD

We start again form the variance-covariance matrix of joint data matrix $(\mathbf{X} \ \mathbf{Y})$ and multiply it by matrices from left and right as follows:

$$\begin{pmatrix} \mathbf{S}_{\mathbf{XX}}^{-1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_{\mathbf{YY}}^{-1/2} \end{pmatrix} \begin{pmatrix} \mathbf{S}_{\mathbf{XX}} & \mathbf{S}_{\mathbf{XY}} \\ \mathbf{S}_{\mathbf{YX}} & \mathbf{S}_{\mathbf{YY}} \end{pmatrix} \begin{pmatrix} \mathbf{S}_{\mathbf{XX}}^{-1/2} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_{\mathbf{YY}}^{-1/2} \end{pmatrix} \\ = \begin{pmatrix} \mathbf{I} & \mathbf{S}_{\mathbf{XX}}^{-1/2} \mathbf{S}_{\mathbf{XY}} \mathbf{S}_{\mathbf{YY}}^{-1/2} \\ \mathbf{S}_{\mathbf{YY}}^{-1/2} \mathbf{S}_{\mathbf{YX}} \mathbf{S}_{\mathbf{XX}}^{-1/2} & \mathbf{I} \end{pmatrix}$$

where $\mathbf{A}^{-1/2}$ a matrix such that $\mathbf{A}^{-1/2} \mathbf{A}^{-1/2} = \mathbf{A}^{-1}$

We then apply SVD to the matrix (the other one is its transpose)

$$\mathbf{S}_{\mathbf{XX}}^{-1/2} \mathbf{S}_{\mathbf{XY}} \mathbf{S}_{\mathbf{YY}}^{-1/2} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^T$$

The singular values are canonical correlations now; the columns of matrices $\mathbf{S}_{\mathbf{XX}}^{-1/2} \mathbf{U}$ and $\mathbf{S}_{\mathbf{YY}}^{-1/2} \mathbf{V}$ give respectively the vectors of coefficients.

Qualitative data: the anatomy of χ^2 -statistic

Recall: we want to test independence in a $r \times c$ contingency table. The probabilities of observations in cells are p_{ij} ; under the hypothesis of independence, $p_{ij} = p_{i.}p_{.j}$, where $p_{i.}$ and $p_{.j}$ are column and row sums - marginal probabilities. We observe cells frequencies n_{ij} ; the estimates for $p_{i.}$ and $p_{.j}$ are $\hat{p}_{i.} = n_{i.}/n$ and $\hat{p}_{.j} = n_{.j}/n$, respectively; n is the total number of observations. Under the hypothesis of independence, the estimate for the cell probability is $\hat{p}_{ij} = \hat{p}_{i.}\hat{p}_{.j} = (n_{i.}/n)(n_{.j}/n)$, and therefore, while the observed number is $O = n_{ij}$, the predicted number of observations is

$$P = n \frac{n_{i.}n_{.j}}{n^2} = \frac{n_{i.}n_{.j}}{n}; \quad \text{the test statistics is } \sum_{\text{all cells}} \frac{(O_k - P_k)^2}{P_k}$$

- the sum of squares of "Pearson residuals" $\frac{O_k - P_k}{\sqrt{P_k}}$

We use χ^2 distribution with $(r - 1)(c - 1)$ degrees of freedom to assess how large is this statistic is large enough, via its right tail value, which gives the p-value for the hypothesis of independence. If this p-value is low, we may reject the hypothesis: good, but what then?

Correspondence analysis

Suppose that \mathbf{E} is the matrix formed from n_{ij}/n (the estimates of cell probabilities not assuming the independence hypothesis) and \mathbf{R} , \mathbf{C} are diagonal matrices formed from vectors \mathbf{r} and \mathbf{c} , with elements $r_i = n_{i.}/n$ and $c_j = n_{.j}/n$, respectively.

Consider the matrix $\mathbf{R}^{-1/2}\mathbf{E}\mathbf{C}^{-1/2}$ (it is easy to form the square roots of diagonal matrices with positive elements). This matrix has elements

$$\frac{e_{ij}}{\sqrt{r_i c_j}}$$

SVD of this matrix can be viewed as returning scores giving maximal “correlations” for rows and columns. The largest singular value is always one, corresponding to constant scores; hence we dismiss it, and look only for nontrivial solutions corresponding to singular values beginning with the second largest. That is, we form the SVD of

$$\mathbf{R}^{-1/2}(\mathbf{E} - \mathbf{r}\mathbf{c}^T)\mathbf{C}^{-1/2} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$$

instead, and then we may take first one or two singular values.

Interpretation I

Can be thought of as analysis of the χ^2 statistic for independence, because the elements of the matrix $\mathbf{R}^{-1/2}(\mathbf{E} - \mathbf{rc}^T)\mathbf{C}^{-1/2}$ are Pearson residuals, up to a factor \sqrt{n} .

```
> class(haireye)='table'
> matrix(residuals(glm(Freq~Hair+Eye,family=poisson,
data=as.data.frame(haireye)),type='pearson'),4,4)/sqrt(sum(haireye))
      [,1]      [,2]      [,3]      [,4]
[1,] 0.180773066 -0.12615064 -0.01961905 -0.08029590
[2,] 0.050694815 -0.08012300  0.05561963 -0.01418351
[3,] -0.003081574 -0.07110772  0.03502737  0.09381990
[4,] -0.240474512  0.28973637 -0.09156384  0.02518174
> diag(1/sqrt(r)) %*% (E - r %*% t(c)) %*% diag(1/sqrt(c))
      [,1]      [,2]      [,3]      [,4]
[1,] 0.180773066 -0.12615064 -0.01961905 -0.08029590
[2,] 0.050694815 -0.08012300  0.05561963 -0.01418351
[3,] -0.003081574 -0.07110772  0.03502737  0.09381990
[4,] -0.240474512  0.28973637 -0.09156384  0.02518174
```

Another interpretation - and plotting

Can be also viewed as a search for the linear combination giving maximal contingency (“correlation”) - not accounting for the trivial constant solution

can be a comparison of distances between “profiles” - rowwise or columnwise conditional distributions.

If the resulting SVD is $\mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$, then of interest are first columns of $\mathbf{A} = \mathbf{R}^{-1/2}\mathbf{U}\mathbf{\Lambda}$ and $\mathbf{B} = \mathbf{C}^{-1/2}\mathbf{V}\mathbf{\Lambda}$

Inertia: the sum of squares of omitted singular values

Plotting:

“Asymmetric approach”: plots either first two columns of \mathbf{A} with first two columns of $\mathbf{C}^{-1/2}\mathbf{V}$ (rows) or \mathbf{B} with first two columns of $\mathbf{R}^{-1/2}\mathbf{U}$ (columns). Row plot can be viewed as that \mathbf{A} is a convex combination of row profiles, given by $\mathbf{C}^{-1/2}\mathbf{V}$ - and similarly the column one

Or, in “classical correspondence analysis”, “symmetric approach”, first two columns of \mathbf{A} and \mathbf{B} are plotted on the same figure

Aggregated hair/eye color data: $r = c = 4$

```
> haireye=apply(HairEyeColor,1:2,sum)
```

```
> haireye
```

	Eye			
Hair	Brown	Blue	Hazel	Green
Black	68	20	15	5
Brown	119	84	54	29
Red	26	17	14	14
Blond	7	94	10	16

First, some testing of the method:

```
> r = apply(haireye,1,sum)/sum(haireye)
```

```
> c = apply(haireye,2,sum)/sum(haireye)
```

```
> E = haireye/sum(haireye)
```

```

> svd(diag(1/sqrt(r)) %*% E %*% diag(1/sqrt(c)))
$d
[1] 1.00000000 0.45691646 0.14908593 0.05097489
$u
      [,1]      [,2]      [,3]      [,4]
[1,] -0.4271211  0.47166009  0.6154461  0.4651134
[2,] -0.6950598  0.22552151 -0.1522951 -0.6654608
[3,] -0.3463126  0.09817011 -0.7424993  0.5649115
[4,] -0.4631706 -0.84678181  0.2161646  0.1473309
$v
      [,1]      [,2]      [,3]      [,4]
[1,] -0.6096078  0.6566258  0.3611439  0.25844921
[2,] -0.6026406 -0.7220003  0.3353208 -0.05567605
[3,] -0.3963516  0.1844169 -0.4450167 -0.78157274
[4,] -0.3287980 -0.1163980 -0.7477267  0.56502056
> svd(diag(1/sqrt(r)) %*% (E - r %*% t(c)) %*% diag(1/sqrt(c)))
$d
[1] 4.569165e-01 1.490859e-01 5.097489e-02 2.929785e-19
$u
      [,1]      [,2]      [,3]      [,4]
[1,] -0.47166009  0.6154461 -0.4651134  0.4271211
[2,] -0.22552151 -0.1522951  0.6654608  0.6950598
[3,] -0.09817011 -0.7424993 -0.5649115  0.3463126
[4,]  0.84678181  0.2161646 -0.1473309  0.4631706
$v
      [,1]      [,2]      [,3]      [,4]
[1,] -0.6566258  0.3611439 -0.25844921 -0.6096078
[2,]  0.7220003  0.3353208  0.05567605 -0.6026406
[3,] -0.1844169 -0.4450167  0.78157274 -0.3963516
[4,]  0.1163980 -0.7477267 -0.56502056 -0.3287980

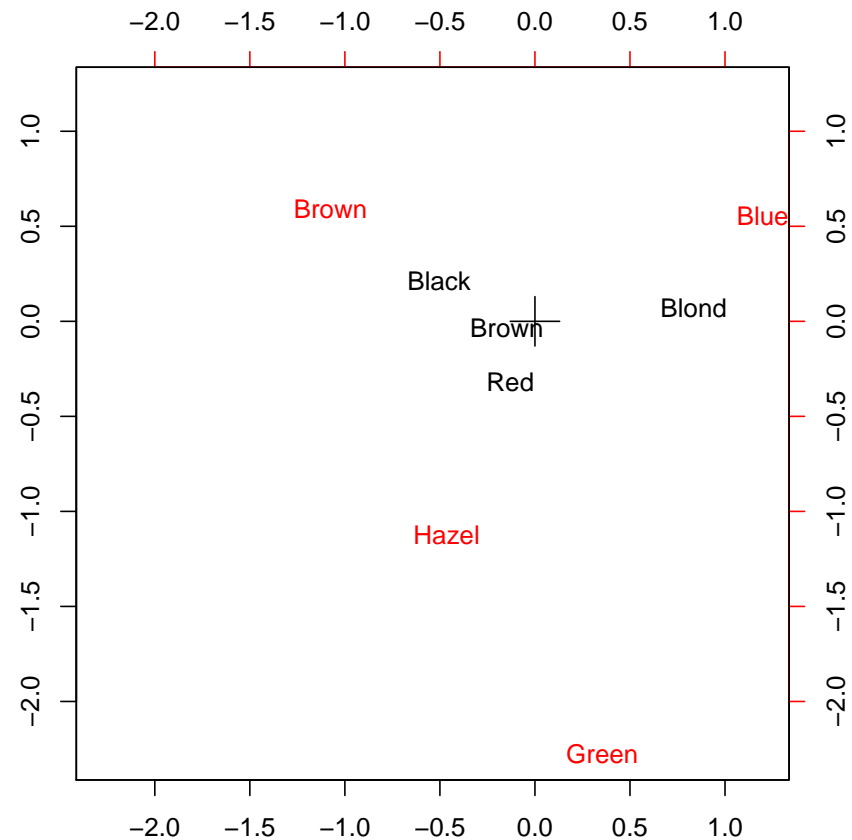
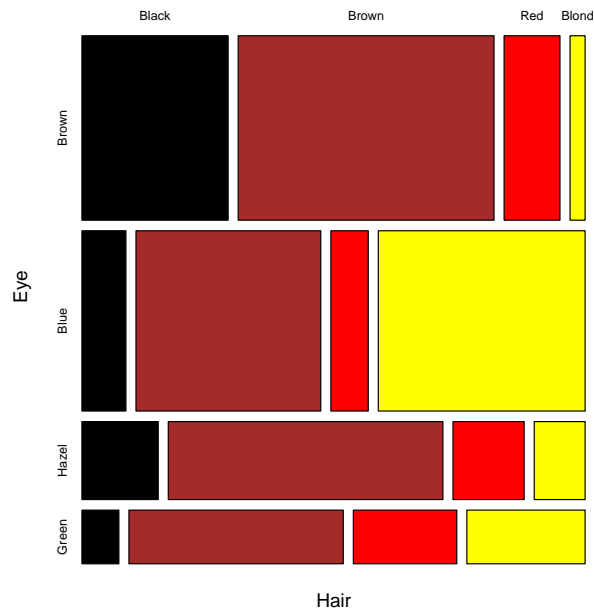
```


And now the mechanized way

```
> library(MASS)
> hc1 = corresp(haireye)
First canonical correlation(s): 0.4569165
Hair scores:
      Black      Brown      Red      Blond
-1.1042772 -0.3244635 -0.2834725  1.8282287
Eye scores:
      Brown      Blue      Hazel      Green
-1.0771283  1.1980612 -0.4652862  0.3540108

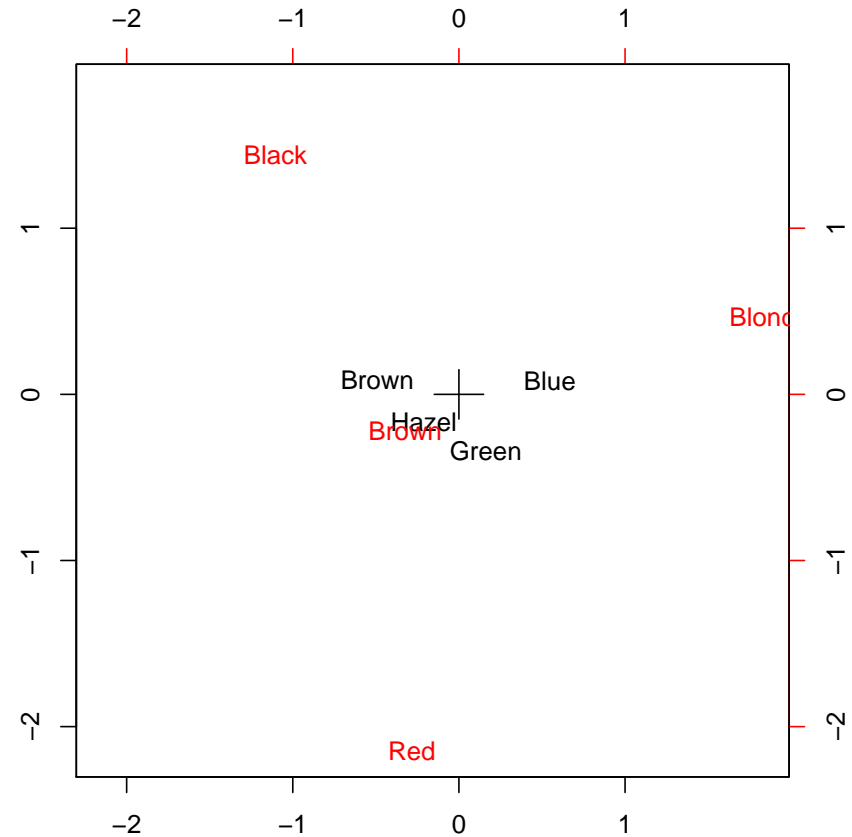
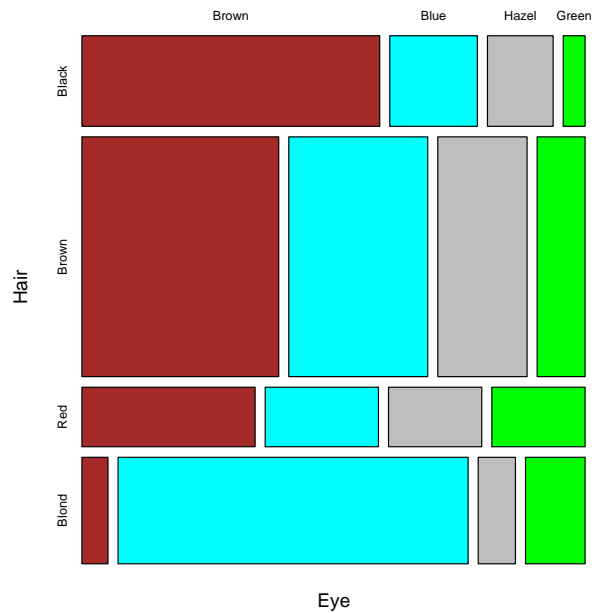
> hc2 = corresp(haireye,nf=2)
First canonical correlation(s): 0.4569165 0.1490859
Hair scores:
           [,1]      [,2]
Black -1.1042772  1.4409170
Brown -0.3244635 -0.2191109
Red    -0.2834725 -2.1440145
Blond  1.8282287  0.4667063
Eye scores:
           [,1]      [,2]
Brown -1.0771283  0.5924202
Blue   1.1980612  0.5564193
Hazel  -0.4652862 -1.1227826
Green  0.3540108 -2.2741218
```

Asymmetric view: rows



```
> plot(hc2,type="rows")
> biplot(hc2,type="rows")
> mosaicplot(haireye,sort=c(2,1),dir=c('v','h'))
```

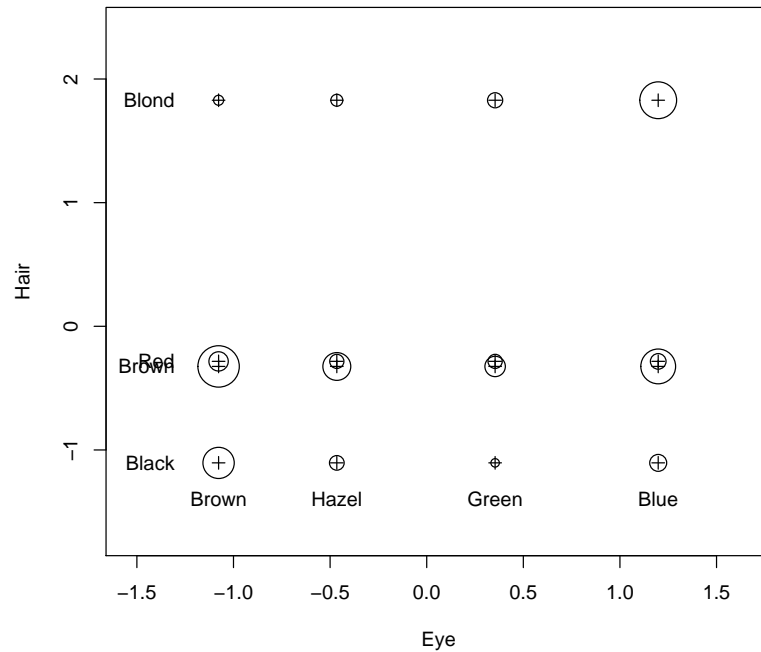
Asymmetric view: columns



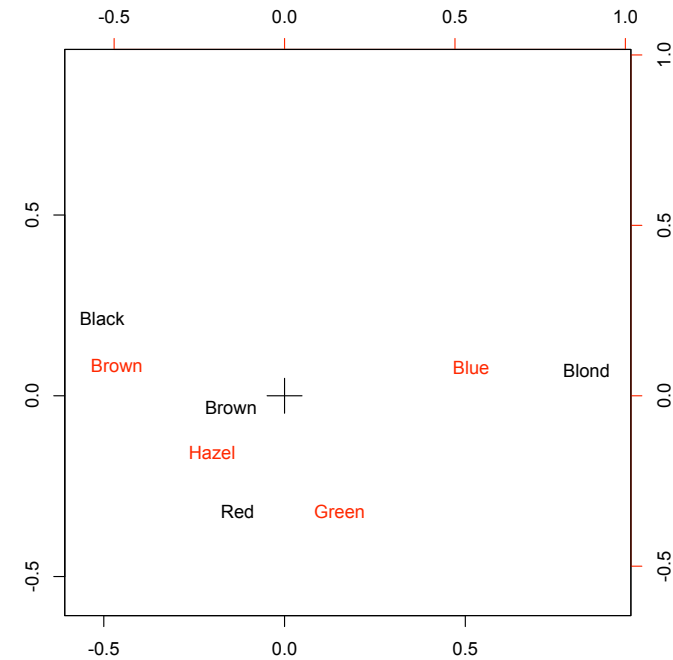
```
> plot(hc2,type="columns")
> biplot(hc2,type="columns")
> mosaicplot(haireye,sort=c(1,2),dir=c('h','v'))
```

And now, symmetric view

First column only



First two columns (more common)



```
> plot(hc2)
> biplot(hc2)
> biplot(hc2,xlim=c(-0.55,0.9),ylim=c(-0.55,0.9))
```

**Extending classics:
multivariate normal distribution and all around**

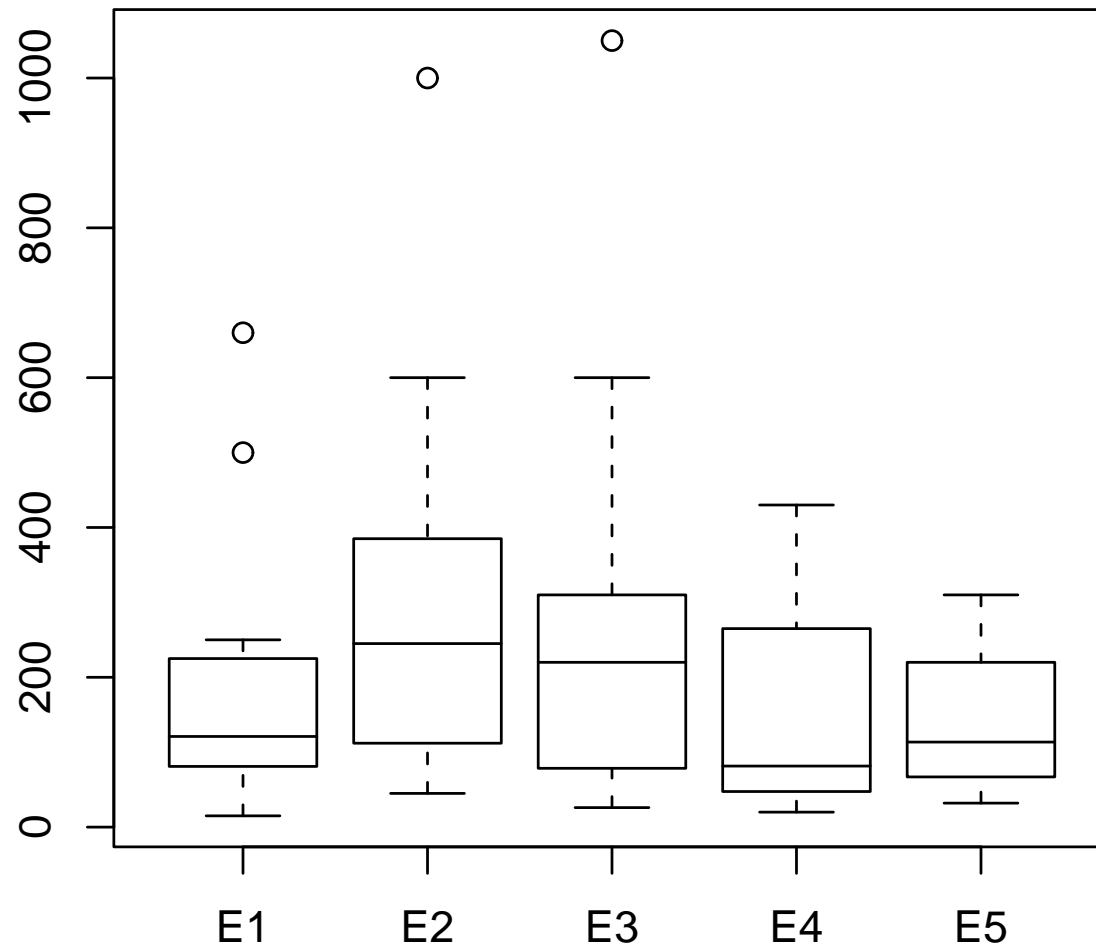
Recall: electrodes

Various electrodes have been tried successively on arms of 16 subjects.

```
> read.table("electro.d",header=T,row.names=1)
```

	E1	E2	E3	E4	E5
1	500	400	98	200	250
2	660	600	600	75	310
3	250	370	220	250	220
4	72	140	240	33	54
5	135	300	450	430	70
6	27	84	135	190	180
7	100	50	82	73	78
8	105	180	32	58	32
9	90	180	220	34	64
10	200	290	320	280	135
11	15	45	75	88	80
12	160	200	300	300	220
13	250	400	50	50	92
14	170	310	230	20	150
15	66	1000	1050	280	220
16	107	48	26	45	51

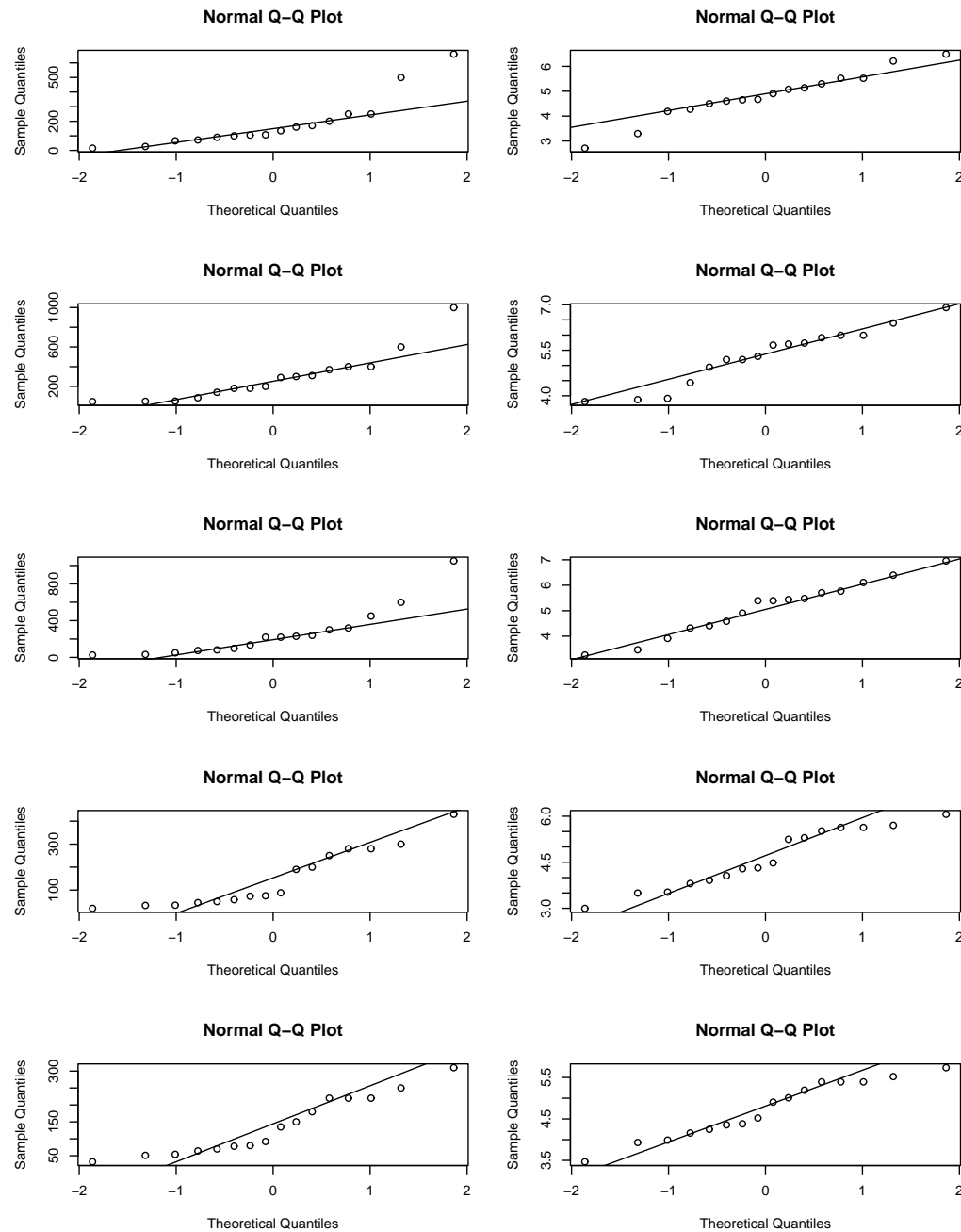
A picture (to figure out whether normal distribution of results is plausible here)



Seems like a bit of asymmetry there... take logs!

```
> elel=log(read.table("electro.d",header=T,row.names=1))
> par(mfcol=c(5,2))
> for (i in 1:5)
+ {
+ qqnorm(ele[,i])
+ qqline(ele[,i])
+ }
> for (i in 1:5)
+ {
+ qqnorm(elel[,i])
+ qqline(elel[,i])
+ }
```


Normal qqplots: left before, right after the logs



Normal distribution: definition

The most straightforward way to define the general, that is multivariate normal distribution (including univariate as a special case) is via its characteristic function

We say that a p -dimensional random vector \mathbf{X} has **normal distribution**, if and only if its characteristic function is

$$\varphi(\mathbf{t}) = e^{i\mathbf{t}^\top \boldsymbol{\mu} - \frac{1}{2}\mathbf{t}^\top \boldsymbol{\Sigma} \mathbf{t}}$$

for some p -dimensional vector $\boldsymbol{\mu}$ and some nonnegative definite $p \times p$ symmetric matrix $\boldsymbol{\Sigma}$; in such a case, we write that \mathbf{X} has the $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ distribution

This definition and notation is justified by the fact that the characteristic function unambiguously determines the probability distribution, and $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ uniquely determine the characteristic function given here

The definition, as given here, allows for singular (degenerate) alternatives; the version precluding those would require that $\boldsymbol{\Sigma}$ is *positive definite*

Normal distribution: univariate case

In the univariate case, normal distribution is uniquely determined by an arbitrary number μ and an arbitrary nonnegative number σ^2 . The characteristic function of normal distribution reduces to

$$\varphi(t) = e^{it\mu - \frac{1}{2}t^2\sigma^2}$$

For $\sigma^2 > 0$ it is the characteristic function of the distribution with the density

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

(This can be shown in a slightly involved, but yet accessible way)

The singular (degenerate) cases are those with $\sigma^2 = 0$; in such case there is no density, as $P[X = \mu] = 1$. These cases can be viewed as certain limits when $\sigma^2 \rightarrow 0$ for fixed μ

Also, it can be shown via direct calculation with characteristic function that if X has univariate normal distribution with parameters σ^2 and μ , then $aX + b$ has also univariate normal distribution with respective parameters $(a\sigma)^2$ and $a\mu + b$

Normal distribution: moments - univariate

The general characteristic function of normal distribution has continuous derivatives of all orders, which implies the existence of all moments. Thus a random vector \mathbf{X} with normal distribution has well-defined and finite $E(\mathbf{X})$ and $\text{Var}(\mathbf{X})$

In the univariate case, when a random variable X has univariate normal distribution, then the differentiation of its characteristic function at 0 (or direct calculation) yields

$$E(X) = \mu$$

$$\text{Var}(X) = \sigma^2$$

This includes also singular situations and is consistent with the distribution of the transformed variable $aX + b$, as

$$E(aX + b) = a\mu + b \quad \text{and} \quad \text{Var}(aX + b) = a^2\sigma^2$$

Normal distribution: general multivariate

Once certain properties of the univariate normal distribution (in particular, the correspondence between the characteristic function and the density, and also the closeness under affine transformations) are established, it is possible to bypass (to an extent) characteristic functions and give an equivalent characterization (and thus an equivalent definition) of the (multivariate) normal distribution via the distributions of linear combinations.

A random vector \mathbf{X} has (multivariate) normal distribution, if and only if any linear combination, $\ell^T \mathbf{X}$, of the components of \mathbf{X} has univariate normal distribution

This property immediately implies the transformation property for general normal distribution: if a random vector \mathbf{X} has normal distribution, then also a vector $\mathbf{A}\mathbf{X} + \mathbf{b}$ has normal distribution, for arbitrary \mathbf{A} and \mathbf{b} . Thus, if a vector has normal distribution, then its every subvector (created by taking certain components, not necessarily adjacent ones) has normal distribution; and in particular, every component has normal distribution

Normal distribution: moments - general

The transformation property then also implies the existence of the first and second moments. Let the vector ℓ_i has i -th component equal to 1 and all others to 0

If a random vector \mathbf{X} has normal distribution, then all its components $X_i = \ell_i^T \mathbf{X}$ have univariate normal distributions, with means μ_i ; thus, we can introduce $\boldsymbol{\mu}$ to denote the mean of the general normal distribution

$$E(\mathbf{X}) = (\mu_1, \mu_2, \dots, \mu_p)^T = \boldsymbol{\mu}$$

The existence of all componentwise variances yields, via the Cauchy-Schwarz inequality, the existence of $\text{Cov}(\ell_i^T \mathbf{X}, \ell_j^T \mathbf{X})$ for all i and j - these covariances form the corresponding elements of the variance-covariance matrix $\text{Var}(\mathbf{X})$; the latter is to be denoted by $\boldsymbol{\Sigma}$

Given all this, one can conclude that if \mathbf{X} has a general normal distribution with mean $\boldsymbol{\mu}$ and variance-covariance matrix $\boldsymbol{\Sigma}$, then $\ell^T \mathbf{X}$, for any ℓ , has univariate normal distribution with mean $\ell^T \boldsymbol{\mu}$ and variance $\ell^T \boldsymbol{\Sigma} \ell$

Normal distribution: proof of the characterization

Once again: after defining univariate normal distribution and establishing some of its properties, we can define the general normal distribution by the property that any linear combination, $\ell^T \mathbf{X}$, of the components of \mathbf{X} has univariate normal distribution.

The fact that the distribution of \mathbf{X} is completely characterized by the collection of one-dimensional distributions of $\ell^T \mathbf{X}$ is the Cramér-Wold theorem. Its proof is also via characteristic functions:

$$\text{if } Y = \ell^T \mathbf{X} \quad \text{then} \quad \varphi_Y(s) = E(e^{isY}) = E(e^{is\ell^T \mathbf{x}})$$

and for $s = 1$, $\varphi_Y(1) = E(e^{i\ell^T \mathbf{Y}})$, which, regarded as a function of ℓ , is a characteristic function of the random vector \mathbf{X} .

Normal distribution: characterization proof continued

Having defined general normal distribution via the linear combinations, we can derive several properties of it, as shown above. At some point, however, we need the characteristic function of the general normal distribution: we derive it from that of the univariate one. In that way, we prove the “only if” part of the characterization of the normal distribution given above; the “if” part follows by the manipulations with general characteristic function

Knowing that $Y = \ell^T \mathbf{X}$ has normal distribution with mean $\ell^T \boldsymbol{\mu}$ and variance $\ell^T \boldsymbol{\Sigma} \ell$, we obtain the characteristic function of Y as

$$\varphi_Y(t) = e^{it\ell^T \boldsymbol{\mu} - \frac{1}{2}t^2 \ell^T \boldsymbol{\Sigma} \ell}$$

This yields

$$\varphi_{\mathbf{X}}(\boldsymbol{\ell}) = \mathbb{E}(e^{i\boldsymbol{\ell}^T \mathbf{X}}) = \mathbb{E}(e^{iY}) = \varphi_Y(1) = e^{i\boldsymbol{\ell}^T \boldsymbol{\mu} - \frac{1}{2}\boldsymbol{\ell}^T \boldsymbol{\Sigma} \boldsymbol{\ell}}$$

- which is identical to the characteristic function introduced at the beginning

Normal distribution and independence

If \mathbf{X}_1 is $N(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$, \mathbf{X}_2 is $N(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$, and they are independent

then $\mathbf{X} = \begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \end{pmatrix}$ is $N\left(\begin{pmatrix} \boldsymbol{\mu}_1 \\ \boldsymbol{\mu}_2 \end{pmatrix}, \begin{pmatrix} \boldsymbol{\Sigma}_1 & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Sigma}_2 \end{pmatrix}\right)$

Conversely, if \mathbf{X} has normal distribution, and the structure of the variance-covariance matrix is as above - which mean that \mathbf{X}_1 and \mathbf{X}_2 are uncorrelated - then not only \mathbf{X}_1 and \mathbf{X}_2 both have normal distribution, but they are also *independent*

Both of these assertions can be now verified by manipulations with characteristic functions - and obviously, they are valid not only for two, but for any finite collection of random vectors \mathbf{X}

Yes, and there are some finessess here:

Suppose that \mathbf{X}_1 has normal distribution, and \mathbf{X}_2 has normal distribution. Does the vector $\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2)^\top$ have normal distribution (we may say then that \mathbf{X}_1 and \mathbf{X}_2 are *jointly* normal, to emphasize that)? Well, if \mathbf{X}_1 and \mathbf{X}_2 are independent, then the property above says that yes, but otherwise it may be one way or another...

Normal distribution has a density...

The independence property immediately yields that if \mathbf{U} is a random vector consisting of p independent components U_i , each with a standard normal distribution $N(0, 1)$, then \mathbf{U} has the $N(\mathbf{0}, \mathbf{I})$ normal distribution. Its density is the product of p standard normal densities

$$g(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^p}} e^{-\frac{1}{2}\mathbf{x}^T\mathbf{x}}$$

In the general case, variance-covariance matrix Σ is a symmetric matrix: thus there is a matrix $\Sigma^{1/2}$ such that $\Sigma^{1/2}\Sigma^{1/2} = \Sigma$

In the *nonsingular*, non-degenerate case, when the variance-covariance matrix Σ is positive definite and thus invertible, then $\Sigma^{1/2}$ is invertible too, and the density transformation theorem says that the distribution of $\mathbf{X} = \Sigma^{1/2}\mathbf{U} + \boldsymbol{\mu}$ - which the examination of moments shows to be $N(\boldsymbol{\mu}, \Sigma)$ - has the density

$$f(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^p \det(\Sigma)}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$

... if its variance-covariance matrix is nonsingular

So, in the nonsingular, non-degenerate case, when the variance-covariance matrix Σ is invertible and thus positive definite, normal distribution $N(\mu, \Sigma)$ has a density

If Σ is singular, then \mathbf{X} does not have a density with respect to the Lebesgue measure on \mathbb{R}^p , but it may have one when restricted to some affine subspace of \mathbb{R}^p , with respect to some appropriately-dimensional Lebesgue measure on that subspace

Summary

Let us summarize the most important properties now:

- Normal is characterized by first and second moments by $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$
- Affine transformation of normal is normal and then it comes again to first and second moments: if \mathbf{X} is $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, then $\mathbf{AX} + \mathbf{b}$ is $N(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T)$

and in particular, all subvectors are normal

- If subvectors of normal are uncorrelated, they are independent (“uncorrelated” means zeros in the appropriate part of $\boldsymbol{\Sigma}$)
- Normal has a density
$$f(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^p \det(\boldsymbol{\Sigma})}} e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$$
 but only if $\boldsymbol{\Sigma}$ is nonsingular, positive definite

And here again beware: random variable X has normal distribution, random variable Y has normal distribution, they are uncorrelated: are they independent?

Extending classics: one-sample Hotelling's T^2

Sampling: recall univariate setting first

We have n numbers, y_1, y_2, \dots, y_n - and we believe that they can be modeled as the outcomes of n random variables Y_1, Y_2, \dots, Y_n - which are iid with the distribution $N(\mu, \sigma^2)$ (iid = “independent identically distributed”)

In such case, we have (for all i) $\mu = E(Y_i)$

and $\sigma^2 = \text{Var}(Y_i) = E[(Y_i - E(Y_i))^2]$

Statistics then suggests to estimate

$$\mu \quad \text{by} \quad \bar{y} = \frac{1}{n} \sum_i y_i$$

$$\text{and } \sigma^2 \quad \text{by} \quad s^2 = \frac{1}{n-1} \sum_i (y_i - \bar{y})^2$$

The subsequent mathematics then yields $\text{Var}(\bar{Y}) = \frac{1}{n} \sigma^2$

which statistics suggests to be estimated by $\frac{1}{n} s^2$

Multivariate sampling: assumptions

Now, we have an array of numbers y_{ij} , forming the data matrix \mathbf{Y}
its lines are n (line) vectors, $i = 1, \dots, n$
of p observations, $j = 1, \dots, p$
We model them via n (column) random vectors $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n$
those that give rows of \mathbf{Y} as their outcomes
each with p components, and independent
that is, independent between themselves
(but not necessarily within, between their components)
with the same distribution $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

Multivariate sampling: estimation

If $\mathbf{y} = (Y_1, Y_2, \dots, Y_p)^\top$ is any of these random vectors, then

$$\boldsymbol{\mu} = \mathbf{E}(\mathbf{y}) = (\mathbf{E}(Y_1), \dots, \mathbf{E}(Y_p))^\top \quad \text{and} \quad \boldsymbol{\Sigma} = \text{Var}(\mathbf{X})$$

We estimate $\boldsymbol{\mu}$ by the vector of columnwise means

$$\bar{\mathbf{y}} = \left(\frac{1}{n} \sum_i y_{i1}, \dots, \frac{1}{n} \sum_i y_{ip} \right)^\top$$

and $\boldsymbol{\Sigma}$ by the sample variance-covariance matrix \mathbf{S} , with elements

$$S_{k\ell} = \frac{1}{n-1} \sum_i (y_{ik} - \bar{y}_k)(y_{i\ell} - \bar{y}_\ell)$$

Note: in what follows, we will abuse notation, using $\bar{\mathbf{y}}$ for the (column) vector of columnwise means, $\frac{1}{n} \mathbf{1}^\top \mathbf{Y}$ (a non-random vector), and also for the average of random vectors \mathbf{y}_i (a random vector)

Multivariate sampling: normal distribution

The sum of independent random vectors with normal distribution is normal; in particular, if $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n$ are iid with $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$\text{then } \bar{\mathbf{y}} = \frac{1}{n} \sum_i \mathbf{y}_i \quad \text{is} \quad N\left(\boldsymbol{\mu}, \frac{1}{n} \boldsymbol{\Sigma}\right)$$

which implies that $\boldsymbol{\Sigma}^{-1/2}(\bar{\mathbf{y}} - \boldsymbol{\mu})\sqrt{n}$ is $N(\mathbf{0}, \mathbf{I})$

- if $\boldsymbol{\Sigma}$ is nonsingular, of course; then we have a matrix $\boldsymbol{\Sigma}^{-1/2}$ inverse to $\boldsymbol{\Sigma}^{1/2}$ and such that $\boldsymbol{\Sigma}^{-1/2}\boldsymbol{\Sigma}^{-1/2} = \boldsymbol{\Sigma}^{-1}$

If $\boldsymbol{\Sigma}$ is nonsingular, then $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n$ have a density which is a product of individual densities; it is possible to derive then the maximum likelihood estimates based on their outcomes $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n$

$$\hat{\boldsymbol{\mu}} = \bar{\mathbf{x}} = \frac{1}{n} \sum_i \mathbf{y}_i$$

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n} \sum_i (\mathbf{y}_i - \bar{\mathbf{y}})(\mathbf{y}_i - \bar{\mathbf{y}})^\top = \frac{n-1}{n} \mathbf{S}$$

where \mathbf{S} is the usual sample variance-covariance matrix

Chi-square: review, mostly univariate

From now on, Σ is always positive definite - nonsingular

Chi-square distribution

If \mathbf{X} is $N(\mathbf{0}, \mathbf{I})$, then $\mathbf{X}^\top \mathbf{X}$ is χ_p^2 with $p = \dim \mathbf{X}$

And then, if $\mathbf{X}_1, \dots, \mathbf{X}_n$ are iid $N(\boldsymbol{\mu}, \Sigma)$

then $n(\bar{\mathbf{X}} - \boldsymbol{\mu})^\top \Sigma^{-1}(\bar{\mathbf{X}} - \boldsymbol{\mu})$ is χ_p^2

Asymptotics

If $\mathbf{X}_1, \dots, \mathbf{X}_n$ are iid and $n - p$ is large

then $\sqrt{n}(\bar{\mathbf{X}} - \boldsymbol{\mu})$ is approximately $N(\mathbf{0}, \Sigma)$

and thus $n(\bar{\mathbf{X}} - \boldsymbol{\mu})^\top \Sigma^{-1}(\bar{\mathbf{X}} - \boldsymbol{\mu})$ is approximately χ_p^2

and thus also $n(\bar{\mathbf{X}} - \boldsymbol{\mu})^\top \mathbf{S}^{-1}(\bar{\mathbf{X}} - \boldsymbol{\mu})$ is approximately χ_p^2

(we may replace Σ by \mathbf{S} if $n - p$ is large)

Univariate: t and F

t distribution

“Student’s t”

If U and V are independent, U is $N(0, 1)$, V is χ_k^2 , then

$$\frac{U}{\sqrt{\frac{V}{k}}} \text{ is } t_k$$

F distribution

“Fisher’s(-Snedecor’s) F”

If U and V are independent, U is χ_ℓ^2 , V is χ_k^2 , then

$$\frac{\frac{U}{\ell}}{\frac{V}{k}} \text{ is } F_{\ell, k}$$

Note: if Z is t_k , then Z^2 is $F_{1, k}$

And now: Wishart distribution, univariate prelude

If X_1, X_2, \dots, X_n are iid $N(\mu, \sigma^2)$

then \bar{X} and s^2 are independent

and $(n-1)\frac{s^2}{\sigma^2}$ is χ_{n-1}^2

We may think of it in a way that $(n-1)s^2$ is $\sigma^2\chi_{n-1}^2$

where U being $\sigma^2\chi_{n-1}^2$ means $\frac{U}{\sigma^2}$ is χ_{n-1}^2

and the distribution of $(n-1)s^2$ is

the distribution of $\sum_{i=1}^{n-1} Z_i^2$, when Z_i are iid $N(0, \sigma^2)$

This is a special case of the Wishart distribution for $\Sigma = (\sigma^2)$.

Wishart distribution: full force, definition

Suppose that random vectors $\mathbf{Z}_1, \mathbf{Z}_2, \dots, \mathbf{Z}_m$ are iid with $N(\mathbf{0}, \Sigma)$

The distribution of $\sum_{i=1}^m \mathbf{Z}_i \mathbf{Z}_i^T$ is called

Wishart distribution with parameters
 m (degrees of freedom, positive integer), and
 Σ (any nonnegative definite symmetric matrix)

Notation: $W_m(\Sigma)$ (it is often assumed that Σ is positive definite)

Also note: if \mathbf{Y} is an $m \times p$ matrix whose rows are \mathbf{Z}_i^T

$$\text{then } \sum_{i=1}^m \mathbf{Z}_i \mathbf{Z}_i^T = \mathbf{Y}^T \mathbf{Y}$$

If \mathbf{L} is a diagonal matrix with diagonal elements ℓ_i

$$\text{then } \mathbf{Y}^T \mathbf{L} \mathbf{Y} = \sum_{i=1}^m \ell_i \mathbf{Z}_i \mathbf{Z}_i^T$$

Wishart distribution: first properties

If \mathbf{B} has $W_m(\boldsymbol{\Sigma})$ distribution

and \mathbf{A} is a fixed (non-random), general $q \times p$ matrix,

then $\mathbf{A}^\top \mathbf{B} \mathbf{A}$ has $W_m(\mathbf{A}^\top \boldsymbol{\Sigma} \mathbf{A})$ distribution

If \mathbf{B}_1 has $W_{m_1}(\boldsymbol{\Sigma})$ and \mathbf{B}_2 has $W_{m_2}(\boldsymbol{\Sigma})$ distribution,

and \mathbf{B}_1 and \mathbf{B}_2 are independent,

then $\mathbf{B}_1 + \mathbf{B}_2$ has $W_{m_1+m_2}(\boldsymbol{\Sigma})$ distribution

If \mathbf{B} has $W_m(\boldsymbol{\Sigma})$ distribution

and \mathbf{a} is an arbitrary fixed (non-random) vector, $\mathbf{a}^\top \boldsymbol{\Sigma} \mathbf{a} \neq 0$,

then $\frac{\mathbf{a}^\top \mathbf{B} \mathbf{a}}{\mathbf{a}^\top \boldsymbol{\Sigma} \mathbf{a}}$ has χ_m^2 distribution

(which is then independent of \mathbf{a})

Wishart distribution: the most important property

Suppose that \mathbf{Y} is an $n \times p$ matrix whose rows are \mathbf{Y}_i^\top ,
where \mathbf{Y}_i are iid random vectors with distribution $N(\mathbf{0}, \Sigma)$;
if \mathbf{P} is a symmetric idempotent matrix,
then $\mathbf{Y}^\top \mathbf{P} \mathbf{Y}$ has $W_m(\Sigma)$ distribution,
where m is equal to the trace (rank) of \mathbf{P}

As a consequence, if \mathbf{S}_Y is the sample variance-covariance matrix
calculated out of \mathbf{Y}_i ,
then the distribution of $(n - 1)\mathbf{S}_Y$ is $W_{n-1}(\Sigma)$

Wishart distribution: more properties

For $m > p$ and arbitrary $p \times p$ symmetric, nonnegative definite Σ ,
 $W_m(\Sigma)$ is (absolutely) continuous (and thus has a density)

If \mathbf{B} has $W_m(\Sigma)$ distribution

and \mathbf{a} is an arbitrary fixed (non-random) vector,

then $\frac{\mathbf{a}^\top \Sigma^{-1} \mathbf{a}}{\mathbf{a}^\top \mathbf{B}^{-1} \mathbf{a}}$ has χ_{m-p+1}^2 distribution

(which is then independent of \mathbf{a})

An important corollary

If \mathbf{d} and \mathbf{B} are independent, \mathbf{d} is $N(\mathbf{0}, \Sigma)$, \mathbf{B} is $W_m(\Sigma)$, then

$$\frac{m-p+1}{p} \mathbf{d}^\top \mathbf{B}^{-1} \mathbf{d} = \frac{\frac{\mathbf{d}^\top \Sigma^{-1} \mathbf{d}}{p}}{\frac{\mathbf{d}^\top \Sigma^{-1} \mathbf{d}}{\mathbf{d}^\top \mathbf{B}^{-1} \mathbf{d}} \frac{\mathbf{d}^\top \mathbf{B}^{-1} \mathbf{d}}{m-p+1}} \quad \text{which is} \quad \frac{\frac{\chi_p^2}{p}}{\frac{\chi_{m-p+1}^2}{m-p+1}}$$

- well, the latter is not a rigorous math formula, only some shorthand, memory aid, for expressing that if U has χ_p^2 , V has χ_{m-p+1}^2 and U and V are independent (do not forget the latter!), and that the expression above is equal to

$$\frac{\frac{U}{p}}{\frac{V}{m-p+1}} \quad \text{which has the same distribution as} \quad \frac{m-p+1}{p} \mathbf{d}^\top \mathbf{B}^{-1} \mathbf{d}$$

- and thus the latter has distribution $F_{p, m-p+1}$

Univariate sampling once again...

We have n numbers, y_1, y_2, \dots, y_n

they can be modeled as the outcomes of n random variables Y_1, Y_2, \dots, Y_n are iid with the distribution $N(\mu, \sigma^2)$

In such case, we have (for all i) $\mu = E(Y_i)$

and $\sigma^2 = \text{Var}(Y_i) = E[(Y_i) - E(Y_i)]^2]$

Statistics then suggests to estimate

$$\mu \quad \text{by} \quad \bar{y} = \frac{1}{n} \sum_i y_i$$

$$\text{and } \sigma^2 \quad \text{by} \quad s^2 = \frac{1}{n-1} \sum_i (y_i - \bar{y})^2$$

The subsequent mathematics then yields $\text{Var}(\bar{Y}) = \frac{1}{n} \sigma^2$

which statistics suggests to be estimated by $\frac{1}{n} s^2$

and also the standard deviation of \bar{Y} is, $\frac{1}{\sqrt{n}} \sigma$, by $\frac{1}{\sqrt{n}} s$

... concluded by the t-ratio (univariate)

t-ratio: $\frac{\bar{Y} - \mu}{\frac{s}{\sqrt{n}}} = \sqrt{n} \frac{\bar{Y} - \mu}{s}$ ("Student's t-ratio")

has distribution t_{n-1} , that is, $\frac{N(0,1)}{\sqrt{\frac{\chi_{n-1}^2}{n-1}}}$ (symbolically)

which may be approximated by $N(0,1)$ for large n

And now: t-ratio squared: $n \frac{(\bar{Y} - \mu)^2}{s^2}$

has distribution $F_{1,n-1}$, that is $\frac{\frac{\chi_1^2}{1}}{\frac{\chi_{n-1}^2}{n-1}}$ (again symbolically)

and may be for large n approximated by χ_1^2

symbolically: $N(0,1)^2$

Recall multivariate sampling now

Now, we have an array of numbers y_{ij} , forming the data matrix \mathbf{Y}

- n vectors, $i = 1, \dots, n$, of p observations, $j = 1, \dots, p$

We model them via n random vectors $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_n$

those that give rows of \mathbf{Y} as their outcomes

each with p components, and independent

that is, between themselves

(but not necessarily within, between their components)

with the same distribution $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

If \mathbf{y} is any of these random vectors,

then we have $\boldsymbol{\mu} = E(\mathbf{y})$ and $\boldsymbol{\Sigma} = \text{Var}(\mathbf{y})$

And then

We estimate $\boldsymbol{\mu}$ by the vector of the columnwise means

as we know that $\bar{\mathbf{y}} = \frac{1}{n} \sum_{i=1}^n \mathbf{y}_i$ has distribution $N\left(\boldsymbol{\mu}, \frac{1}{n}\boldsymbol{\Sigma}\right)$

Then we estimate $\boldsymbol{\Sigma}$ by the sample variance-covariance matrix \mathbf{S} ,

as we know that $(n-1)\mathbf{S}$ has distribution $W_{n-1}(\boldsymbol{\Sigma})$

And after we observe that $(n-1)\mathbf{S}$ and $\bar{\mathbf{y}}$ are independent

We form not the t-ratio, but its square

t-ratio (squared): multivariate (Hotelling's T^2)

$$T^2 = n(\bar{\mathbf{y}} - \boldsymbol{\mu})^\top \mathbf{S}^{-1}(\bar{\mathbf{y}} - \boldsymbol{\mu}) \quad \text{which has}$$

(under all the assumptions above)

$$\text{the distribution } \frac{(n-1)p}{n-p} F_{p, n-1-p+1} = \frac{(n-1)p}{n-p} F_{p, n-p},$$

which actually means that

$$\frac{n-p}{(n-1)p} T^2 = \frac{n-p}{(n-1)p} n(\bar{\mathbf{y}} - \boldsymbol{\mu})^\top \mathbf{S}^{-1}(\bar{\mathbf{y}} - \boldsymbol{\mu})$$

has distribution $F_{p, n-p}$

(which for large n may be approximated by χ_p^2)

Note: for $p = 1$ the first fraction is 1 and the distributions are $F_{1, n-1}$ and χ_p^2 - same as for the univariate squared t-ratio.

Once again: we keep abusing the notation, using $\bar{\mathbf{y}}$ for the (column) vector of columnwise means, $\frac{1}{n} \mathbf{1}^\top \mathbf{Y}$ (a non-random vector), and at the same time for the average of random vectors \mathbf{y}_i (a random vector)

First applications

First applications are sort of analogs of univariate ones: we can **test a hypothesis**

$$H_0: \boldsymbol{\mu} = \boldsymbol{\mu}_0$$

using $T^2 = n(\bar{\mathbf{y}} - \boldsymbol{\mu}_0)^\top \mathbf{S}^{-1}(\bar{\mathbf{y}} - \boldsymbol{\mu}_0)$ (substitute $\boldsymbol{\mu} = \boldsymbol{\mu}_0$)

rejecting H_0 if $T^2 > \frac{(n-1)p}{n-p} F_{p, n-p}(\alpha)$

In the similar vein, we can form

confidence sets

$\boldsymbol{\mu}$ in T^2 becomes a variable

yielding a confidence set which is an ellipsoid such that

$$P\left[(\bar{\mathbf{y}} - \boldsymbol{\mu})^\top \mathbf{S}^{-1}(\bar{\mathbf{y}} - \boldsymbol{\mu}) \leq \frac{(n-1)p}{n(n-p)} F_{p, n-p}(\alpha)\right] = 1 - \alpha.$$

Paired comparisons

This is still an application in the univariate style: a paired t-test is generalized to the situation when there are not pairs of one, but several variables (the pairing is one-to-one)

The observations come as are n pairs of vectors \mathbf{y}_{1i} and \mathbf{y}_{2i}

similarly to the univariate, classical paired t-test

\mathbf{y}_{1i} and \mathbf{y}_{2i} are *jointly normal*

not necessary independent within or between themselves

but *pairs of vectors* are independent for different $i = 1, 2, \dots, n$

and have the same distribution (independent of $i = 1, 2, \dots, n$)

In such case, the (vector) differences $\mathbf{z}_i = \mathbf{y}_{1i} - \mathbf{y}_{2i}$ can be modeled by iid random vectors with normal distribution $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

The hypothesis $H_0 : \boldsymbol{\mu} = \mathbf{0}$ is then rejected if

$$T^2 = n\bar{\mathbf{z}}^T \mathbf{S}^{-1} \bar{\mathbf{z}} > \frac{(n-1)p}{n-p} F_{p, n-p}(\alpha)$$

A technology of its own: repeated measures

Truly multivariate application: repeated measures

In a sense, it is a generalization of paired t-test again, but in different direction: now we do not compare two paired groups of vectors, but do it in a more involved way

We do it using a data matrix \mathbf{Y} using **contrasts**, believing, as before, that the rows of \mathbf{Y} are realizations of iid random vectors \mathbf{y}_i

A **contrast matrix** is defined to be any $k \times p$ matrix \mathbf{C} that has sums of rows equal to zero; the comparisons we are after are expressed through $\mathbf{C}\mathbf{y}_i$

Let us have a look at some examples with $p = 4$

Examples of contrasts that carry special meaning

Compare all to control:

```
> t(contr.sum(4))
```

	1	2	3	4
[1,]	1	0	0	-1
[2,]	0	1	0	-1
[3,]	0	0	1	-1

Compare first to second, second to third, third to fourth,...:

```
> t(array(dim=c(4,3),c(1,-1,0,0,0,1,-1,0,0,0,1,-1)))
```

	[,1]	[,2]	[,3]	[,4]
[1,]	1	-1	0	0
[2,]	0	1	-1	0
[3,]	0	0	1	-1

Of course, we do not have to have $k = 3$ lines in each contrast; we can consider contrasts also with $k = 1$ or $k = 2$ - but $k = p - 1$ is the maximum possible number of *linearly independent* lines in a contrast

More elaborate contrasts

Let a and A be two levels of the first factor, b and B two levels of the second factor, and the observations at every item correspond to ab , aB , Ab , AB . Then the first contrast evaluates the effect of the first factor, the second of the second factor, and the third one the interaction:

```
> t(array(dim=c(4,3),c(1,1,-1,-1,1,-1,1,-1,1,-1,-1,1)))
      [,1] [,2] [,3] [,4]
[1,]     1     1    -1    -1
[2,]     1    -1     1    -1
[3,]     1    -1    -1     1
```

Such an elaborate contrast is possible for $p = 4$ (or similar)

Incidentally, cannot a contrast - for $p = 4$ - have different number of lines than three?

And how about $p = 5$? For our data, we have $p = 5$, so we have to use rather some of the previous contrasts

Distribution of repeated measures

Rows of the data matrix - (row) vectors $(Y_{i1}, Y_{i2}, \dots, Y_{ip})$
are modeled as (column) random vectors \mathbf{y}_i

Vectors \mathbf{y}_i are considered iid, with normal distribution $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$\mathbf{z}_i = \mathbf{C}\mathbf{y}_i$ can be then modeled as iid random vectors
with normal distribution $N(\mathbf{C}\boldsymbol{\mu}, \mathbf{C}\boldsymbol{\Sigma}\mathbf{C}^T)$

and we can use again the distributional mathematics (abusing the notation and using $\bar{\mathbf{y}}$ also for columnwise means of \mathbf{Y} made into a column vector) for

$$T^2 = n\bar{\mathbf{z}}^T \mathbf{S}_{\mathbf{Y}\mathbf{C}^T}^{-1} \bar{\mathbf{z}} = n(\mathbf{C}\bar{\mathbf{y}})^T (\mathbf{C}\mathbf{S}_{\mathbf{Y}}\mathbf{C}^T)^{-1} (\mathbf{C}\bar{\mathbf{y}})$$

which in the model has the distribution $\frac{(n-1)k}{n-k} F_{k, n-k}$

Typically, we can test the hypothesis that all contrasts are zero
but also other hypothesis, for confidence sets, etc.

And it is all pretty much nothing else but applying the T^2 : not to the original variables, but rather to the specific linear combinations of those

So, do we see now what can be the dimension k of \mathbf{C} ?

It is all in the formula for T^2

The formula for T^2 calls for the invertibility of \mathbf{CSC}^T ; as this matrix has dimension $k \times k$, its rank must be k then

Now, the rank of a product of matrices is at most the maximum or ranks of the matrices involved; consequently, the rank of \mathbf{CSC}^T is not greater than the rank of \mathbf{S} - so if we assume it is p , then k cannot be greater than p . And the condition that rows sum to zero - in matrix terms expressible as $\mathbf{1}^T \mathbf{C} = \mathbf{0}$ further drives rank one more down: that is, k cannot be greater than $p - 1$, otherwise \mathbf{CSC}^T cannot have rank k

Of course, if $k = p - 1$, it is not guaranteed mathematically that the rank is k ; but from the statistical point of view, we can always believe that elements of \mathbf{S} are sufficiently “in a general position”

(Try generating a random matrix with components that come from independent realizations of a distribution with a density; the result is then invertible with probability one - and indeed in R, you likely never encounter a noninvertible matrix this way

```
> solve(matrix(rnorm(100),10,10)) # repeat or alter if you wish  
...
```

Recall first again: the data

```
> read.table("electro.d",header=T,row.names=1)
```

	E1	E2	E3	E4	E5
1	500	400	98	200	250
2	660	600	600	75	310
3	250	370	220	250	220
4	72	140	240	33	54
5	135	300	450	430	70
6	27	84	135	190	180
7	100	50	82	73	78
8	105	180	32	58	32
9	90	180	220	34	64
10	200	290	320	280	135
11	15	45	75	88	80
12	160	200	300	300	220
13	250	400	50	50	92
14	170	310	230	20	150
15	66	1000	1050	280	220
16	107	48	26	45	51

We want to compare E1, E2, E3, E4, E5 - somehow in total. Lines are related to a certain subject, hence independence within a line may not be realistic; but independence between lines perhaps yes

First taking logs (more conforming to normal)

```
> elel=log(read.table("electro.d",header=T,row.names=1))  
> elel
```

	E1	E2	E3	E4	E5
1	6.214608	5.991465	4.584967	5.298317	5.521461
2	6.492240	6.396930	6.396930	4.317488	5.736572
3	5.521461	5.913503	5.393628	5.521461	5.393628
4	4.276666	4.941642	5.480639	3.496508	3.988984
5	4.905275	5.703782	6.109248	6.063785	4.248495
6	3.295837	4.430817	4.905275	5.247024	5.192957
7	4.605170	3.912023	4.406719	4.290459	4.356709
8	4.653960	5.192957	3.465736	4.060443	3.465736
9	4.499810	5.192957	5.393628	3.526361	4.158883
10	5.298317	5.669881	5.768321	5.634790	4.905275
11	2.708050	3.806662	4.317488	4.477337	4.382027
12	5.075174	5.298317	5.703782	5.703782	5.393628
13	5.521461	5.991465	3.912023	3.912023	4.521789
14	5.135798	5.736572	5.438079	2.995732	5.010635
15	4.189655	6.907755	6.956545	5.634790	5.393628
16	4.672829	3.871201	3.258097	3.806662	3.931826

Contrasts and their transposes

Now, contrasts were defined to be $k \times p$ matrices, with each row summing to 0 - that was convenient in the stochastic assumptions, where observations were modeled as column $p \times 1$ vectors.

With an $n \times p$ data matrix \mathbf{Y} , these observations correspond to its *rows*. Hence we have to multiply \mathbf{Y} from right right by a $p \times k$ *transposed* contrast - a matrix that has *columns*, not rows, now summing to zero.

In what follows, we show these contrasts as they appear in R - that is, in their transposed form

Once again some of the examples, now in this setting

Compare all to control

```
> contr.sum(4)
  [,1] [,2] [,3]
1     1     0     0
2     0     1     0
3     0     0     1
4    -1    -1    -1
```

Compare first to second, second to third, third to fourth,...

```
> array(dim=c(4,3),c(1,-1,0,0,0,1,-1,0,0,0,1,-1))
  [,1] [,2] [,3]
[1,]     1     0     0
[2,]    -1     1     0
[3,]     0    -1     1
[4,]     0     0    -1
```

More elaborate contrasts again

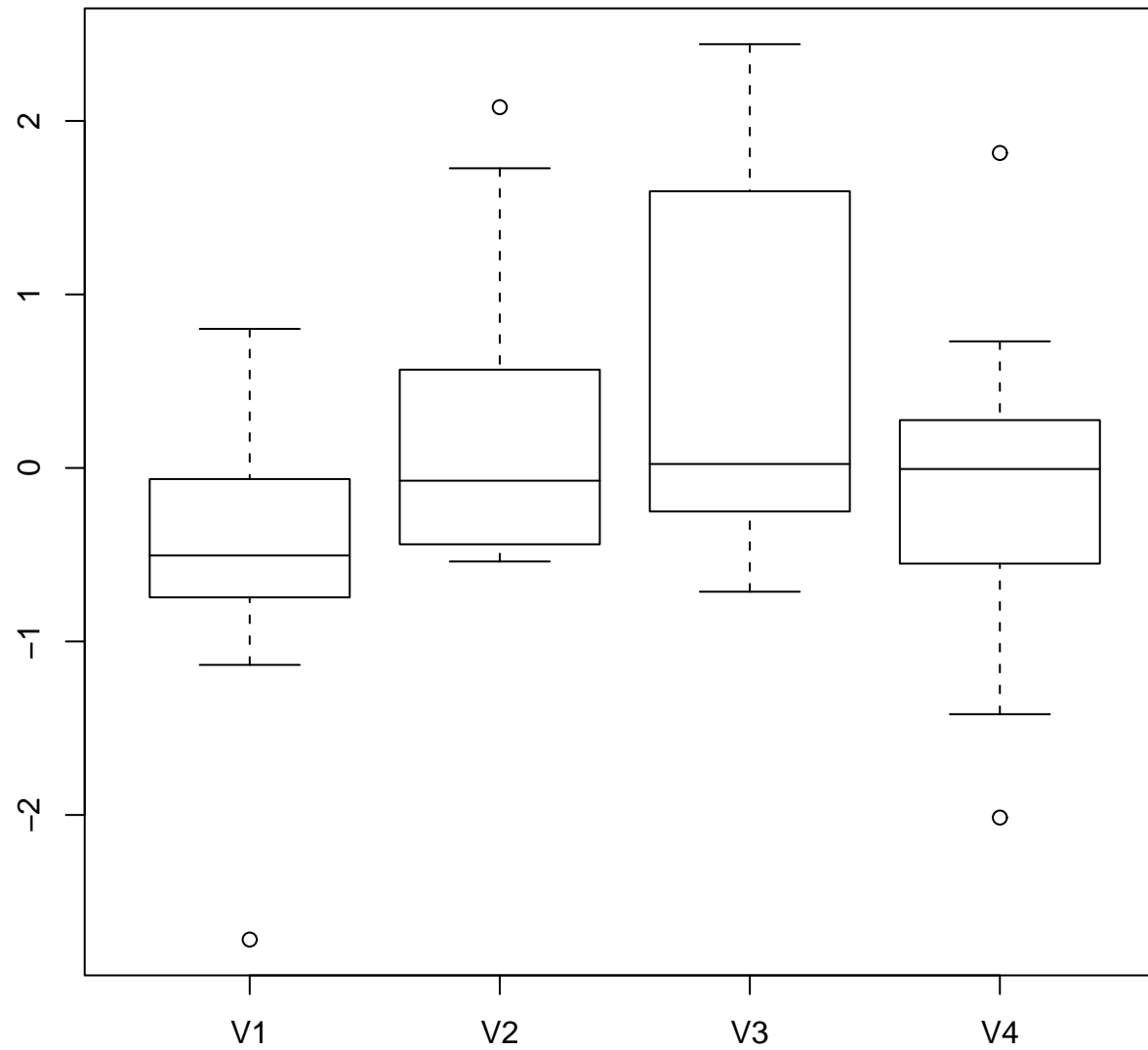
Let a and A be two levels of the first factor, b and B two levels of the second factor, and the observations at every item correspond to ab , aB , Ab , AB . Then the first contrast (first column) evaluates the effect of the first factor, the second (column) of the second factor, and the third one the interaction (between those):

```
> array(dim=c(4,3),c(1,1,-1,-1,1,-1,1,-1,1,-1,-1,1))
      [,1] [,2] [,3]
[1,]    1    1    1
[2,]    1   -1   -1
[3,]   -1    1   -1
[4,]   -1   -1    1
```

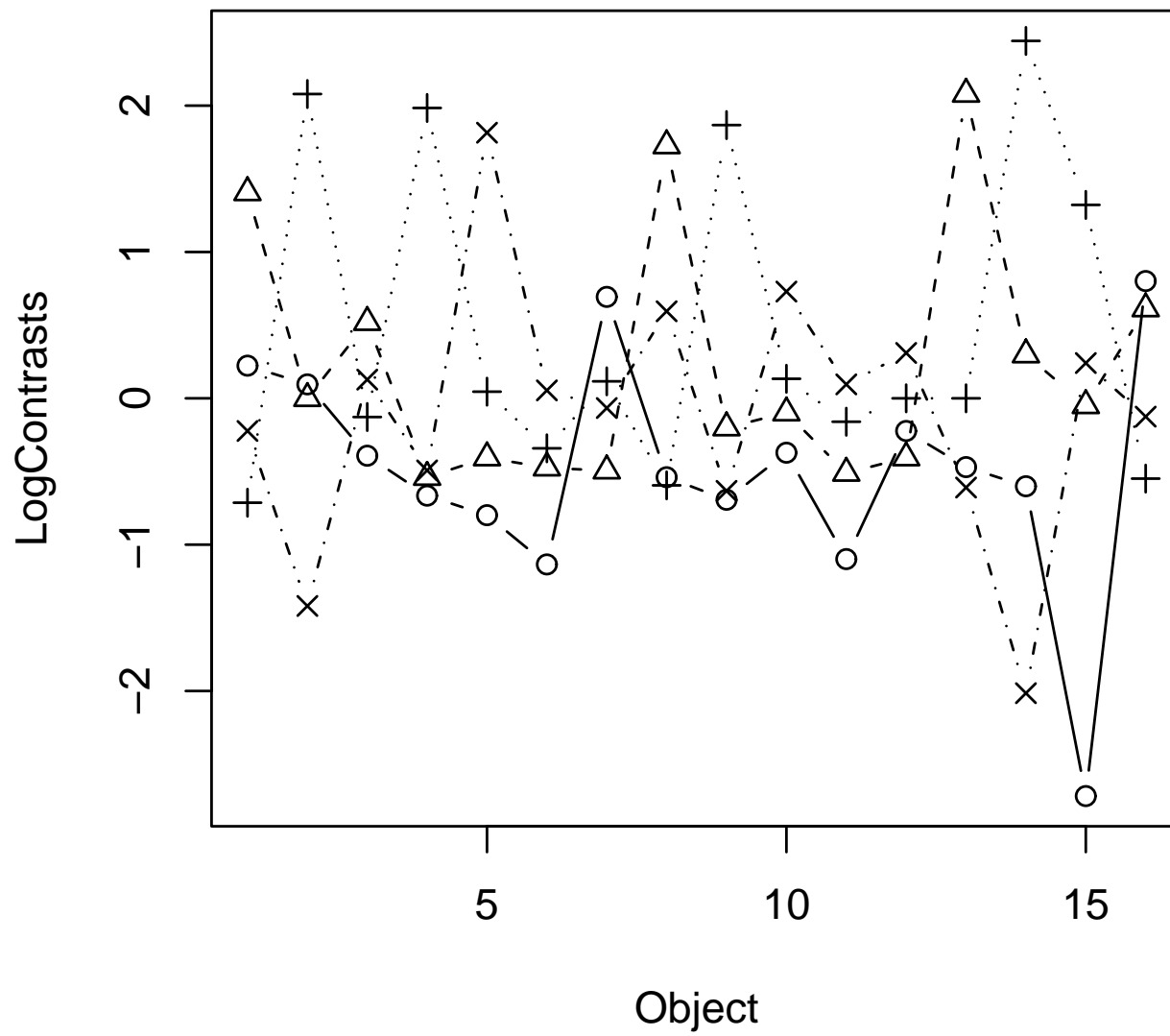
And now: contrasts for (logarithms of) electrodes

```
> elec = array(dim=c(5,4),c(1,-1,0,0,0,0,1,-1,0,0,0,0,1,-1,0,0,0,0,1,-1))
> elec
      [,1] [,2] [,3] [,4]
[1,]     1     0     0     0
[2,]    -1     1     0     0
[3,]     0    -1     1     0
[4,]     0     0    -1     1
[5,]     0     0     0    -1
> elelc=as.matrix(elec) %*% elec # see note below
> plot(as.ts(elelc),plot.t="single",type="b",pch=1:4,lty=1:4)
> boxplot(as.data.frame(elelc))
```

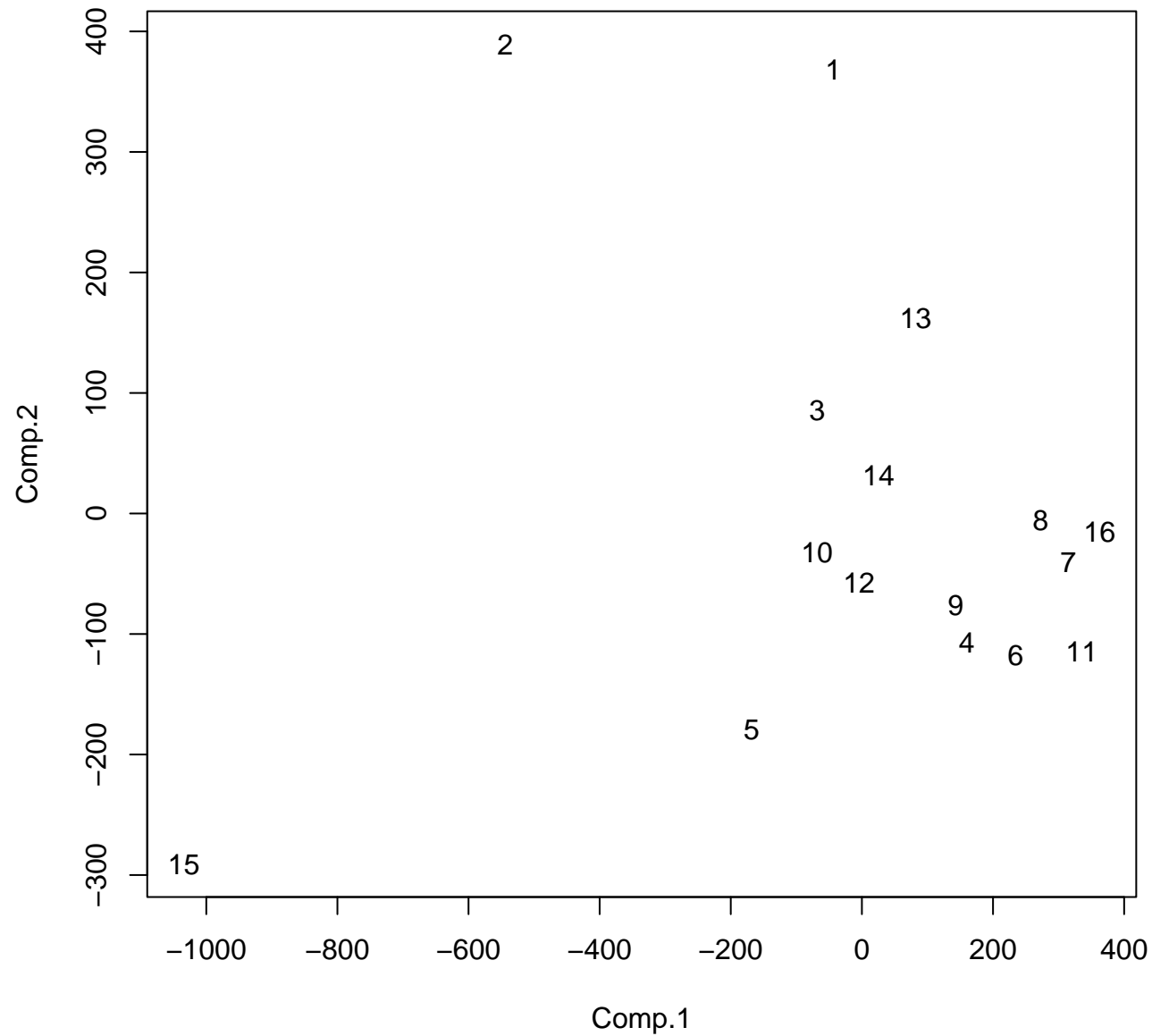
Electrodes: boxplots of contrasts



Contrasts: objectwise



Contrasts: principal components



We can finally look at Hotelling's T^2

```
> dim(elelc)
[1] 16  4
> elmu = apply(elelc,2,mean); elmu
[1] -0.4932261  0.2166766  0.4690089 -0.1009543
> elis = solve(var(elelc)) # oh: I am not supposed to do this!
> 1-pf(elmu %*% elis %*% elmu*16*12/(4*15),4,12)
0.1044359
```

First p-value here. Now, there is a suspicion that 15th subject is somewhat out of the ordinary (an “outlier”, so to say) - how about trying the analysis without it?

```
> elmu=apply(elelc[-15,],2,mean)
> elis=solve(var(elelc[-15,]))
> 1-pf( elmu %*% elis %*% elmu * 15*11/(4*14),4,11)
0.1278355
```

How about looking only on (all) the 1st and 3rd contrasts?

```
> elmu = apply(elelc[,c(1,3)],2,mean)
> elis = solve(var(elelc[,c(1,3)]))
> 1-pf(elmu %*% elis %*% elmu*16*14/(2*15),2,14)
0.06439189
```


T² continued

And now, only one of those (1st and 3rd) contrasts at a time

```
> elmu = mean(elelc[,3])
> elis = solve(var(elelc[,3]))
> 1-pf(elmu %*% elis %*% elmu*16*15/(1*15),1,15)
0.1010562
> elmu = mean(elelc[,1])
> elis = solve(var(elelc[,1]))
> 1-pf(elmu %*% elis %*% elmu*16*15/(1*15),1,15)
0.02852685
```

Yeah, so the 1st one would yield some significance - only, we could arrive to this by a simple paired t-test...

```
> 4*mean(elelc[,1])/sqrt(var(elelc[,1]))
-2.422740
> qt(.025,15)
-2.131450
> 2*(1-pt(abs(4*mean(elelc[,1]))/sqrt(var(elelc[,1])),15))
0.02852685
```

Isn't there a function for t-test in R?

Surely is!

```
> t.test(ele1[,1],ele1[,2],paired=TRUE)
```

Paired t-test

data: ele1[, 1] and ele1[, 2]

t = -2.4227, df = 15, p-value = 0.02853

alternative hypothesis: true difference in means is not equal to 0

95 percent confidence interval:

-0.92715075 -0.05930155

sample estimates:

mean of the differences

-0.4932261

Isn't there any package for Hotelling?

```
> summary(manova(elelc~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)
(Intercept)  1           0.81125   2.43374      4    12 0.1044
Residuals    15

> summary(manova(elelc~1),intercept=T,test="W")
              Df   Wilks approx F num Df den Df Pr(>F)
(Intercept)  1 0.55211   2.43374      4    12 0.1044
Residuals    15

> summary(manova(elelc[-15,]~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)
(Intercept)  1           0.82388   2.26568      4    11 0.1278
Residuals    14

> summary(manova(elelc[-15,]~1),intercept=T,test="W")
              Df   Wilks approx F num Df den Df Pr(>F)
(Intercept)  1 0.54828   2.26568      4    11 0.1278
Residuals    14

> summary(manova(elelc[,c(1,3)]~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)
(Intercept)  1           0.4797   3.3577      2    14 0.06439
Residuals    15
```

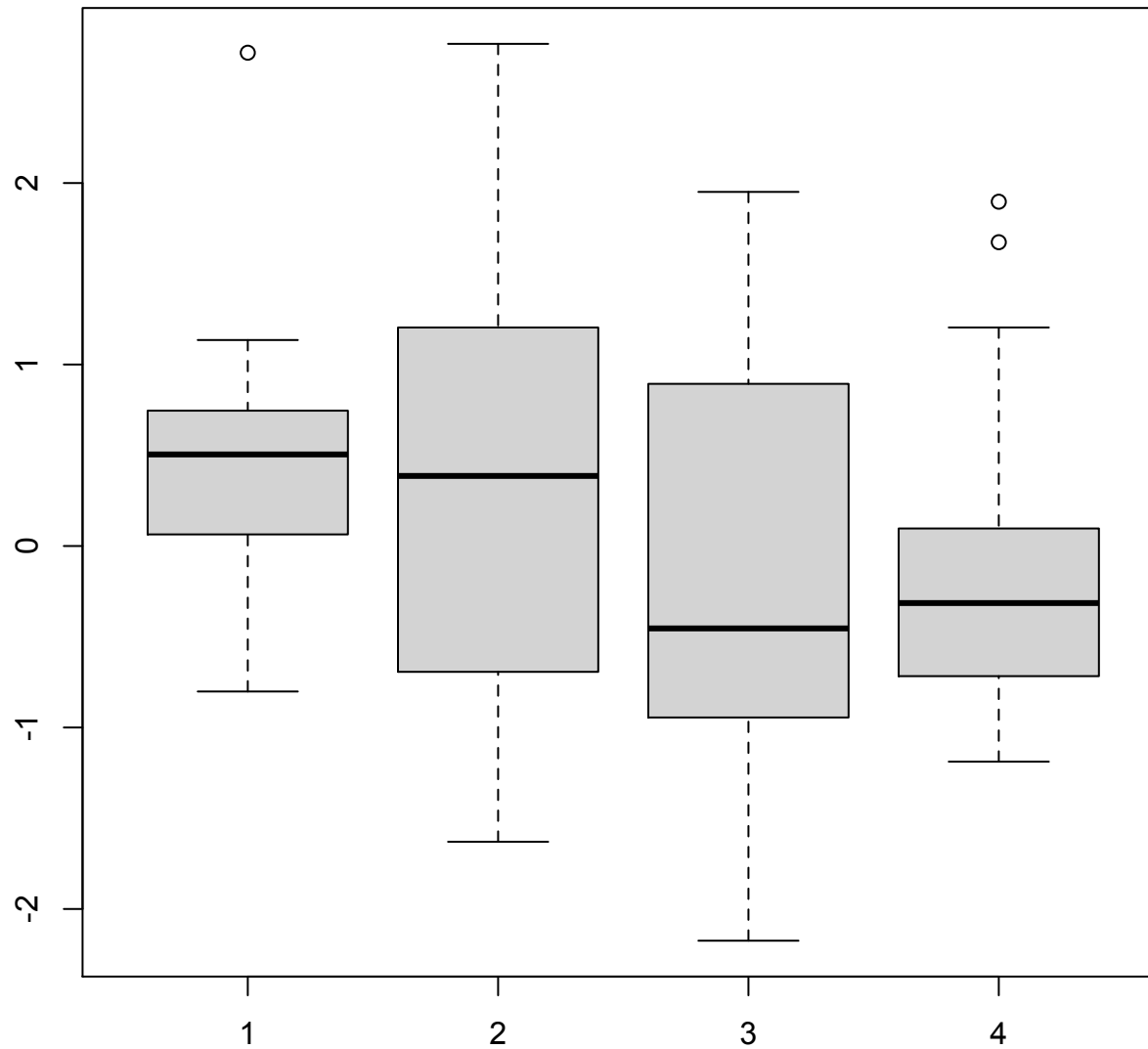
Hotelling package continued

```
> summary(manova(elelc[,1]~1),intercept=T,test="H")
Error in manova(elelc[, 1] ~ 1) : need multiple response
> summary(aov(elelc[,1]~1),intercept=T)
              Df Sum Sq Mean Sq F value  Pr(>F)
(Intercept)  1  3.8924   3.8924   5.8697 0.02853 *
Residuals    15  9.9469   0.6631
```

Second thoughts: how about trying some other contrast matrix?

```
> contr.sum(5)[c(5,1:4),]  
  [,1] [,2] [,3] [,4]  
5   -1   -1   -1   -1  
1    1    0    0    0  
2    0    1    0    0  
3    0    0    1    0  
4    0    0    0    1  
> elc=as.matrix(ele1) %*% contr.sum(5)[c(5,1:4),]  
> boxplot(elc)
```

Boxplots of contrasts: not that bad



Oops... was this expected?

```
> summary(manova(elc~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)
(Intercept)   1           0.81125    2.4337     4    12 0.1044
Residuals    15
```

Well, was to be expected... or not? Also

```
> summary(manova(elc[-15,]~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)
(Intercept)   1           0.82388    2.2657     4    11 0.1278
Residuals    14
```

For subsets, however...

```
> summary(manova(elc[,c(1,2,3)]~1),intercept=T,test="W")
              Df   Wilks approx F num Df den Df  Pr(>F)
(Intercept)   1 0.57287    3.2309      3    13 0.05757 .
Residuals    15

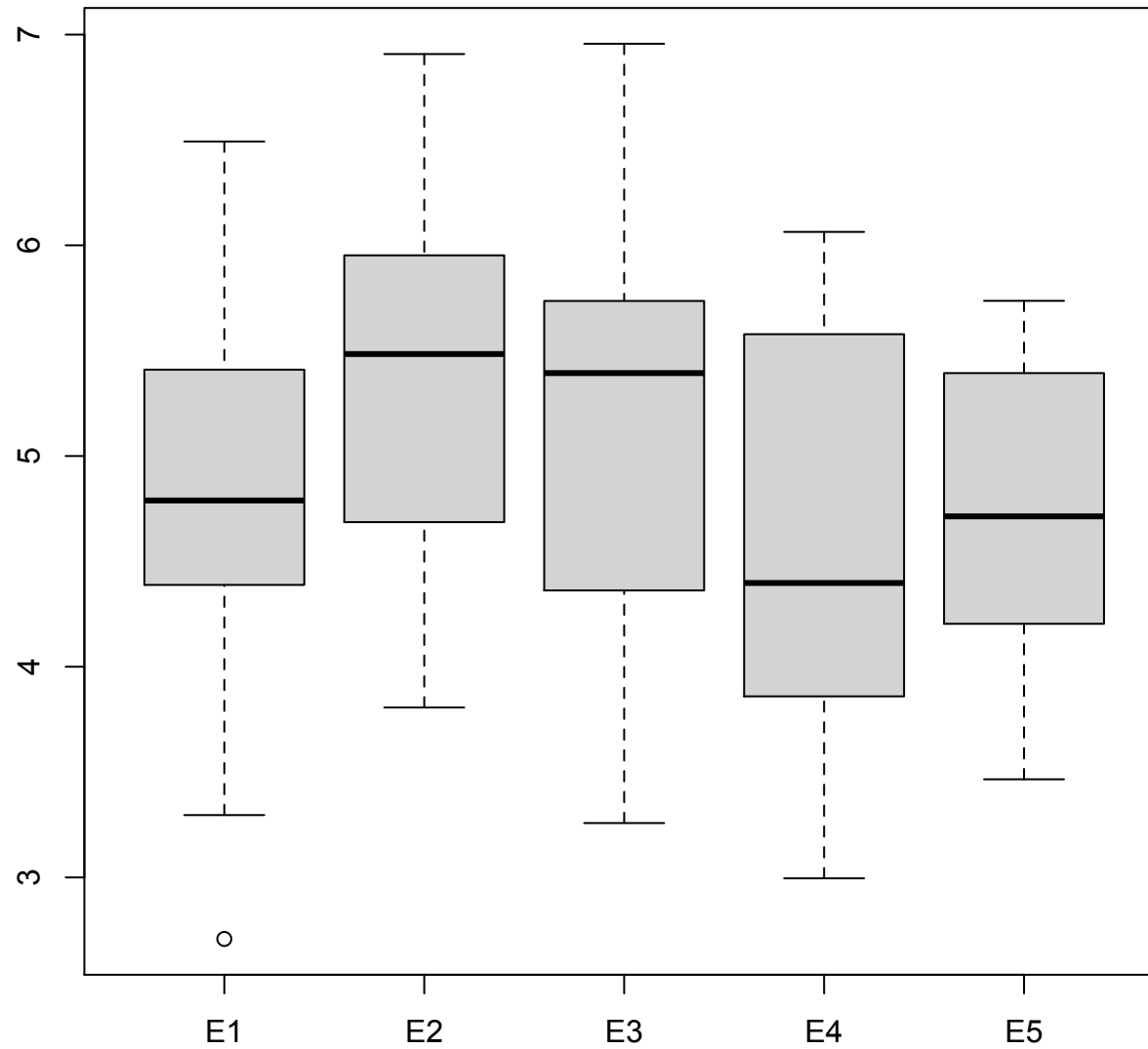
> summary(manova(elc[,c(1,2)]~1),intercept=T,test="W")
              Df   Wilks approx F num Df den Df  Pr(>F)
(Intercept)   1 0.6451    3.851      2    14 0.0465 *
Residuals    15

> summary(manova(elc[,c(1,3)]~1),intercept=T,test="W")
              Df   Wilks approx F num Df den Df  Pr(>F)
(Intercept)   1 0.5806    5.0564      2    14 0.02224 *
Residuals    15
```

Note the “progress”: originally we have been only able to isolate one contrast significant at $\alpha = 0.05$. Now we are able to pick up two...

Shall we continue? (I did...)

Incidentally, the boxplots of original logarithms



Perhaps one can still move on...

Some impasses are inevitable:

```
> cn = rbind(c(-1,-1,0,0),c(1,0,-1,0),c(0,0,0,-1),  
+ c(0,0,0,1),c(0,1,1,0))
```

```
> cn
```

```
      [,1] [,2] [,3] [,4]  
[1,]   -1   -1    0    0  
[2,]    1    0   -1    0  
[3,]    0    0    0   -1  
[4,]    0    0    0    1  
[5,]    0    1    1    0
```

```
> ecn=as.matrix(elel) %*% cn
```

```
> summary(manova(ecn[,c(1,2,3)]~1),intercept=T,test="H")
```

```
Error in summary.manova(manova(ecc[, c(1, 2, 3)] ~ 1), intercept = T  
  residuals have rank 2 < 3
```

```
> summary(manova(ecn[,c(1,3)]~1),intercept=T,test="H")
```

	Df	Hotelling-Lawley	approx F	num Df	den Df	Pr(>F)
(Intercept)	1	0.74424	5.2097	2	14	0.02036 *
Residuals	15					

I see...

A better shot?

```
> con = rbind(c(-1,0,0,0),c(1,-1,0,0),c(0,0,1,0),
+ c(0,0,0,1),c(0,1,-1,-1))
> con
      [,1] [,2] [,3] [,4]
[1,]   -1    0    0    0
[2,]    1   -1    0    0
[3,]    0    0    1    0
[4,]    0    0    0    1
[5,]    0    1   -1   -1
> econ=as.matrix(ele1) %*% con
```

We have already seen this

```
> summary(manova(econ~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)
(Intercept)   1             0.81125    2.4337     4    12 0.1044
Residuals    15

> summary(manova(ecc[,c(1,2,3)]~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)
(Intercept)   1             0.74923    3.2467     3    13 0.05686 .
Residuals    15

> summary(manova(econ[,c(1,2)]~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)
(Intercept)   1             0.74424    5.2097     2    14 0.02036 *
```

This not - but who cares...

```
> summary(manova(econ[,c(1,3)]~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)
(Intercept)   1             0.41386    2.897     2    14 0.08854 .
Residuals    15
```

But this!!

```
> summary(manova(ecc[,c(1,2,4)]~1),intercept=T,test="H")
              Df Hotelling-Lawley approx F num Df den Df  Pr(>F)
(Intercept)   1             0.81014    3.5106      3    13 0.04628 *
Residuals    15
```

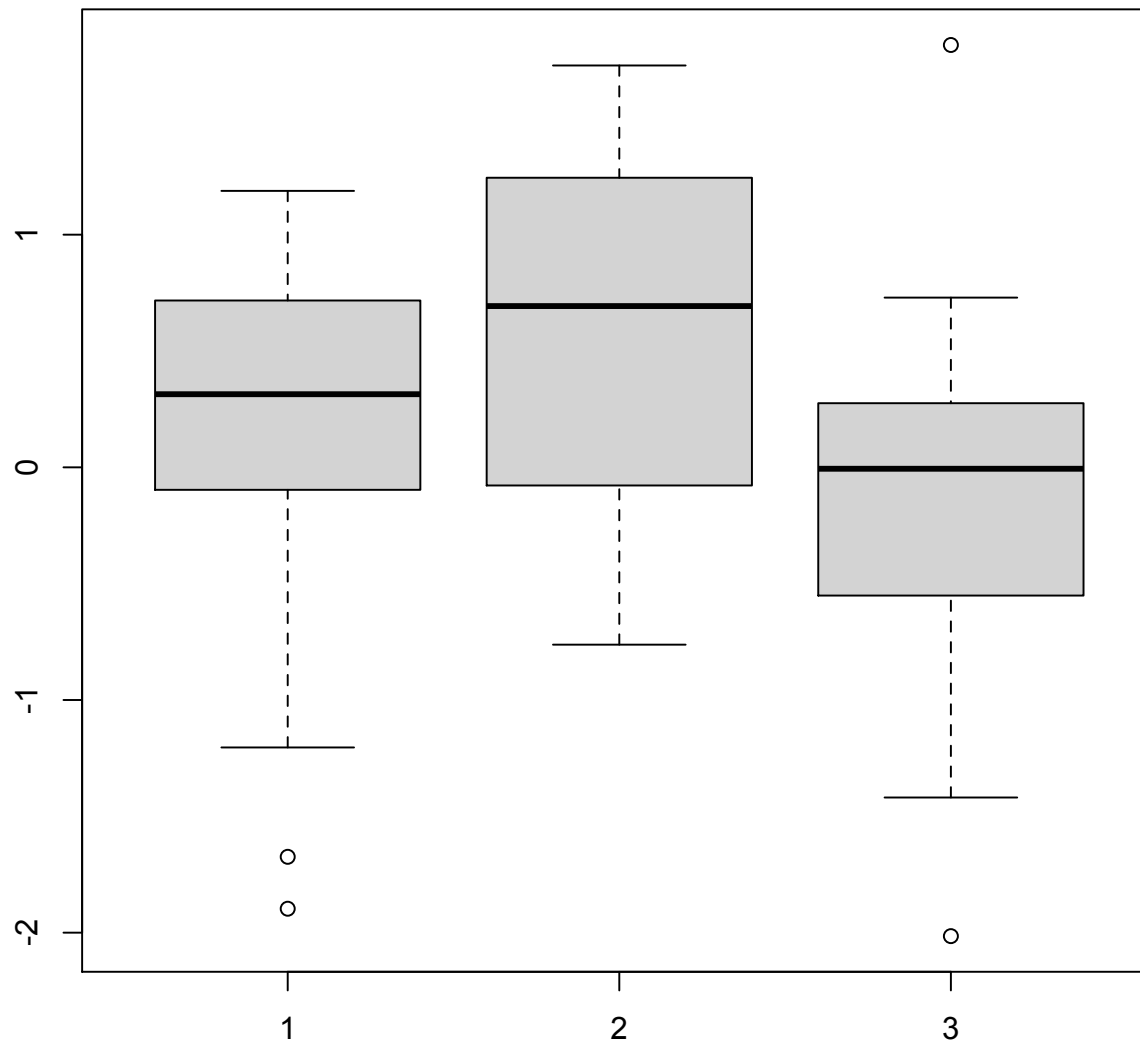
Recall:

```
> con
      [,1] [,2] [,3] [,4]
[1,]   -1   -1    0    0
[2,]    1    0   -1   -1
[3,]    0    0    1    0
[4,]    0    1    0    0
[5,]    0    0    0    1
```

But this!!

```
> eln = as.matrix(ele1[,-3]) %*% contr.sum(4)
> ele1[,-3]
      E1      E2      E4      E5
1  6.214608 5.991465 5.298317 5.521461
...
16 4.672829 3.871201 3.806662 3.931826
> summary(manova(eln~1),intercept=T,test="H")
      Df Hotelling-Lawley approx F num Df den Df  Pr(>F)
(Intercept)  1          0.81014    3.5106     3    13 0.04628 *
Residuals   15
> boxplot(eln)
```

Boxplot of contrasts: things do not always look as they appear



Still extending classics: two-sample Hotelling's T^2

And now: two-sample, first again univariate

Two-sample t-test: if

y_{1i} , $i = 1, \dots, n_1$ are modeled iid with $N(\mu_1, \sigma_1^2)$, and

y_{2i} , $i = 1, \dots, n_2$ are modeled iid with $N(\mu_2, \sigma_2^2)$, and

it is believed that those random variables are all independent

(between, but also within groups - “samples” - as well)

and it is also believed that $\sigma_1^2 = \sigma_2^2$

then $\frac{\bar{x}_1 - \bar{x}_2}{s_{\text{pooled}}} \sqrt{\frac{n_1 n_2}{n_1 + n_2 - 2}}$ is modeled by $t_{n_1 + n_2 - 2}$,

or equivalently, $\left(\frac{n_1 n_2}{n_1 + n_2 - 2} \right) \frac{(\bar{x}_1 - \bar{x}_2)^2}{s_{\text{pooled}}^2}$ by $F_{1, n_1 + n_2 - 2}$.

The important component here is the “pooled” estimate of the common variance

$$s_{\text{pooled}}^2 = \frac{1}{n_1 + n_2 - 2} \left(\sum_{i=1}^{n_1} (x_{1i} - \bar{x}_1)^2 + \sum_{i=1}^{n_2} (x_{2i} - \bar{x}_2)^2 \right)$$

Two-sample: multivariate

Hotelling T^2 : if

\mathbf{y}_{1i} , $i = 1, \dots, n_1$ are modeled iid with $N(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$, and

\mathbf{y}_{2i} , $i = 1, \dots, n_2$ are modeled iid with $N(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$, and

those random vectors are believed to be independent

(between and within groups)

(but not necessarily within vectors)

and $\boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2$, then (writing $\boldsymbol{\mu} = \boldsymbol{\mu}_1 - \boldsymbol{\mu}_2$)

$$\frac{n_1 + n_2 - 1 - p}{(n_1 + n_2 - 2)p} \frac{n_1 n_2}{n_1 + n_2} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2 - \boldsymbol{\mu})^\top \mathbf{S}_{\text{pooled}}^{-1} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2 - \boldsymbol{\mu})$$

can be considered $F_{p, n_1 + n_2 - 1 - p}$ or also

$$T^2 = \frac{n_1 n_2}{n_1 + n_2} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2 - \boldsymbol{\mu})^\top \mathbf{S}_{\text{pooled}}^{-1} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2 - \boldsymbol{\mu})$$

can be considered $\frac{(n_1 + n_2 - 2)p}{n_1 + n_2 - 1 - p} F_{p, n_1 + n_2 - 1 - p}$

The pooled estimate of Σ

The estimate of the common variance-covariance matrix is analogously the $p \times p$ matrix $\mathbf{S}_{\text{pooled}}$ whose element in k -th row and ℓ -th column is

$$\frac{1}{n_1 + n_2 - 2} \left(\sum_{i=1}^{n_1} (y_{1ik} - \bar{y}_{1k})(y_{1i\ell} - \bar{y}_{1\ell}) + \sum_{i=1}^{n_2} (y_{2ik} - \bar{y}_{2k})(y_{2i\ell} - \bar{y}_{2\ell}) \right)$$

Applications akin to univariate ones

Two-sample comparisons

testing $H_0: \mu_1 = \mu_2$.

Two-sample confidence intervals

for $\mu = \mu_1 - \mu_2$

Truly multivariate application: profile analysis

Profile analysis is again more general:

we test $H_0 : \mathbf{C}\boldsymbol{\mu}_1 = \mathbf{C}\boldsymbol{\mu}_2$, where \mathbf{C} is $k \times p$

using
$$T^2 = \frac{n_1 n_2}{n_1 + n_2} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2)^\top \mathbf{C}^\top [\mathbf{C} \mathbf{S}_{\text{pooled}} \mathbf{C}^\top]^{-1} \mathbf{C} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2)$$

with the distribution
$$\frac{(n_1 + n_2 - 2)k}{n_1 + n_2 - 1 - k} F_{k, n_1 + n_2 - 1 - k}$$

Example

V1, V2 and V3, V4 are the same measurements made in two labs.

```
> eff
```

	V1	V2	V3	V4
1	6	27	25	15
2	6	23	28	13
3	18	64	36	22
4	8	44	35	29
5	11	30	15	31
6	34	75	44	64
7	28	26	42	30
8	71	124	54	64
9	43	54	34	56
10	33	30	29	20
11	20	14	39	21

Paired T^2

Let's try the paired Hotelling first:

```
> summary(manova(cbind(V1-V3,V2-V4)~1,data=eff),  
+ intercept=T,test="H")  
              Df Hotelling-Lawley approx F num Df den Df  Pr(>F)  
(Intercept)  1              1.3639    6.1377      2      9 0.02083 *  
Residuals    10  
> 1-pf(13.6*9/20,2,9)  
[1] 0.02098437
```

And two-sample T^2

And then the two-sample Hotelling:

```
> respon=cbind(c(eff$V1,eff$V3),c(eff$V2,eff$V4))
> sam=factor(rep(c(0,1),c(11,11)))
> sam
 [1] 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1
Levels: 0 1
> summary(manova(respon~sam),test="H")
              Df Hotelling-Lawley approx F num Df den Df    Pr(>F)
sam           1           0.6332    6.0158     2    19 0.009463 **
Residuals    20
```


Review of t-tests: one-sample

Notation: $\bar{y} = \frac{1}{n} \sum_i y_i$, $s^2 = \frac{1}{n-1} \sum_i (y_i - \bar{y})^2$

the *t statistic* $\sqrt{n} \frac{\bar{y} - \mu}{s}$ is t_{n-1} (abusing the notation)

if y_1, y_2, \dots, y_n are iid, each is $N(\mu, \sigma^2)$; then it follows that

- \bar{y} is $N(\mu, \frac{1}{n}\sigma^2)$, and then $\frac{\bar{y} - \mu}{\frac{\sigma}{\sqrt{n}}} = \sqrt{n} \frac{\bar{y} - \mu}{\sigma}$ is $N(0, 1)$
- $\frac{(n-1)s^2}{\sigma^2} = \frac{\sum_i (x_i - \bar{x})^2}{\sigma^2}$ is χ_{n-1}^2
- \bar{x} and s^2 , and thus $\sqrt{n} \frac{\bar{x} - \mu}{\sigma}$ and $\frac{(n-1)s^2}{\sigma^2}$ are independent

which together yields the t_{n-1} distribution of

$$\frac{\sqrt{n} \frac{\bar{x} - \mu}{\sigma}}{\sqrt{\frac{(n-1)s^2}{\sigma^2}} \frac{1}{\sqrt{n-1}}} = \sqrt{n} \frac{\bar{x} - \mu}{s}$$

For large n , this distribution is approximately $N(0, 1)$

Two sample (t) test: univariate

If y_{1i} , $i = 1, \dots, n_1$ are iid with $N(\mu_1, \sigma_1^2)$,

and y_{2i} , $i = 1, \dots, n_2$ are iid with $N(\mu_2, \sigma_2^2)$,

and they are independent also between samples, and $\sigma_1^2 = \sigma_2^2$,

then $\frac{\bar{y}_1 - \bar{y}_2}{\bar{s}} \sqrt{\frac{n_1 n_2}{n_1 + n_2 - 2}}$ is $t_{n_1 + n_2 - 2}$ (\bar{s} is “pooled” estimate)

or, alternatively, $\left(\frac{n_1 n_2}{n_1 + n_2 - 2} \right) \frac{(\bar{y}_1 - \bar{y}_2)^2}{\bar{s}^2}$ is $F_{1, n_1 + n_2 - 2}$.

Two sample (T^2) test: multivariate

If \mathbf{y}_{1i} , $i = 1, \dots, n_1$ are iid with $N(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$,

and \mathbf{y}_{2i} , $i = 1, \dots, n_2$ are iid with $N(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2)$,

and they are independent also between samples,

and $\boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2$,

then ($\boldsymbol{\mu} = \boldsymbol{\mu}_1 - \boldsymbol{\mu}_2$)

$$\frac{n_1 + n_2 - 1 - p}{(n_1 + n_2 - 2)p} \frac{n_1 n_2}{n_1 + n_2} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2 - \boldsymbol{\mu})^\top \mathbf{S}_{\text{pooled}}^{-1} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2 - \boldsymbol{\mu})$$

is F_{p, n_1+n_2-1-p} , or, alternatively,

$$T^2 = \frac{n_1 n_2}{n_1 + n_2} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2 - \boldsymbol{\mu})^\top \mathbf{S}_{\text{pooled}}^{-1} (\bar{\mathbf{y}}_1 - \bar{\mathbf{y}}_2 - \boldsymbol{\mu})$$

is $\frac{(n_1 + n_2 - 2)p}{n_1 + n_2 - 1 - p} F_{p, n_1+n_2-1-p}$

where $\mathbf{S}_{\text{pooled}}$ is the pooled sample variance-covariance matrix with elements

$$\frac{1}{n_1 + n_2 - 2} \left(\sum_{i=1}^{n_1} (y_{1ik} - \bar{y}_{1k})(y_{1il} - \bar{y}_{1l}) + \sum_{i=1}^{n_2} (y_{2ik} - \bar{y}_{2k})(y_{2il} - \bar{y}_{2l}) \right)$$

**Trying to extend classics:
linear model and ANOVA**

One-way layout: univariate

response y_{ki} , $i = 1, \dots, n$, coming in $k = 1, \dots, K$ groups

model $y_{ki} = \mu_k + \varepsilon_{ki}$ (or some equivalent form)

the size of groups not necessarily equal: $n = n_1 + \dots + n_k$

errors ε_{ki} are independent and $N(0, \sigma^2)$
(the same variance for all errors)

the hypothesis of interest: all μ_k equal

fit by least-squares method

under model, and

under restricted model (hypothesis)

One-way layout: univariate - testing

restricted model: we fit the same μ to all y_{ki}

its estimate is grand mean \bar{y} , over all y_{ki}

the minimized sum of squares is $T = \sum (y_{ki} - \bar{y})^2$

divided by $n - 1$ degrees of freedom gives the estimate s_T^2

full model: we fit not necessarily same μ_k to each group of y_{ki}

the estimates are group means \bar{y}_k

the minimized sum of squares is $W = \sum (y_{ki} - \bar{y}_k)^2$

divided by $n - K$ degrees of freedom gives $s^2 = s_W^2$

the ratio $\frac{\frac{T - W}{n - 1 - (n - K)}}{\frac{W}{n - K}} = \frac{\frac{T - W}{K - 1}}{\frac{W}{n - K}}$ is good for testing

if the assumptions hold, its distribution is $F_{(K-1)(n-K)}$

and if the hypothesis is true, it tends to be small

One-way layout: multivariate

Multivariate: $j = 1, \dots, p$, p is the dimension of the response
response y_{kij} , $i = 1, \dots, n$, coming in $k = 1, \dots, K$ groups

model $y_{kij} = \mu_{kj} + \varepsilon_{kij}$

the size of groups not necessarily equal: $n = n_1 + \dots + n_k$

errors ε_{ki} are independent and $N(\mathbf{0}, \Sigma)$

(the same variance-covariance matrix for all errors)

the hypothesis of interest: all μ_k equal

fit by least-squares method

under model, and

under restricted model (hypothesis)

On more graduate level: multivariate linear model

$$\mathbf{Y} = \mathbf{XB} + \mathbf{E}$$

\mathbf{Y} - an $n \times p$ response matrix;

\mathbf{X} - an $n \times r$ matrix of covariates (stimuli)

\mathbf{B} - an $r \times p$ matrix of parameters

\mathbf{E} - an $n \times p$ matrix of errors

If $p = 1$, it is univariate linear model; in fact, a multivariate linear model can be viewed as p univariate linear models together

$$\begin{aligned} \mathbf{y}_{\cdot j} &= \mathbf{X}\boldsymbol{\beta}_{\cdot j} + \boldsymbol{\varepsilon}_{\cdot j}, \quad j = 1, \dots, p & \mathbf{Y} &= (\mathbf{y}_{\cdot 1} \quad \dots \quad \mathbf{y}_{\cdot j} \quad \dots \quad \mathbf{y}_{\cdot p}) \\ & & \mathbf{B} &= (\boldsymbol{\beta}_{\cdot 1} \quad \dots \quad \boldsymbol{\beta}_{\cdot j} \quad \dots \quad \boldsymbol{\beta}_{\cdot p}) \\ & & \mathbf{E} &= (\boldsymbol{\varepsilon}_{\cdot 1} \quad \dots \quad \boldsymbol{\varepsilon}_{\cdot j} \quad \dots \quad \boldsymbol{\varepsilon}_{\cdot p}) \end{aligned}$$

Even more componentwise

$$y_{ij} = \mathbf{x}_{i.}^T \boldsymbol{\beta}_{.j} + \varepsilon_{ij}, \quad i = 1, \dots, n, \quad j = 1, \dots, p \quad \mathbf{X} = \begin{pmatrix} \mathbf{x}_{1.}^T \\ \vdots \\ \mathbf{x}_{i.}^T \\ \vdots \\ \mathbf{x}_{n.}^T \end{pmatrix}$$

Typical modeling assumptions: ε_i are now **rows** of $\mathbf{E} = \begin{pmatrix} \boldsymbol{\varepsilon}_{1.}^T \\ \vdots \\ \boldsymbol{\varepsilon}_{i.}^T \\ \vdots \\ \boldsymbol{\varepsilon}_{n.}^T \end{pmatrix}$

$$E(\boldsymbol{\varepsilon}_{i.}) = \mathbf{0}$$

$$\text{Var}(\boldsymbol{\varepsilon}_{i.}) = \boldsymbol{\Sigma} \quad (\text{not depending on } j)$$

$$\text{Cov}(\boldsymbol{\varepsilon}_{i.}, \boldsymbol{\varepsilon}_{k.}) = \mathbf{0} \quad \text{for } i \neq k, \quad \text{or stronger: rows } \boldsymbol{\varepsilon}_{i.} \text{ are independent}$$

$$\text{also normality assumption: } \boldsymbol{\varepsilon}_{i.} \text{ are independent, each } N(\mathbf{0}, \boldsymbol{\Sigma})$$

Estimation

Least squares, motivated by

1. Numerical convenience: quadratic minimization problem leads to linear equations;
2. Gauss-Markov theory (best linear unbiased estimate)
3. Maximum likelihood under normality assumption

Assumption: Σ is nonsingular (\rightarrow density exists)

a particular advantage in the multivariate context: estimation of a multivariate model splits to the estimation of p univariate ones - minimizing the left-hand sum amount to separate minimizations of the right-hand sums in

$$\sum_{i,j} (y_{ij} - \mathbf{x}_i^\top \boldsymbol{\beta}_j)^2 = \sum_i (y_{i1} - \mathbf{x}_i^\top \boldsymbol{\beta}_1)^2 + \cdots + \sum_i (y_{ip} - \mathbf{x}_i^\top \boldsymbol{\beta}_p)^2$$

$$\hat{\boldsymbol{\beta}}_j = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}_j \quad \hat{\mathbf{B}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{Y}$$

Beware: not true in general (when it's *not* least squares)

The verification of the least-squares formula

$$\sum_{i,j} (y_{ij} - \mathbf{x}_i^\top \boldsymbol{\beta}_j)^2 = \text{tr}(\mathbf{Y} - \mathbf{XB})^\top (\mathbf{Y} - \mathbf{XB})$$

$$= \text{tr}\left((\mathbf{Y} - \mathbf{XB} + \mathbf{XB} - \mathbf{XB})^\top (\mathbf{Y} - \mathbf{XB} + \mathbf{XB} - \mathbf{XB})\right)$$

$$= \text{tr}\left((\mathbf{Y} - \mathbf{XB})^\top (\mathbf{Y} - \mathbf{XB})\right) + \text{tr}\left((\mathbf{XB} - \mathbf{XB})^\top (\mathbf{XB} - \mathbf{XB})\right)$$

due to the fact that $(\mathbf{Y} - \mathbf{XB})^\top (\mathbf{XB} - \mathbf{XB}) = \mathbf{0}$

Verifying the maximum likelihood claim

The negative of the log-likelihood is, up to an additive and multiplicative constants that don't affect the outcomes of minimization,

$$\begin{aligned} & \sum_i \log \det(\boldsymbol{\Sigma}) + (\mathbf{y}_{i\cdot} - \mathbf{x}_{i\cdot}^\top \mathbf{B}) \boldsymbol{\Sigma}^{-1} (\mathbf{y}_{i\cdot} - \mathbf{x}_{i\cdot}^\top \mathbf{B})^\top \\ &= n \log \det(\boldsymbol{\Sigma}) + \sum_i \text{tr} \left((\mathbf{y}_{i\cdot} - \mathbf{x}_{i\cdot}^\top \mathbf{B}) \boldsymbol{\Sigma}^{-1} (\mathbf{y}_{i\cdot} - \mathbf{x}_{i\cdot}^\top \mathbf{B})^\top \right) \\ &= n \log \det(\boldsymbol{\Sigma}) + \text{tr} \left(\sum_i (\mathbf{y}_{i\cdot} - \mathbf{x}_{i\cdot}^\top \mathbf{B})^\top (\mathbf{y}_{i\cdot} - \mathbf{x}_{i\cdot}^\top \mathbf{B}) \boldsymbol{\Sigma}^{-1} \right) \\ &= n \log \det(\boldsymbol{\Sigma}) + \text{tr} \left((\mathbf{Y} - \mathbf{XB})^\top (\mathbf{Y} - \mathbf{XB}) \boldsymbol{\Sigma}^{-1} \right) \\ &= n \log \det(\boldsymbol{\Sigma}) + \text{tr} \left((\mathbf{Y} - \mathbf{XB})^\top (\mathbf{Y} - \mathbf{XB}) \boldsymbol{\Sigma}^{-1} \right) \end{aligned}$$

If $\boldsymbol{\Sigma}$ is fixed, then the first term does not depend on \mathbf{B} and the second one is minimized by \mathbf{B} equal to the least squares estimator $\hat{\mathbf{B}}$:

Verifying continued

$$\begin{aligned} & \text{tr}\left((\mathbf{Y} - \mathbf{XB})^\top (\mathbf{Y} - \mathbf{XB}) \boldsymbol{\Sigma}^{-1}\right) \\ &= \text{tr}\left((\mathbf{Y} - \mathbf{X}\hat{\mathbf{B}})^\top (\mathbf{Y} - \mathbf{X}\hat{\mathbf{B}}) \boldsymbol{\Sigma}^{-1}\right) + \text{tr}\left((\mathbf{X}\hat{\mathbf{B}} - \mathbf{XB})^\top (\mathbf{X}\hat{\mathbf{B}} - \mathbf{XB}) \boldsymbol{\Sigma}^{-1}\right) \\ &= \text{tr}\left((\mathbf{Y} - \mathbf{X}\hat{\mathbf{B}})^\top (\mathbf{Y} - \mathbf{X}\hat{\mathbf{B}}) \boldsymbol{\Sigma}^{-1}\right) + \text{tr}\left((\mathbf{X}\hat{\mathbf{B}} - \mathbf{XB}) \boldsymbol{\Sigma}^{-1} (\mathbf{X}\hat{\mathbf{B}} - \mathbf{XB})^\top\right) \end{aligned}$$

and the last term is the trace of the nonnegative definite matrix.

Put $\mathbf{B} = \hat{\mathbf{B}}$; let $\mathbf{A} = (\mathbf{Y} - \mathbf{X}\hat{\mathbf{B}})^\top (\mathbf{Y} - \mathbf{X}\hat{\mathbf{B}})$

the negative log-likelihood becomes, if \mathbf{A} is nonsingular,

$$\begin{aligned} n \log \det(\boldsymbol{\Sigma}) + \text{tr}(\mathbf{A}\boldsymbol{\Sigma}^{-1}) &= -n \log \det(\boldsymbol{\Sigma}^{-1}) + \text{tr}(\mathbf{A}\boldsymbol{\Sigma}^{-1}) \\ &= -n \log \det(\mathbf{A}\boldsymbol{\Sigma}^{-1}) + n \log \det \mathbf{A} + \text{tr}(\mathbf{A}\boldsymbol{\Sigma}^{-1}) \end{aligned}$$

which is minimized by $\hat{\boldsymbol{\Sigma}} = \frac{1}{n} \mathbf{A}$ if \mathbf{A} is fixed (and nonsingular)

One-way layout: multivariate - testing

restricted model: we fit the same μ to all y_{ki}

its estimate is the grand mean $\bar{y} = (\bar{y}_1, \dots, \bar{y}_p)^T$

the estimate of variance-covariance matrix is obtained from

the matrix \mathbf{T} with elements $T_{rs} = \sum_{k,i} (y_{kir} - \bar{y}_r)(y_{kis} - \bar{y}_s)$

by dividing it by $n - 1$ degrees of freedom

full model: we fit not necessarily same μ_k to each group of y_{ki}

the estimates are group means $\bar{y}_k = (\bar{y}_{k1}, \dots, \bar{y}_{kp})^T$

the estimate of variance-covariance matrix is obtained from

the matrix \mathbf{W} with elements $W_{rs} = \sum (y_{kir} - \bar{y}_{kr})(y_{kis} - \bar{y}_{ks})$

by dividing it by $n - K$ degrees of freedom

ANOVA decomposition: univariate and multivariate

In univariate setting, we have the decomposition

$$RSS_H = RSS + (RSS_H - RSS)$$

in our notation it is $T = W + (T - W)$

They are minimized sum of squares, and serve also as a basis for variance estimation. We then take, up to some constants, a ratio of $T - W$ and W as a testing statistic

In the multivariate setting, we cannot decompose minimized sums of squares in this way; we can do that, however, for matrices that serve for the estimation of the variance-covariance matrices

$$\mathbf{T} = \mathbf{W} + (\mathbf{T} - \mathbf{W})$$

The problem is then: what is the ratio of $\mathbf{T} - \mathbf{W}$ and \mathbf{W} ?

Four possibilities for the ratio

Essentially (given tractability and other considerations), there are four possibilities to consider.

Note that after getting $\mathbf{W}^{-1}(\mathbf{T} - \mathbf{W})$ or similar matrix, we need still to evaluate - by one number - how much this matrix differs from \mathbf{O}

The possibilities (some of them) are:

1. Hotelling's—Lawley's trace: $\text{tr}[\mathbf{W}^{-1}(\mathbf{T} - \mathbf{W})]$
2. Roy's maximal eigenvalue of $\mathbf{W}^{-1}(\mathbf{T} - \mathbf{W})$
3. Pillai's trace $\text{tr}[\mathbf{T}^{-1}(\mathbf{T} - \mathbf{W})]$
4. Wilks's $\lambda = \frac{\det \mathbf{W}}{\det \mathbf{T}}$

Some insights

AB and **BA** have the same nonzero eigenvalues

$\text{tr } \mathbf{AB} = \text{tr } \mathbf{BA}$; also, trace is the sum of eigenvalues

Maximal eigenvalues of **AB** and **BA** are equal

Determinant is the product of eigenvalues

Let $\lambda_1 \geq \lambda_2 \geq \dots$ be eigenvalues of $\mathbf{W}^{-1}(\mathbf{T} - \mathbf{W})$

Let $\xi_1 \geq \xi_2 \geq \dots$ be eigenvalues of $\mathbf{T}^{-1}(\mathbf{T} - \mathbf{W})$

We have that $\xi_i = \frac{\lambda_i}{1 + \lambda_i}$, $\lambda_i = \frac{\xi_i}{1 - \xi_i}$

$$1. \text{tr}[\mathbf{W}^{-1}(\mathbf{T} - \mathbf{W})] = \sum \lambda_i = \sum \frac{\xi_i}{1 - \xi_i}$$

$$2. \text{The maximal eigenvalue of } \mathbf{W}^{-1}(\mathbf{T} - \mathbf{W}) \text{ is } \lambda_1 = \frac{\xi_1}{1 - \xi_1}$$

$$3. \text{tr}[\mathbf{T}^{-1}(\mathbf{T} - \mathbf{W})] = \sum \frac{\lambda_i}{1 + \lambda_i} = \sum \xi_i$$

$$4. \frac{\det(\mathbf{W})}{\det(\mathbf{T})} = \prod \frac{1}{1 + \lambda_i} = \prod (1 - \xi_i)$$

Tales about distributions

ν - “residual degrees of freedom”: $n - \dim \mathcal{M}(\mathbf{X})$

ν_H - “hypothesis degrees of freedom”: $\dim \mathcal{M}(\mathbf{X}) - \dim \mathcal{M}(\mathbf{X}_H)$

p - the dimension of the response

$t = \min\{p, \nu_H\}$, $u = \max\{p, \nu_H\}$, $\lambda = \frac{1}{4}(p\nu_H - 2)$,

$r = \frac{1}{2}(|p - \nu_H| - 1)$, $k = \nu - p - 1$, $m = \nu + \frac{1}{2}\nu_H - \frac{1}{2}(p + 1)$,

There we quite a few approximations proposed; the following are not the only ones

1. Hotelling's-Lawley's trace U

$\frac{(tk + 2)}{t^2(2r + t + 1)} U$ is approximately $F_{t(2r+t+1), tk+2}$

2. Roy's maximal eigenvalue (root) Θ : $\frac{u}{\nu - u - 1} F_{u, \nu - u - 1}$

gives only a lower bound on approximate p-value

(hence its significance is often ignored - especially when other criteria contraindicate it)

More tales about distributions

3. Pillai's trace V :

$\frac{k+t+1}{2r+t+1} \frac{V}{t-V}$ is approximately $F_{t(2r+t+1), t(k+t+1)}$

4. Wilks's Λ :

Bartlett's approximation: $-m \log \Lambda$ is approximately $\chi^2_{p\nu_H}$

Rao's transformation: $\frac{1 - \Lambda^{1/s}}{\Lambda^{1/s}} \frac{ms - 2\lambda}{p\nu_H}$ is

approximately (exactly if $t \leq 2$) $F_{p\nu_H, ms-2\lambda}$

non-integer degrees of freedom possible here

$s = \sqrt{\frac{p^2\nu_H^2-4}{p^2+\nu_H^2-5}}$ if $p^2 + \nu_H^2 - 5 > 0$, otherwise $s = 1$

Distributions: summary

All of the alternatives approximate F for certain constant multiples, as listed above; some of them possess also some alternative approximations, or even “exact” distributions (exact under exact normality).

Only lower bound on p -value for Roy; hence generally disregarded if others are not significant.

Wilks has also another approximation, by χ^2 ; its F approximation may have non-integer second degrees of freedom.

All four are approximately equivalent for large sample sizes.

All four are equivalent *exactly*

for $p = 1$, that is, in the univariate case
then they reduce to the usual F -ratio

in one-sample or two-sample models - then equivalent to
one-sample or two-sample Hotelling T^2 , respectively.

Some authors recommend as first choice Pillai's trace V , because of its robustness; then Wilks's Λ ; then Hotelling's-Lawley's trace U

Likelihood ratio motivation for Wilks' Λ

Under normal distribution of errors

the maximized value of the likelihood is $\frac{e^{-np/2}}{(2\pi)^{np/2}(\det \hat{\Sigma})^{n/2}}$

where $\hat{\Sigma}$ is the maximum likelihood estimate of Σ

The likelihood ratio for testing the submodel is thus

$$\frac{(\det \hat{\Sigma}_H)^{-n/2}}{(\det \hat{\Sigma})^{-n/2}} = \left(\frac{\det \hat{\Sigma}}{\det \hat{\Sigma}_H} \right)^{n/2} \quad \text{which is}$$

equivalent to Wilks's $\Lambda = \frac{\det \hat{\Sigma}}{\det \hat{\Sigma}_H} = \frac{\det \mathbf{W}}{\det \mathbf{T}}$

Note that in the univariate case, this is equal to $\frac{RSS}{RSS_H}$

which is equivalent to the usual F-ratio, as it is equivalent to

$$\frac{RSS_H}{RSS} = \frac{RSS + RSS_H - RSS}{RSS} = 1 + \frac{RSS_H - RSS}{RSS}$$

Example: dogs

5 groups:

```
> levels(as.factor(Canine$Group))
```

```
[1] "Cuon" "GoldenJackal" "IndianWolf"
```

```
[4] "ModernThaiDog" "PrehistoricThaiDog"
```

```
> Canine
```

	Sample	X1	X2	X3	X4	X5	X6	X7	X8	X9	Sex	Group
1	1	123	10.1	23	23	19	7.8	32	33	5.6	Male	ModernThaiDog
2	2	137	9.6	19	22	19	7.8	32	40	5.8	Male	ModernThaiDog
3	3	121	10.2	18	21	21	7.9	35	38	6.2	Male	ModernThaiDog
4	4	130	10.7	24	22	20	7.9	32	37	5.9	Male	ModernThaiDog
5	5	149	12.0	25	25	21	8.4	35	43	6.6	Male	ModernThaiDog

...

```
> attach(Canine)
```

```
> nrow(Canine)
```

```
[1] 77
```

Is there a way to visualize this?

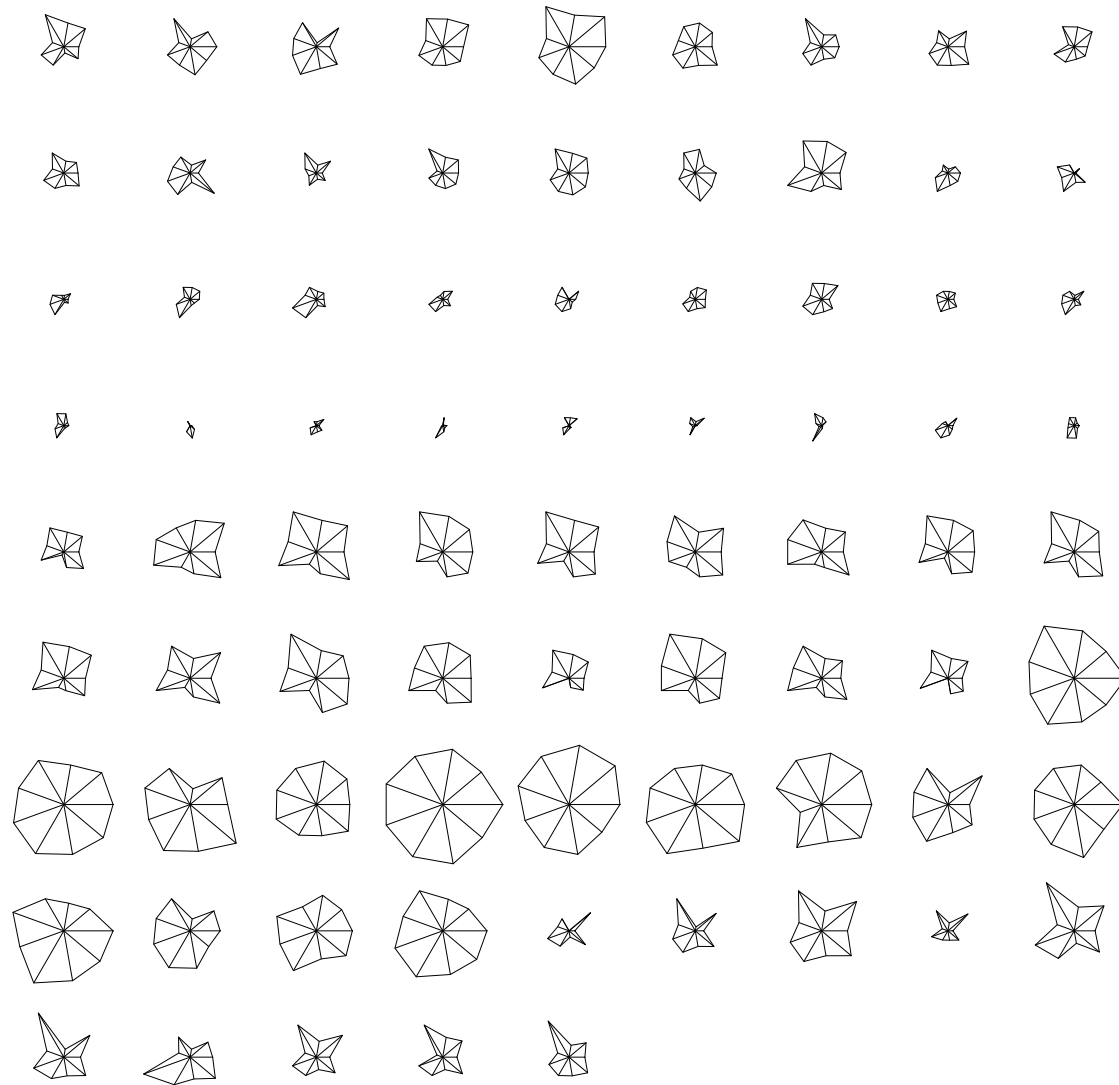
Dogs: plotting (one way of)

```
> stars(Canine[,2:10])
> stars(Canine[,2:10],labels=Canine$Group,lwd=1)
> stars(Canine[,2:10],labels=as.numeric(as.factor(Canine$Group)),
+ lwd=1)
> stars(dogs[,2:10],lwd=0.7,
+ labels=strtrim(as.character(dogs$Group),6), cex=0.7, flip=F,
+ col.stars=
+ c("pink","grey","white")[as.numeric(as.factor(dogs$Sex))],ncol=7)
```

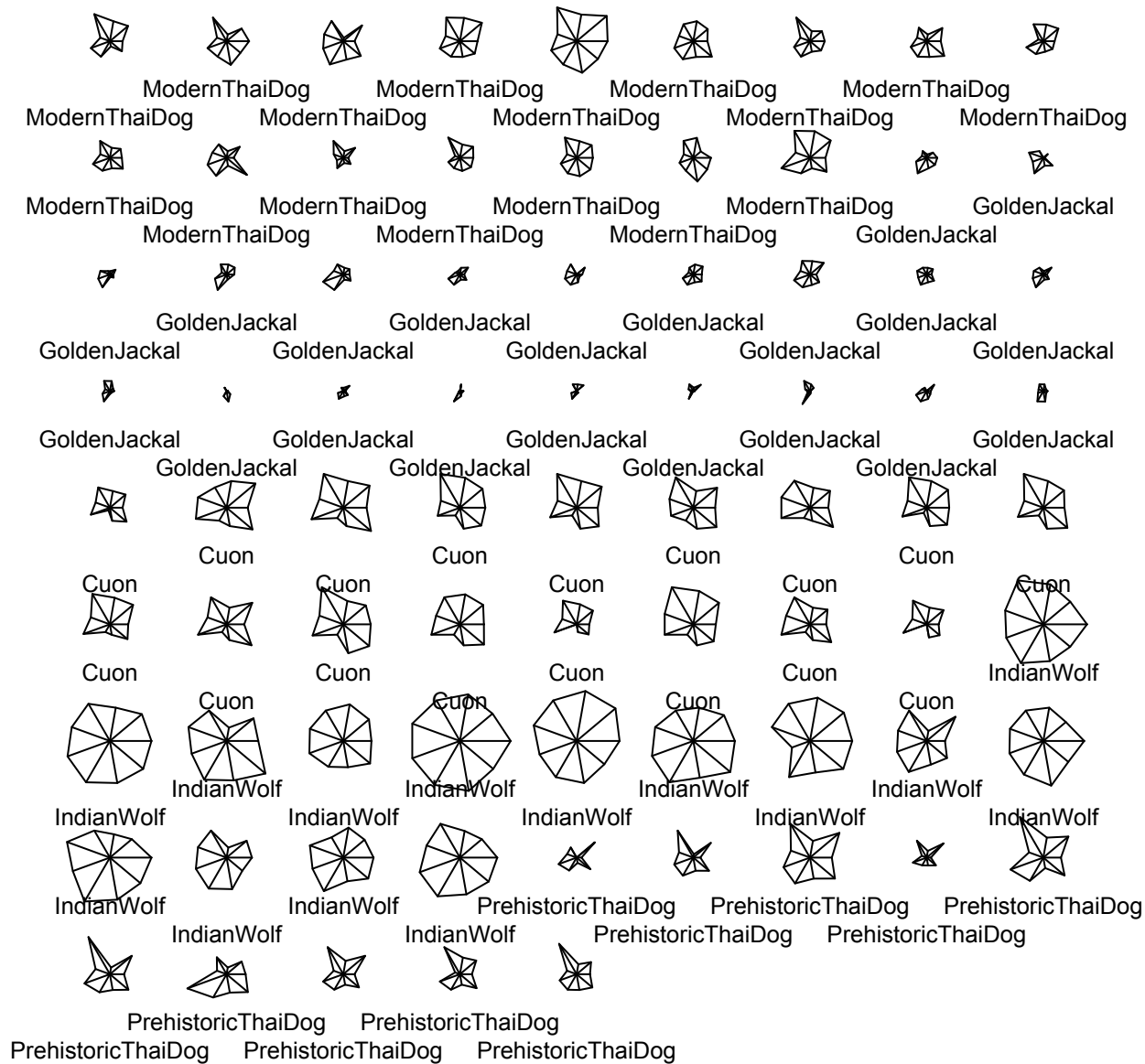
Dogs: profiles (another plotting method)

```
> plot(c(1:9,1:9),
+ c(apply(Canine[,2:10],2,max),apply(Canine[,2:10],2,min)),
+ type='n',xlab='',ylab='')
> for (k in (1:77)[Group=="Cuon"] )
+ lines(1:9,Canine[k,2:10],pch=1,type='b',col='black')
> for (k in (1:77)[Group=="GoldenJackal"] )
+ lines(1:9,Canine[k,2:10],pch=2,type='b',col='yellow')
> for (k in (1:77)[Group=="IndianWolf"] )
+ lines(1:9,Canine[k,2:10],pch=3,type='b',col='green')
> for (k in (1:77)[Group=="ModernThaiDog"] )
+ lines(1:9,Canine[k,2:10],pch=4,type='b',col='magenta')
> for (k in (1:77)[Group=="PrehistoricThaiDog"] )
+ lines(1:9,Canine[k,2:10],pch=5,type='b',col='blue')
```

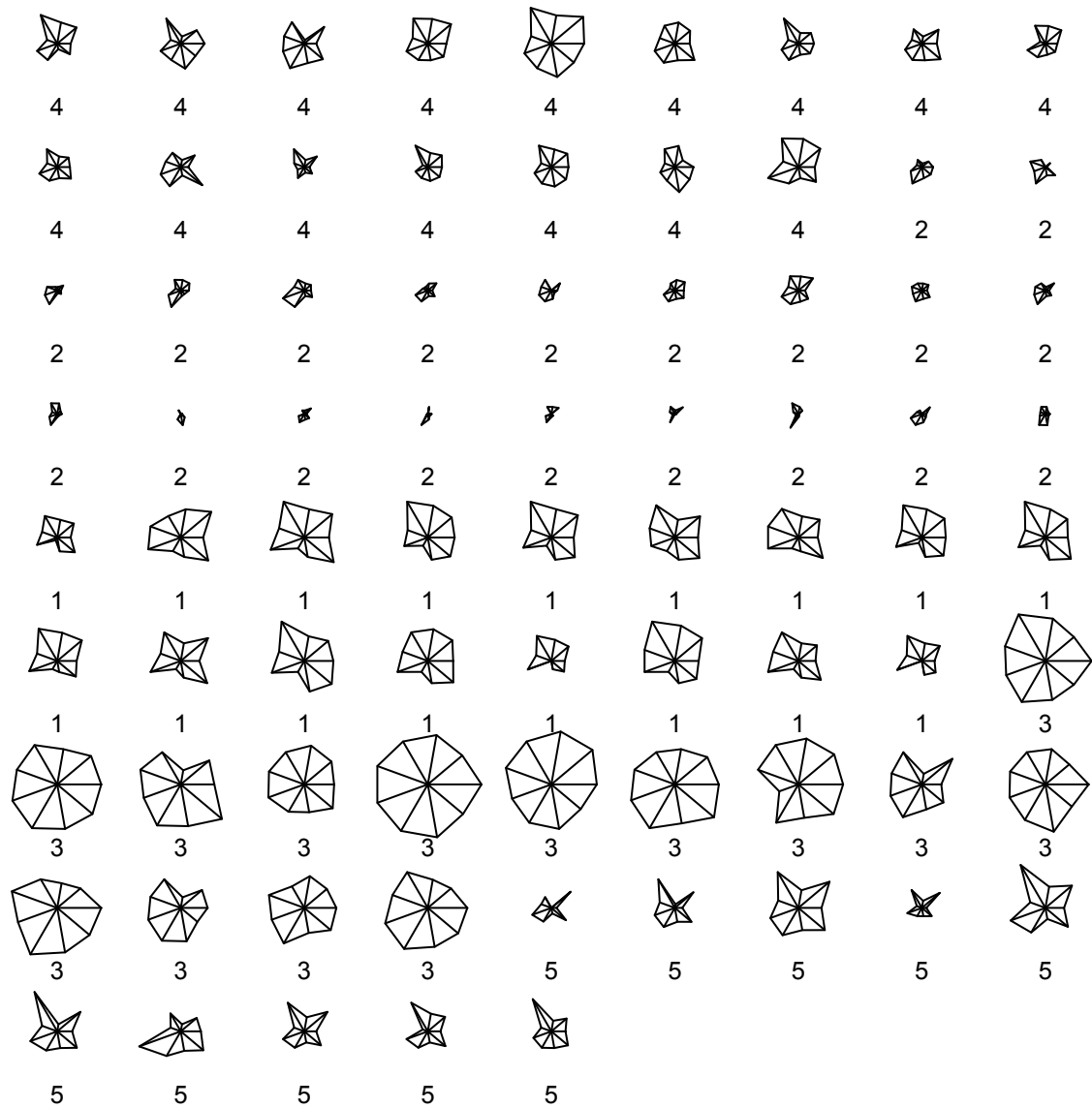

Star plot: this is the default now



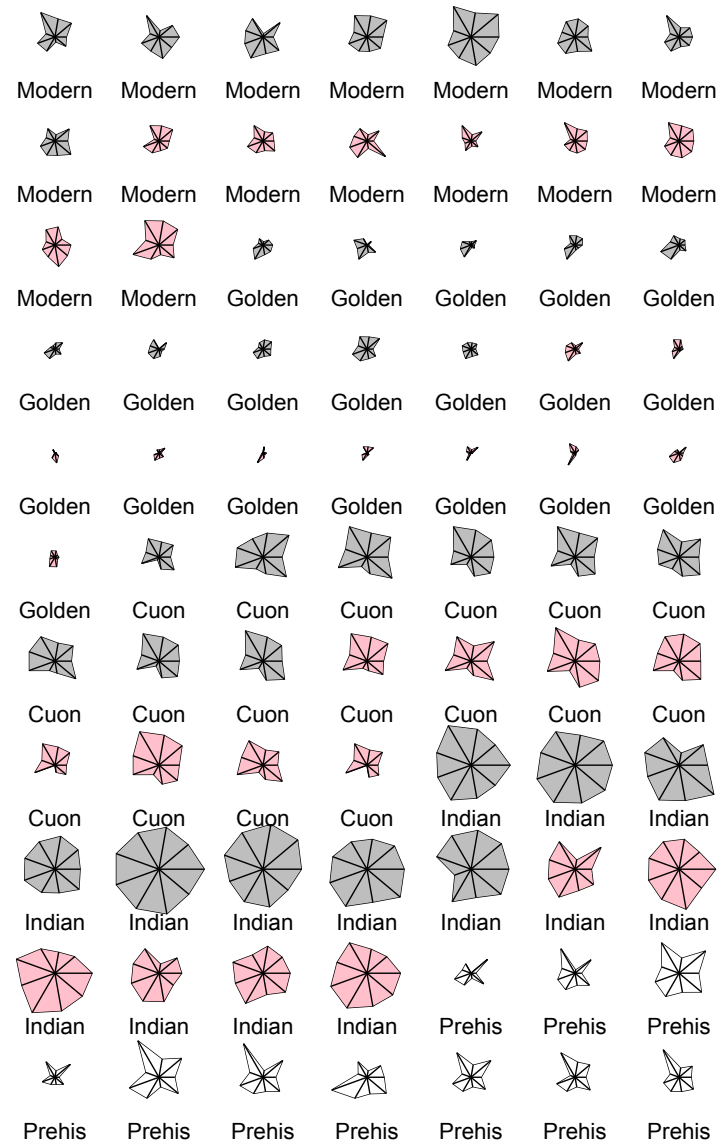
Is this one better?



Or this one?

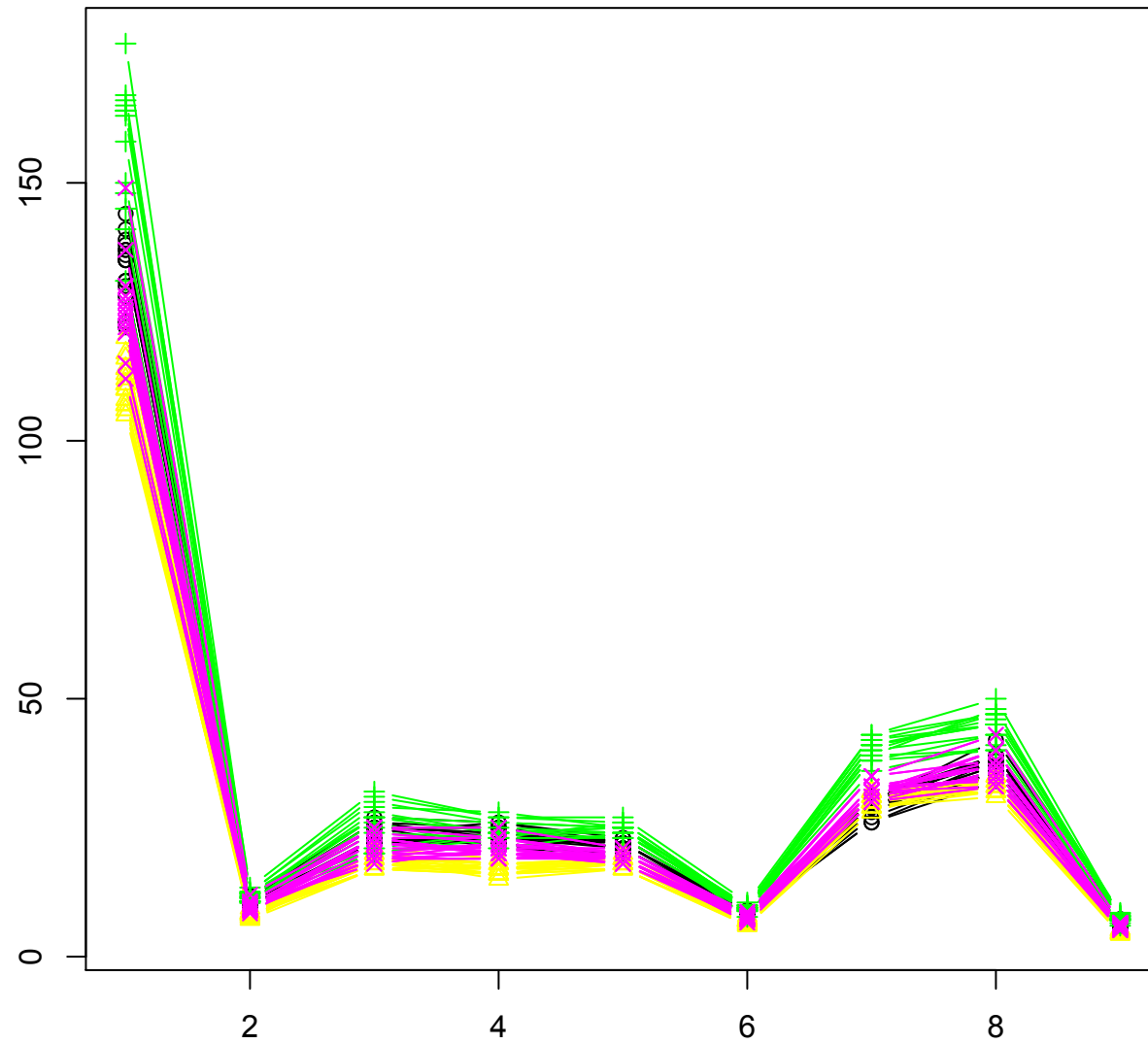


How about this one?

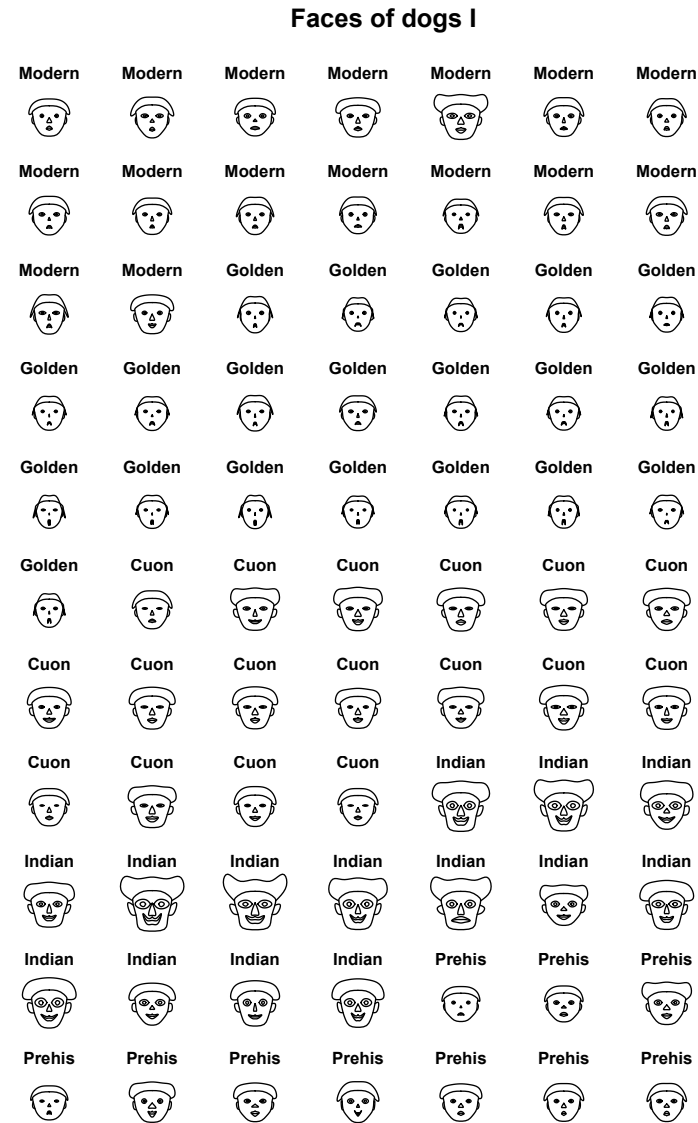


(Colors show sex: male, female, or unknown)

Profiles

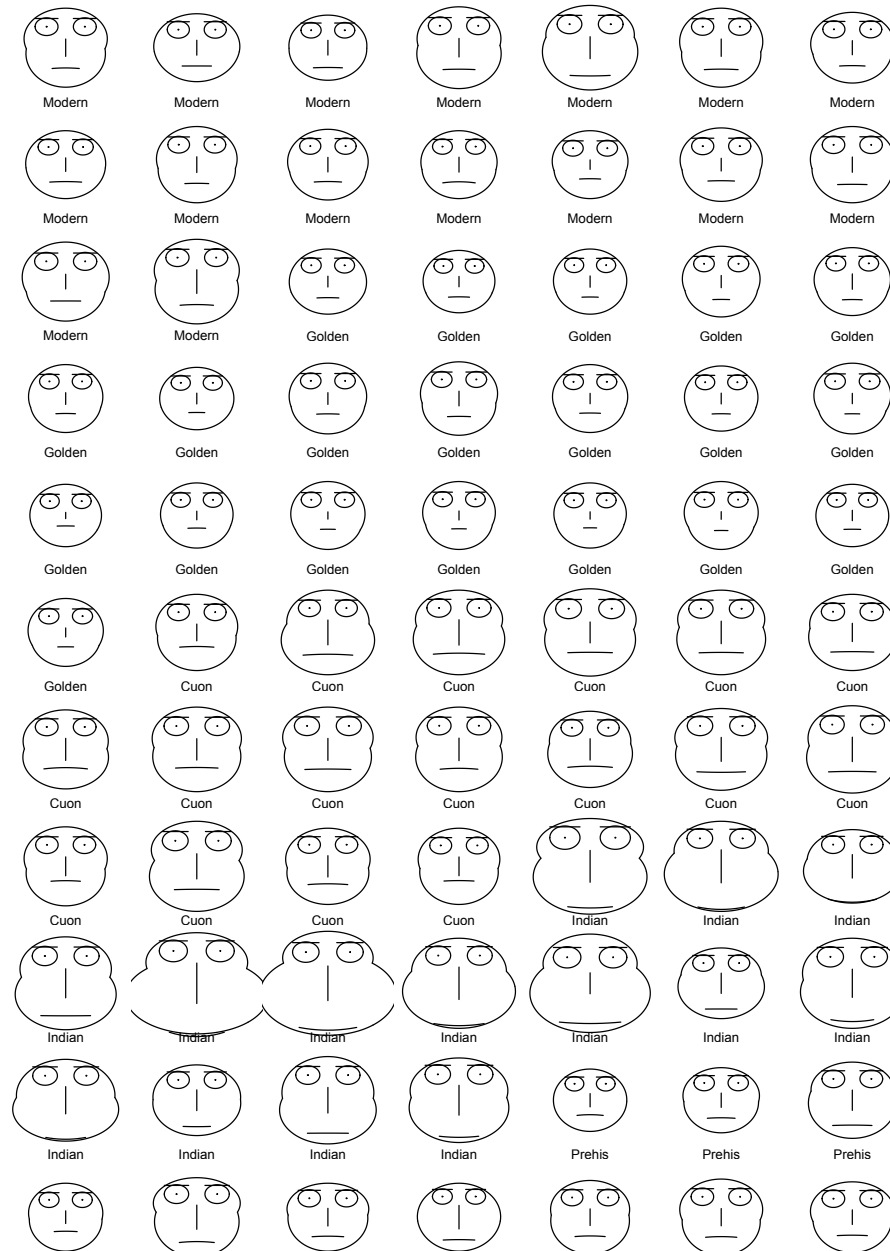


Fancy plotting through glyphs: Chernoff faces



Visualizing variables by various facial characteristics

More original look



For how to do it in R, google up “Chernoff faces R”

And now the rigorous stuff

```
> respo <- cbind(X1,X2,X3,X4,X5,X6,X7,X8,X9)
> summary(manova(respo~Group, data=Canine), test='H')
```

	Df	Hotelling-Lawley	approx F	num Df	den Df	Pr(>F)
Group	4	25.129	43.627	36	250	< 2.2e-16 ***
Residuals	72					

```
> summary(manova(respo~Group, data=Canine), test='R')
```

	Df	Roy	approx F	num Df	den Df	Pr(>F)
Group	4	16.348	121.699	9	67	< 2.2e-16 ***
Residuals	72					

```
> summary(manova(respo~Group, data=Canine), test='P')
```

	Df	Pillai	approx F	num Df	den Df	Pr(>F)
Group	4	2.5892	13.6622	36	268	< 2.2e-16 ***
Residuals	72					

```
> summary(manova(respo~Group, data=Canine), test='W')
```

	Df	Wilks	approx F	num Df	den Df	Pr(>F)
Group	4.00	0.0022	27.6656	36.00	241.57	< 2.2e-16 ***
Residuals	72.00					

More sophisticated modeling possible

```
> summary(manova(respo~Group*Sex, data=Canine),test='H')
```

	Df	Hotelling-Lawley	approx F	num Df	den Df	Pr(>F)
Group	4	31.664	51.454	36	234	< 2.2e-16 ***
Sex	1	0.486	3.242	9	60	0.002866 **
Group:Sex	3	0.656	1.426	27	176	0.091126 .
Residuals	68					

```
> summary(manova(respo~Group*Sex, data=Canine),test='R')
```

	Df	Roy	approx F	num Df	den Df	Pr(>F)
Group	4	21.463	150.242	9	63	< 2.2e-16 ***
Sex	1	0.486	3.242	9	60	0.002866 **
Group:Sex	3	0.412	2.839	9	62	0.007281 **
Residuals	68					

```
> summary(manova(respo~Group*Sex, data=Canine),test='P')
```

	Df	Pillai	approx F	num Df	den Df	Pr(>F)
Group	4	2.6446	13.6581	36	252	< 2.2e-16 ***
Sex	1	0.3272	3.2417	9	60	0.002866 **
Group:Sex	3	0.5054	1.3958	27	186	0.103601
Residuals	68					

```
> summary(manova(respo~Group*Sex, data=Canine),test='W')
```

	Df	Wilks	approx F	num Df	den Df	Pr(>F)
Group	4.00	0.0014	30.2015	36.00	226.59	< 2.2e-16 ***
Sex	1.00	0.6728	3.2417	9.00	60.00	0.002866 **
Group:Sex	3.00	0.5637	1.4125	27.00	175.87	0.096985 .
Residuals	68.00					

And for two-level one-way layout all coincide

... and reduce to two-sample Hotelling T^2 .

```
> summary(manova(respo~Sex,  
+ data=Canine,subset=Sex!="Unknown"),test='H')  
              Df Hotelling-Lawley approx F num Df den Df Pr(>F)  
Sex           1          0.14886  0.94279      9    57 0.4961  
Residuals 65
```

```
> summary(manova(respo~Sex,  
+ data=Canine,subset=Sex!="Unknown"),test='R')  
              Df      Roy approx F num Df den Df Pr(>F)  
Sex           1 0.14886  0.94279      9    57 0.4961  
Residuals 65
```

```
> summary(manova(respo~Sex,  
+ data=Canine,subset=Sex!="Unknown"),test='P')  
              Df  Pillai approx F num Df den Df Pr(>F)  
Sex           1 0.12957  0.94279      9    57 0.4961  
Residuals 65
```

```
> summary(manova(respo~Sex,  
+ data=Canine,subset=Sex!="Unknown"),test='W')  
              Df   Wilks approx F num Df den Df Pr(>F)  
Sex           1 0.87043  0.94279      9    57 0.4961  
Residuals 65
```

**Dual view - reconciling distances:
multidimensional scaling (ordination)**

The principle

Imagine that you have a map, with the distances of cities
and then you lose it, and what remains are distances
and you have to reconstruct the map

Fairmont hotels in Alberta

Caution: only to illustrate methodology - otherwise not quite an example of a real data analysis. Driving distances:

```
> Fairorg      ## original data out of travel claims
      Banff Calgary Edmonton Jasper LakeLouise
Banff         0      128         NA         NA         58
Calgary       128         0      294         NA         NA
Edmonton       NA      294         0      370         NA
Jasper         NA      NA      370         0      229
LakeLouise     58      NA      NA      229         0
```

```
> Fairmont     ## completed by "minimal sum"
      Banff Calgary Edmonton Jasper LakeLouise
Banff         0      128      422      287         58
Calgary       128         0      294      415        186
Edmonton       422      294         0      370        480
Jasper         287      415      370         0        229
LakeLouise     58      186      480      229         0
```

```
> plot(cmdscale(Fairmont),
+ pch=16,xlab='',ylab='',xlimrrank=c(-250,350),ylim=c(-250,200))
> text(cmdscale(Fairmont)-15,lab=row.names(Fairmont))
```


Banff



Edmonton



Calgary



Lake Louise



Jasper



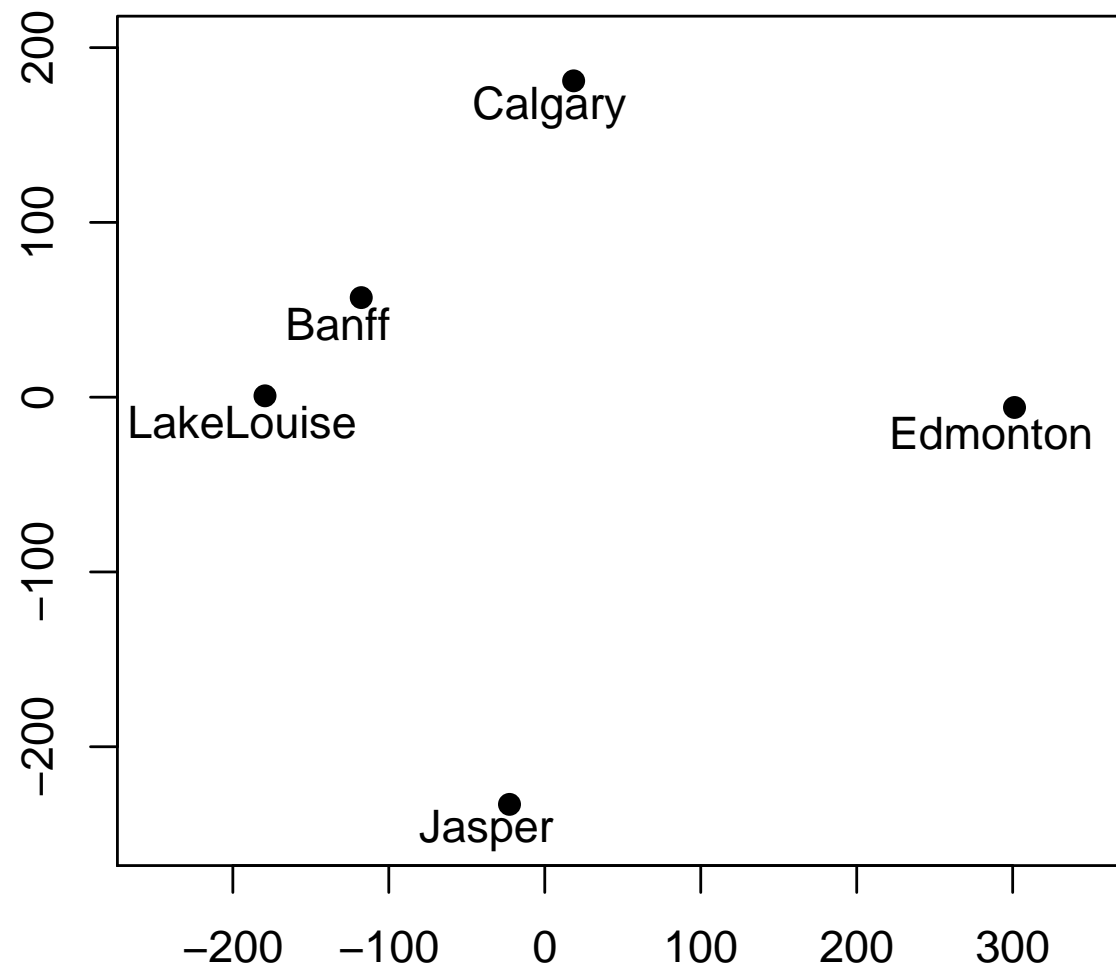
And now something different: Skoki lodge



Even the king goes there by foot



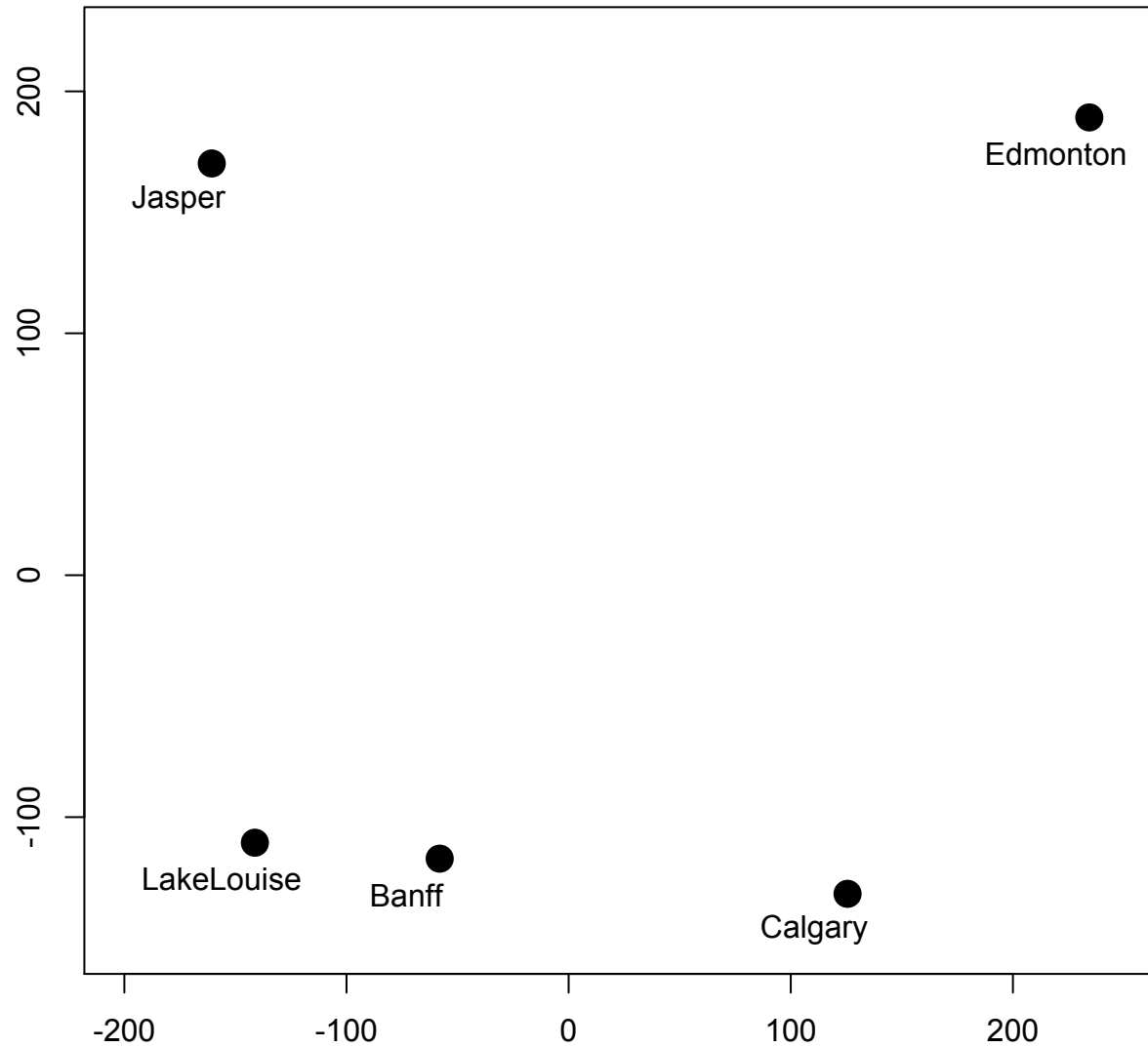
Is this Alberta?



This is Alberta



And now?



```
rbind(c(cos(pi*0.21),sin(pi*0.21)),c(sin(pi*0.21),-cos(pi*0.21)))
```

OK, let's try something closer...

Dojezdová vzdálenost (kilometr)		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Brno	1		296	77	307	216	168	296	146	96	169	337	93	208	176	240
Plzeň	2	296		369	200	137	208	181	213	388	462	81	217	92	469	100
Olomouc	3	77	370		236	290	139	370	135	63	98	411	167	282	104	314
Liberec	4	309	198	237		249	98	96	155	401	434	233	230	110	449	135
České Budějovice	5	217	137	290	250		253	239	258	309	383	218	138	151	389	183
Hradec Králové	6	167	209	140	97	253		190	24	206	238	240	112	116	245	143
Ústí nad Labem	7	298	181	371	96	238	190		196	390	463	122	219	93	470	87
Pardubice	8	146	214	135	154	193	24	196		201	234	246	90	121	240	149
Zlín	9	96	389	62	400	308	206	389	202		124	430	186	300	131	333
Ostrava	10	170	463	94	440	383	239	463	235	125		504	261	375	14	407
Karlovy Vary	11	337	82	410	234	218	241	121	246	429	502		258	127	509	105
Jihlava	12	93	218	167	229	138	113	218	90	186	259	259		130	266	162
Praha	13	209	91	282	109	150	116	92	121	301	375	128	130		382	31
Paskov	14	176	469	100	451	388	244	469	240	131	13	510	266	380		412
Kladno	15	240	99	313	135	181	143	86	148	332	406	105	161	31	412	

But rather better example first: Crimes

After interviewing respondents, we have the following table of **dissimilarities** between various crimes

0												
2	0											
15	13	0										
15	14	6	0									
15	14	3	3	0								
6	4	3	10	12	0							
4	2	14	14	15	13	0						
15	6	5	11	10	6	10	0					
15	10	12	2	2	12	14	7	0				
2	2	15	15	15	14	4	11	15	0			
14	12	2	11	11	6	15	11	12	14	0		
14	15	8	4	3	12	14	11	3	15	11	0	
9	13	6	14	9	5	10	11	7	13	7	11	0

"Murder" "Manslaugh" "Burglary" "Drugs" "Shoplift" "Drunkdrive" "Arson"
"Bodyharm" "Drunkdisord" "Rape" "Cartheft" "Trespass" "Taxes"

The story of multidimensional scaling

Can we summarize these data somehow?

Say, plot them as points on the plane?

Multidimensional scaling: we would like to represent data in a low (usually 2-) dimensional plane while preserving the dissimilarities (distances) between the data points as much as possible (minimizing the possible distortion caused by the reduction of dimensionality).

Alternative name: ordination

Dissimilarities \approx (more or less) distances

The prefix “dis-” means that similar objects would have low dissimilarity and objects not similar high - if it were other way round the name would rather be “similarity”

What constitutes a “distance”? Some desirable properties:

D1. *nonnegativity*: from A to B it is ≥ 0

D2. *symmetry*: from A to B = from B to A

D3. *identification*: from A to A it should be 0

These are usually the minimal properties which we require for “distance” or **dissimilarity**. A **similarity** has scale reversed: it satisfies 1. and 2. but instead of 3. it is required that

S. similarity of A and B is always \leq than similarity of A and A
- and thus also \leq than similarity of B and B

More stringent properties

Possible more stringent properties of dissimilarities are

D4. *triangle inequality*

$$\text{from A to C} \leq \text{from A to B} + \text{from B to C}$$

A dissimilarity satisfying D1-D4 is called a **pseudometric**. A pseudometric is a **metric**, if it also satisfies

D5. if from A to B is 0, then $A = B$

If a dissimilarity satisfies D5 and

D6. $\text{from A to C} \leq \max\{\text{from A to B}, \text{from B to C}\}$

(note that the latter implies triangle inequality, hence D5 and D6 imply a metric), it is called an **ultrametric**. We will see an example in hierarchical clustering, where it arises as a distance on a tree.

Aspects of dissimilarities

Sometimes we may like dissimilarities ranging from 0 to 1, sometimes from 0 to $+\infty$; sometimes we need to convert a similarity measure to a dissimilarity; useful transformations are $1 - d$, $1/d$, $1/(1 + d)$

Another way to transform a similarity c_{ij} into a dissimilarity is to consider the dissimilarity

$$d_{ij} = (c_{ii} - 2c_{ij} + c_{jj})^{1/2}$$

If we are calculating distances from the datapoints, we may want them standardized: all variables mean zero, standard deviation one.

Dissimilarities may be computed from variables, or given explicitly; they can be conveniently organized into a matrix - a symmetric one if the dissimilarities are so.

In R, it is a function: `dist()`

Also, in the widely used R package `cluster` it is `daisy()`

Examples: metrics

Euclidean metric:

$$d_2(A, B) = \sqrt{(A_1 - B_1)^2 + \cdots + (A_p - B_p)^2}$$

Manhattan (“Edmonton”, cityblock) metric

$$d_1(A, B) = |A_1 - B_1| + \cdots + |A_p - B_p|$$

Maximum metric

$$d_\infty(A, B) = \max\{|A_1 - B_1|, \dots, |A_p - B_p|\}$$

These are all special cases (limit for $p = \infty$) of the Minkowski distance

$$d_p(A, B) = (|A_1 - B_1|^p + \cdots + |A_p - B_p|^p)^{1/p}$$

Some dissimilarities aimed at other data types

For binary data, dissimilarities may be based on various association coefficients known from contingency tables, like Yule's $(ad - bc)/(ad + bc)$.

If we interpret contingency table as presence-absence matching, then we have things like $a + d/(a + b + c + d)$ (ordinary matching), $a/\sqrt{(a + b)(a + c)}$ (Ochiai index), or $2a/(2a + b + c)$ (Dice-Sorensen index), or $a/(a + b + c)$ (Jaccard index).

For ordinal data (rankings), dissimilarities may be based on ranks

Canberra metric
$$\frac{n}{n^*} \sum_i \frac{|x_i - y_i|}{|x_i| + |y_i|}$$

is aimed at counts, that is, nonnegative x_i and y_i

hence sometimes also $|x_i + y_i|$ or $x_i + y_i$ in the denominator

the sum is over the n^* terms that are *not* of the form 0/0

(if all have this form, then undefined)

Examples of dissimilarities aimed at 0-1 data

Hamming metric - handy for nominal (categorical) data:

1— proportion of i such that $x_i = y_i$

proportion means: the number of the i 's for which it is true
divided by the total number of the i 's

equivalent: proportion of i such that $x_i \neq y_i$

R function `dist()` has a distance “binary” defined also as

proportion of i such that $x_i \neq y_i$

but the proportion is only among those that are not both 0

Penrose's measure

There are measures of distances between groups (populations and samples), when the information is available only on means, standard deviations, and covariances.

Penrose's measure: suppose there are p variables and several groups: the mean of k -th variable in i -th group is μ_{ki} . If we know that all groups have variance v_k of k -th variable, then

$$P_{ij} = \sum_{k=1}^p \frac{(\mu_{ki} - \mu_{kj})^2}{pv_k}$$

Does not include covariances: may overemphasize correlated variables.

Mahalanobis distance

Euclidean distance after normalizing the data

If we know (or estimate) the variance-covariance matrix Σ , we form its inverse Σ^{-1} , whose elements are σ^{rs} . Then

$$D_{ij} = \sum_{r=1}^p \sum_{s=1}^p (\mu_{ri} - \mu_{rj}) \sigma^{rs} (\mu_{si} - \mu_{sj}) = (\mu_i - \mu_j)^T \Sigma^{-1} (\mu_i - \mu_j)$$

where μ_i is the column vector with components μ_{ki} .

Distances based on proportions

If p_k , q_k are proportions of the k -th attribute in the first and second group respectively, then we may take

$$d = \sum_k \frac{1}{2} |p_k - q_k| \quad \text{or} \quad d = 1 - \frac{\sum_k p_k q_k}{\left(\sum_k p_k^2 \sum_k q_k^2 \right)^{1/2}}$$

(we typically want them to range from 0 to 1)

Classical multidimensional scaling: Euclidean distances

Classical multidimensional scaling is derived under assumption that the distances are **Euclidean** - that is, they arose as the Euclidean distances among points in some high-dimensional space.

The crucial property that distinguishes Euclidean metric from others is the relationship to the inner product. If the dissimilarities d_{ij} between n objects are Euclidean, then there is a collection of points, vectors $\mathbf{y}_i \in \mathbb{R}^p$ for some p (not greater than $n - 1$) such that

$$d_{ij}^2 = (\mathbf{y}_i - \mathbf{y}_j)^\top (\mathbf{y}_i - \mathbf{y}_j) = \mathbf{y}_i^\top \mathbf{y}_i + \mathbf{y}_j^\top \mathbf{y}_j - 2\mathbf{y}_i^\top \mathbf{y}_j = \|\mathbf{y}_i\|^2 + \|\mathbf{y}_j\|^2 - 2\mathbf{y}_i^\top \mathbf{y}_j$$

Given the d_{ij} 's, let \mathbf{A} be the matrix with the elements $-\frac{1}{2}d_{ij}^2$. If the dissimilarities are Euclidean, this matrix must be symmetric, have diagonal elements zero, and off-diagonal elements nonzero. As the Euclidean distances are invariant with respect to translations and rotations, we can choose without loss of generality the coordinate

system so that $\mathbf{0} = \bar{\mathbf{y}}$, that is, $\mathbf{0} = \sum_{i=1}^n \mathbf{y}_i$.

Recovering inner product

Now, given the matrix **A**, we construct the matrix **B** consisting of elements

$$-\frac{1}{2}d_{ij}^2 + \frac{1}{2n} \sum_i d_{ij}^2 + \frac{1}{2n} \sum_j d_{ij}^2 - \frac{1}{2n^2} \sum_{i,j} d_{ij}^2$$

This matrix is always symmetric if the dissimilarities are symmetric; if they are also Euclidean, the elements of **B** are equal to $\mathbf{y}_i^T \mathbf{y}_j$

Thus, **B** “reconstructs” the inner products of the \mathbf{y}_i ’s - and in particular, if \mathbf{y}_i^T are lines of a matrix **Y**, then $\mathbf{B} = \mathbf{Y}\mathbf{Y}^T$

Conversely, if **B** is a symmetric and nonnegative definite $n \times n$ matrix, then it defines an inner product among some collection of \mathbf{y}_i , $i = 1, 2, \dots, n$ - which in turn yields squared distances among the objects corresponding to those \mathbf{y}_i , as given above

The proof

For all i and j we have

$$d_{ij}^2 = d_{ji}^2 = (\mathbf{y}_i - \mathbf{y}_j)^\top (\mathbf{y}_i - \mathbf{y}_j) = \|\mathbf{y}_i\|^2 + \|\mathbf{y}_j\|^2 - 2\mathbf{y}_i^\top \mathbf{y}_j$$

Using the fact that $\sum_i \mathbf{y}_i = \mathbf{0}$, we obtain

$$\frac{1}{n} \sum_i d_{ij}^2 = \frac{1}{n} \sum_i \|\mathbf{y}_i\|^2 + \|\mathbf{y}_j\|^2 \quad \text{and} \quad \frac{1}{n} \sum_j d_{ij}^2 = \|\mathbf{y}_i\|^2 + \frac{1}{n} \sum_j \|\mathbf{y}_j\|^2$$

$$\text{and also} \quad \frac{1}{n^2} \sum_{i,j} d_{ij}^2 = \frac{1}{n} \sum_j \frac{1}{n} \sum_i d_{ij}^2 = \frac{1}{n} \sum_i \|\mathbf{y}_i\|^2 + \frac{1}{n} \sum_j \|\mathbf{y}_j\|^2$$

which yields then

$$d_{ij}^2 - \frac{1}{n} \sum_i d_{ij}^2 - \frac{1}{n} \sum_j d_{ij}^2 + \frac{1}{n^2} \sum_{i,j} d_{ij}^2 = -2\mathbf{y}_i^\top \mathbf{y}_j$$

and subsequently the result. For the converse, just note that

$$\mathbf{B} = \mathbf{U}\mathbf{L}\mathbf{U}^\top = \mathbf{U}\mathbf{L}^{1/2}\mathbf{L}^{1/2}\mathbf{U}^\top$$

yielding the desired $\mathbf{Y} = \mathbf{U}\mathbf{L}^{1/2}$

Note that $\mathbf{B} = \mathbf{H}\mathbf{A}\mathbf{H}$, where $\mathbf{H} = \left(\mathbf{I} - \frac{1}{n} \mathbf{1}\mathbf{1}^\top \right)$

Classical multidimensional scaling

So, it is assumed that the distances are *Euclidean, at least approximately*: they arise, *possibly with some error*, as the Euclidean distances among some points in a Euclidean space. Out of these dissimilarities, the matrices **A** and **B** are constructed as above; this matrices is symmetric as long as the dissimilarities are symmetric

Let $\mathbf{U}\mathbf{L}\mathbf{U}^T$ be the eigenvalue decomposition of **B**. If the distances are Euclidean, then **B** is nonnegative definite, its eigenvalues are all nonnegative, and one can construct its approximation of rank k , a symmetric nonnegative definite matrix $\mathbf{B}_k = \mathbf{U}\mathbf{L}_k\mathbf{U}^T$, where \mathbf{L}_k is constructed from **L** by retaining only k largest eigenvalues (and changing the rest of the diagonal to zero).

In the approximate case, when there may be also negative eigenvalues, a possibility is to increase all eigenvalues by a constant making them nonnegative; another possibility is to use only the k largest eigenvalues, if they are positive

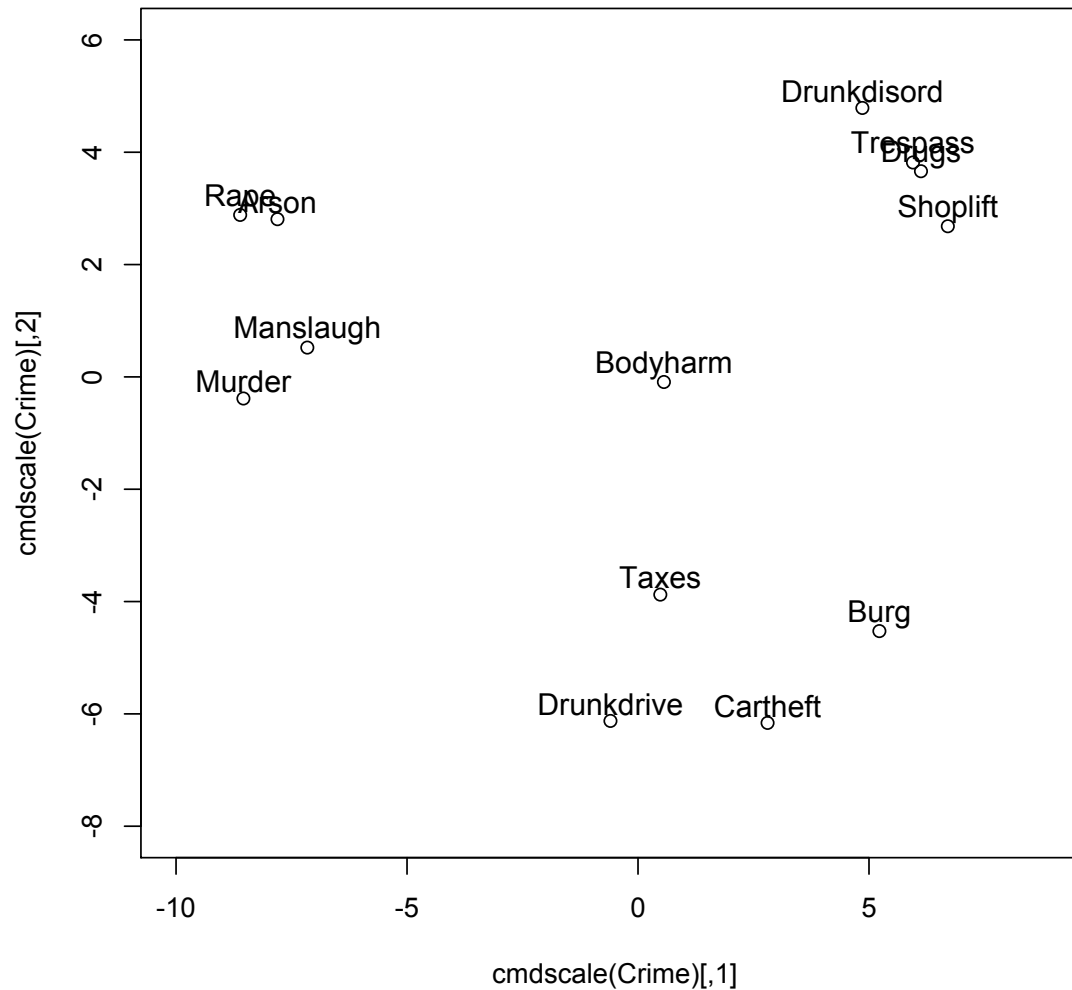
The eigenvalue decomposition $\mathbf{U}\mathbf{L}_k\mathbf{U}^T$ of \mathbf{B}_k then gives the coordinates of the new objects in the desired k -dimensional representation: $\mathbf{Y}_k = \mathbf{U}\mathbf{L}_k^{1/2}$

Duality to principal components

If the dissimilarities d_{ij} arise as the Euclidean distances between the lines of a matrix \mathbf{Y} - which can be, due to the translation and rotation invariance of the distances, considered without loss of generality with centered columns, that is, the columnwise sums of \mathbf{Y} are all zero - then the k -dimensional transformation amounts to obtaining the first k principal components of \mathbf{Y} (without scaling to the correlation matrix)

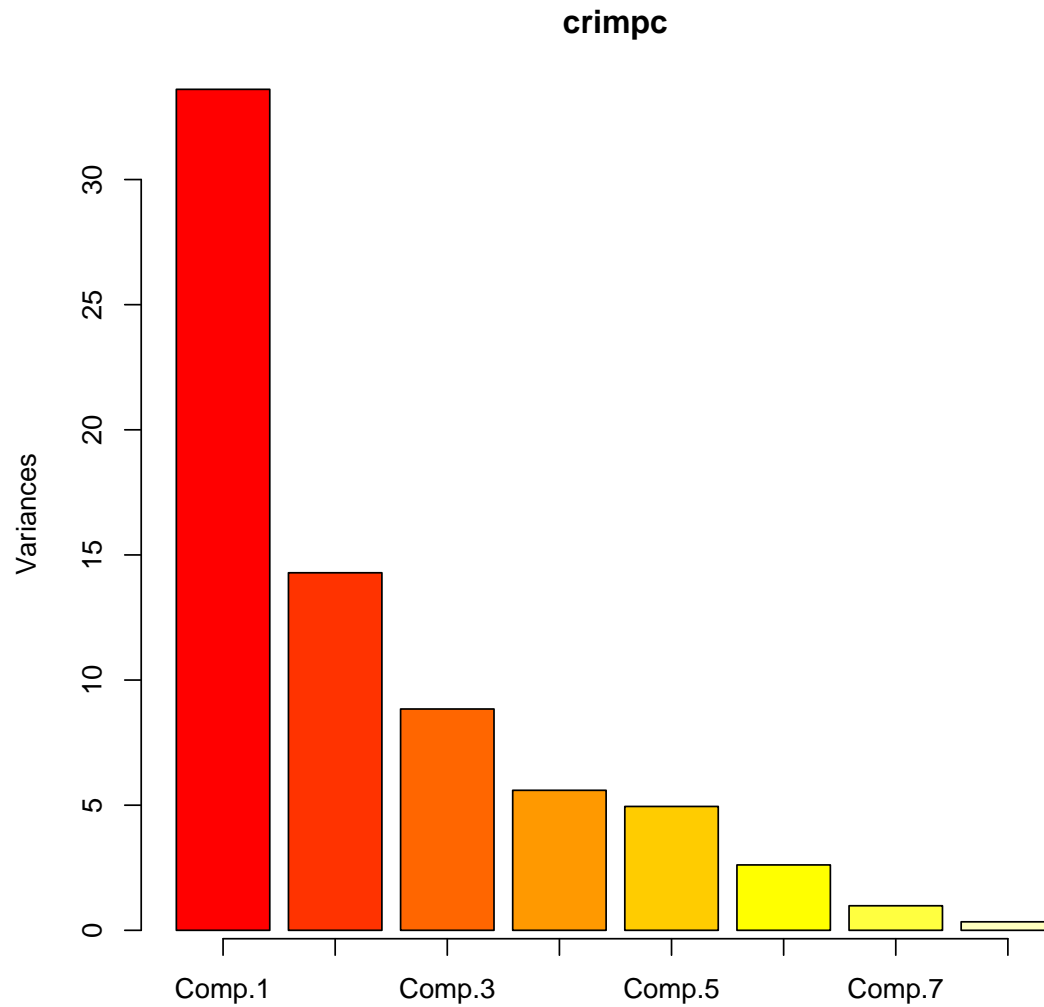
The classical multidimensional scaling can be thus seen as equivalent, or also dual, to obtaining first k (most often $k = 2$, in which this amounts to plotting) principal components

Classical multidimensional scaling



```
> plot(cmdscale(Crime),xlim=c(-10,9),ylim=c(-8,6))  
> text(t(t(cmdscale(Crime))+c(0,0.3)),labels=labels(Crime),cex=1.1)
```

How distorted?



0.6725267 % of variance explained by the first two components

Stress

If the distances are Euclidean, then the new distances, the distances between the new objects constructed by the algorithm of classical multidimensional scaling, are the ones minimizing, *among all linear transformations of the original objects*,

$$\sum_{i,j} (d_{ij}^2 - \hat{d}_{ij}^2) = \sum_{i \neq j} (d_{ij}^2 - \hat{d}_{ij}^2)$$

or equivalently

$$\frac{\sum_{i,j} (d_{ij}^2 - \hat{d}_{ij}^2)}{\sum_{i,j} d_{ij}^2} = \frac{\sum_{i \neq j} (d_{ij}^2 - \hat{d}_{ij}^2)}{\sum_{i \neq j} d_{ij}^2}$$

where d_{ij} are the original and \hat{d}_{ij} the new, transformed distances

The quantities above can be considered as a measure of distortion - **stress**; nonlinear versions of multidimensional scaling optimize (numerically) different stresses

Nonlinear versions

Sammon mapping. The stress is (note that no off-diagonal zero elements allowed)

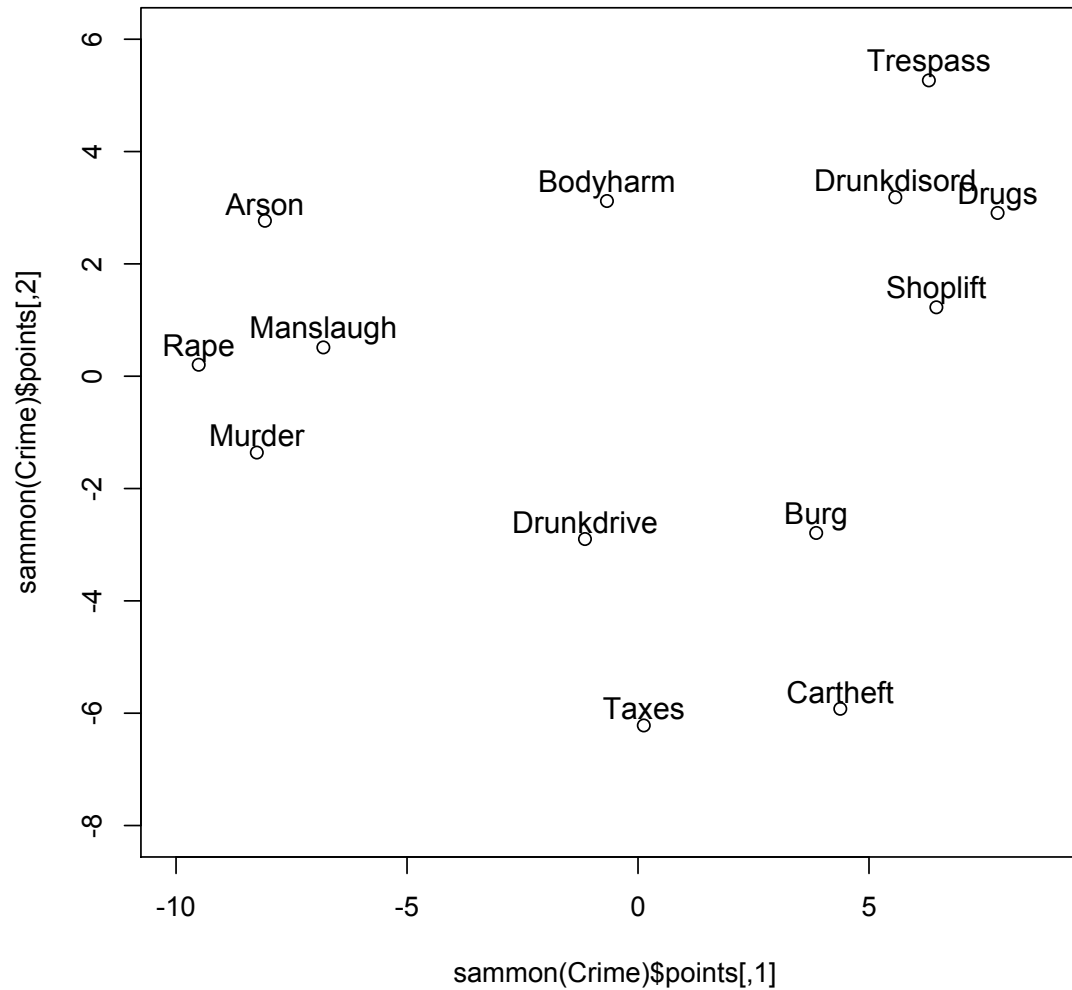
$$\frac{1}{\sum_{i \neq j} d_{ij}} \sum_{i \neq j} \frac{(d_{ij}^2 - \hat{d}_{ij}^2)^2}{d_{ij}}$$

iso-MDS aka **Kruskal nonmetric** MDS: if the original distances are Euclidean, then the (square of) stress is

$$\sum_{i \neq j} \frac{(d_{ij} - \vartheta(\hat{d}_{ij}))^2}{\sum_{i,j} d_{ij}^2}$$

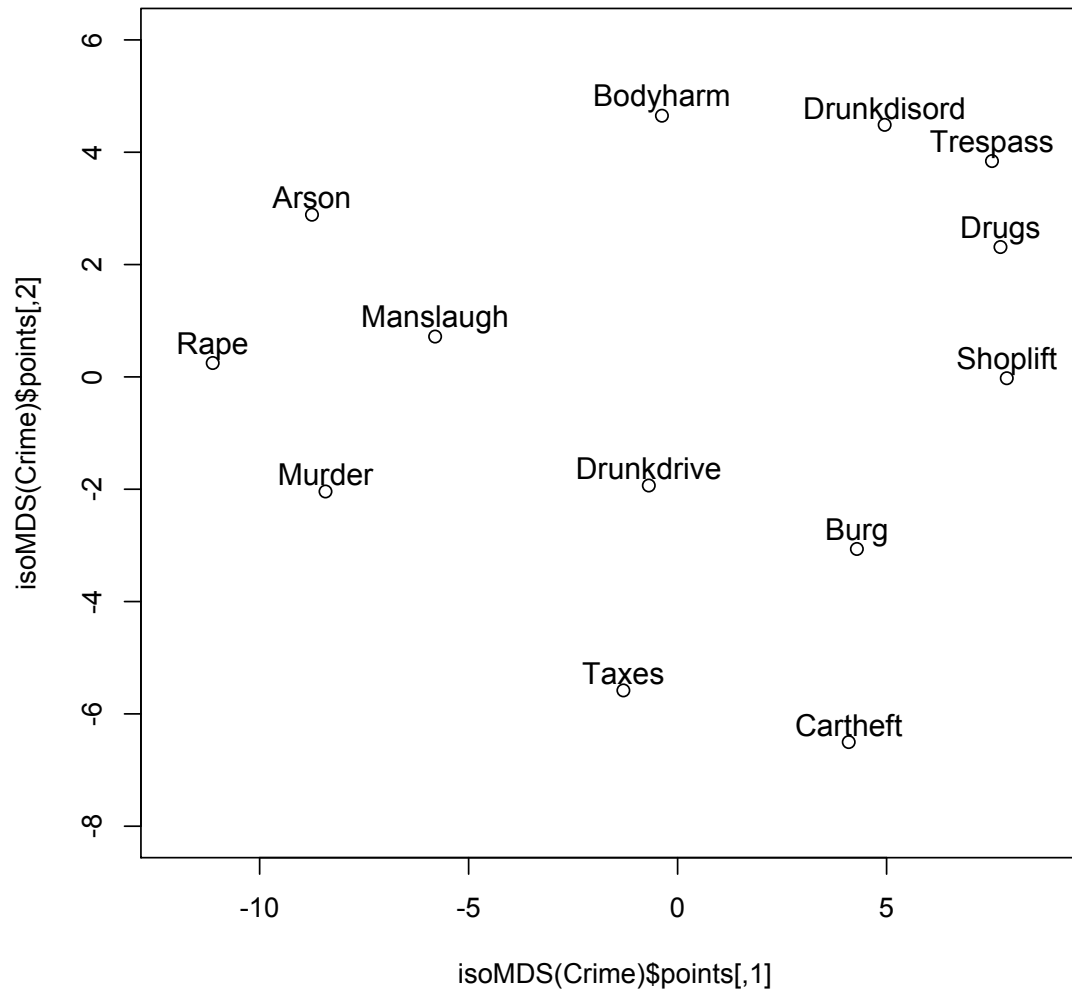
where ϑ is an increasing transformation. The algorithm minimizes over all possible \hat{d}_{ij} as well as ϑ . Idea: to choose a new configuration so that the *ordering* of the distances is as much preserved as possible.

Sammon



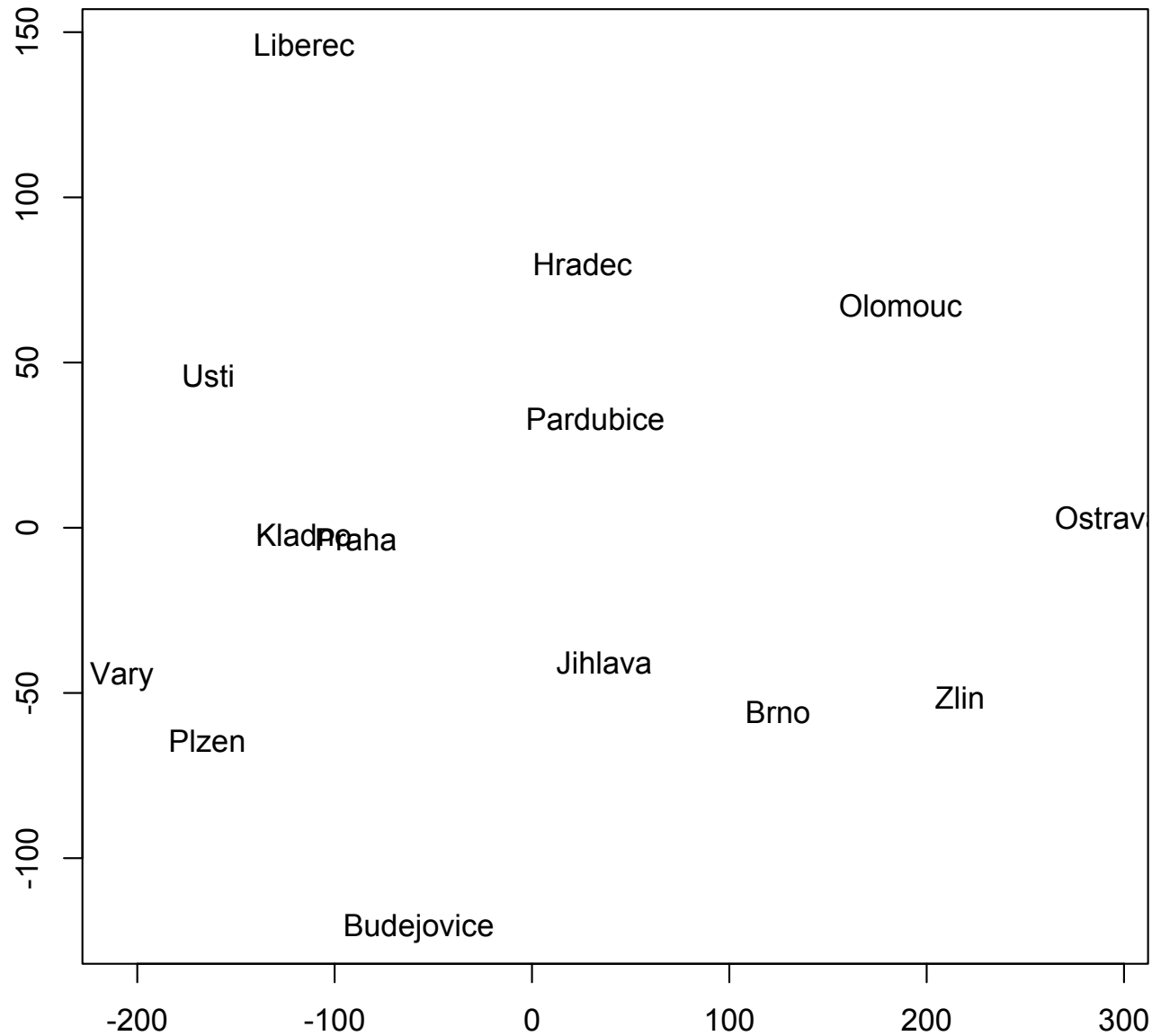
```
> library(MASS)
> plot(sammon(Crime)$points,xlim=c(-10,9),ylim=c(-8,6))
> text(t(t(sammon(Crime)$points)+c(0,0.3)),labels=labels(Crime),cex=1.1)
```

Kruskal nonmetric



```
> library(MASS)
> plot(isoMDS(Crime)$points,xlim=c(-12,9),ylim=c(-8,6))
> text(t(t(isoMDS(Crime)$points)+c(0,0.3)),labels=labels(Crime),cex=1.1)
```

And Czech cities? Not a big deal (Nic moc)



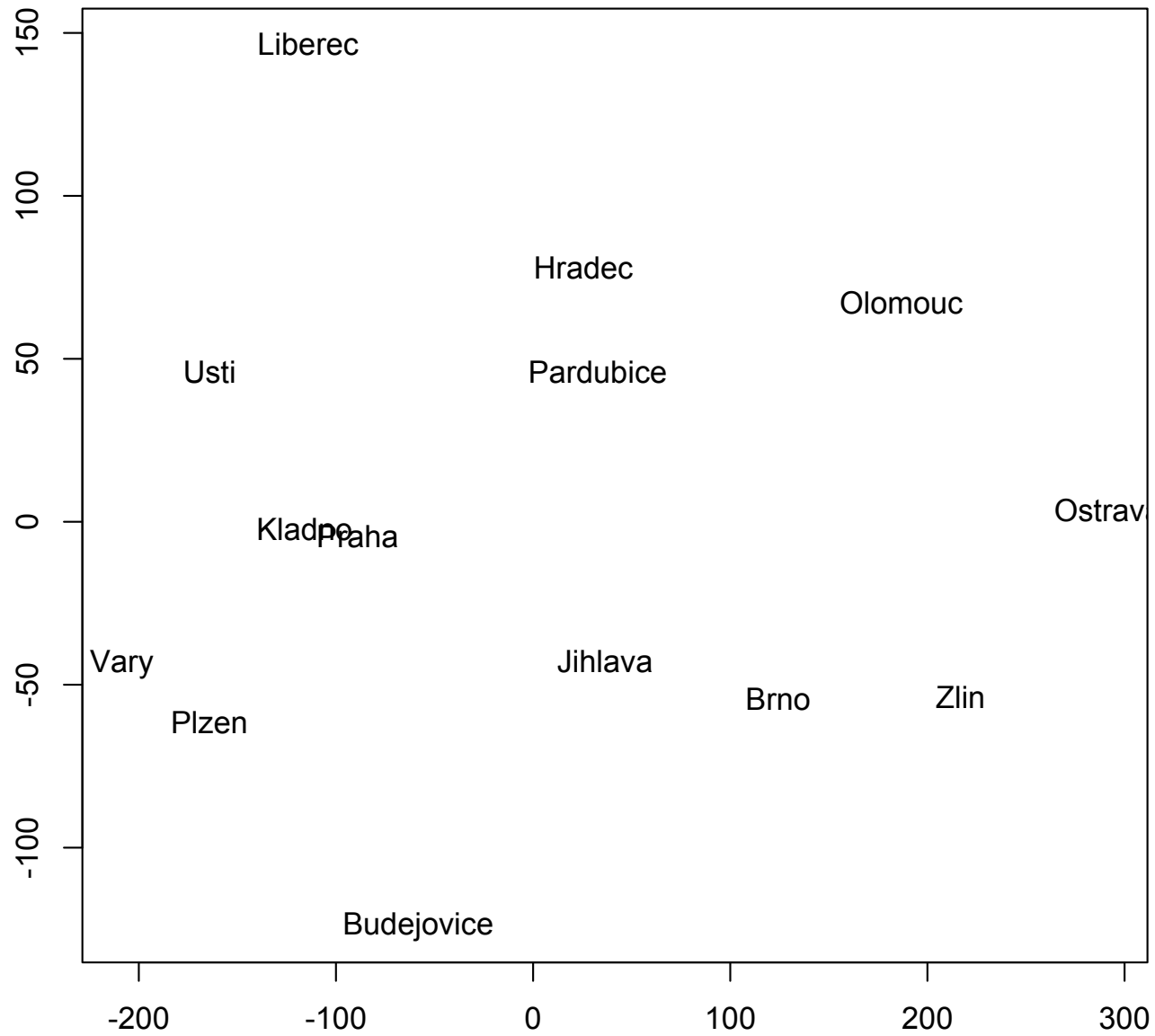
Better data?

More thorough examination shows that the distance matrix is not symmetric... (???)

```
> Czechia=(Czechiaorg+t(Czechiaorg))/2
> Czech.cl=cmdscale(Czechia)
> plot(Czech.cl,type="n",xlab="",ylab="")
> text(Czech.cl,labels=rownames(Czech.cl))
```

	Brno	Plzen	Olomouc	Liberec	Budejovice	Hradec	Usti	Pardubice	Zlin	Ostrava	Vary	Jihlava	Praha	Kladno
Brno	0.0	296.0	77.0	308.0	216.5	167.5	297.0	146.0	96.0	169.5	337.0	93.0	208.5	240.0
Plzen	296.0	0.0	369.5	199.0	137.0	208.5	181.0	213.5	388.5	462.5	81.5	217.5	91.5	99.5
Olomouc	77.0	369.5	0.0	236.5	290.0	139.5	370.5	135.0	62.5	96.0	410.5	167.0	282.0	313.5
Liberec	308.0	199.0	236.5	0.0	249.5	97.5	96.0	154.5	400.5	437.0	233.5	229.5	109.5	135.0
Budejovice	216.5	137.0	290.0	249.5	0.0	253.0	238.5	225.5	308.5	383.0	218.0	138.0	150.5	182.0
Hradec	167.5	208.5	139.5	97.5	253.0	0.0	190.0	24.0	206.0	238.5	240.5	112.5	116.0	143.0
Usti	297.0	181.0	370.5	96.0	238.5	190.0	0.0	196.0	389.5	463.0	121.5	218.5	92.5	86.5
Pardubice	146.0	213.5	135.0	154.5	225.5	24.0	196.0	0.0	201.5	234.5	246.0	90.0	121.0	148.5
Zlin	96.0	388.5	62.5	400.5	308.5	206.0	389.5	201.5	0.0	124.5	429.5	186.0	300.5	332.5
Ostrava	169.5	462.5	96.0	437.0	383.0	238.5	463.0	234.5	124.5	0.0	503.0	260.0	375.0	406.5
Vary	337.0	81.5	410.5	233.5	218.0	240.5	121.5	246.0	429.5	503.0	0.0	258.5	127.5	105.0
Jihlava	93.0	217.5	167.0	229.5	138.0	112.5	218.5	90.0	186.0	260.0	258.5	0.0	130.0	161.5
Praha	208.5	91.5	282.0	109.5	150.5	116.0	92.5	121.0	300.5	375.0	127.5	130.0	0.0	31.0
Kladno	240.0	99.5	313.5	135.0	182.0	143.0	86.5	148.5	332.5	406.5	105.0	161.5	31.0	0.0

Not a big deal either



Hm...

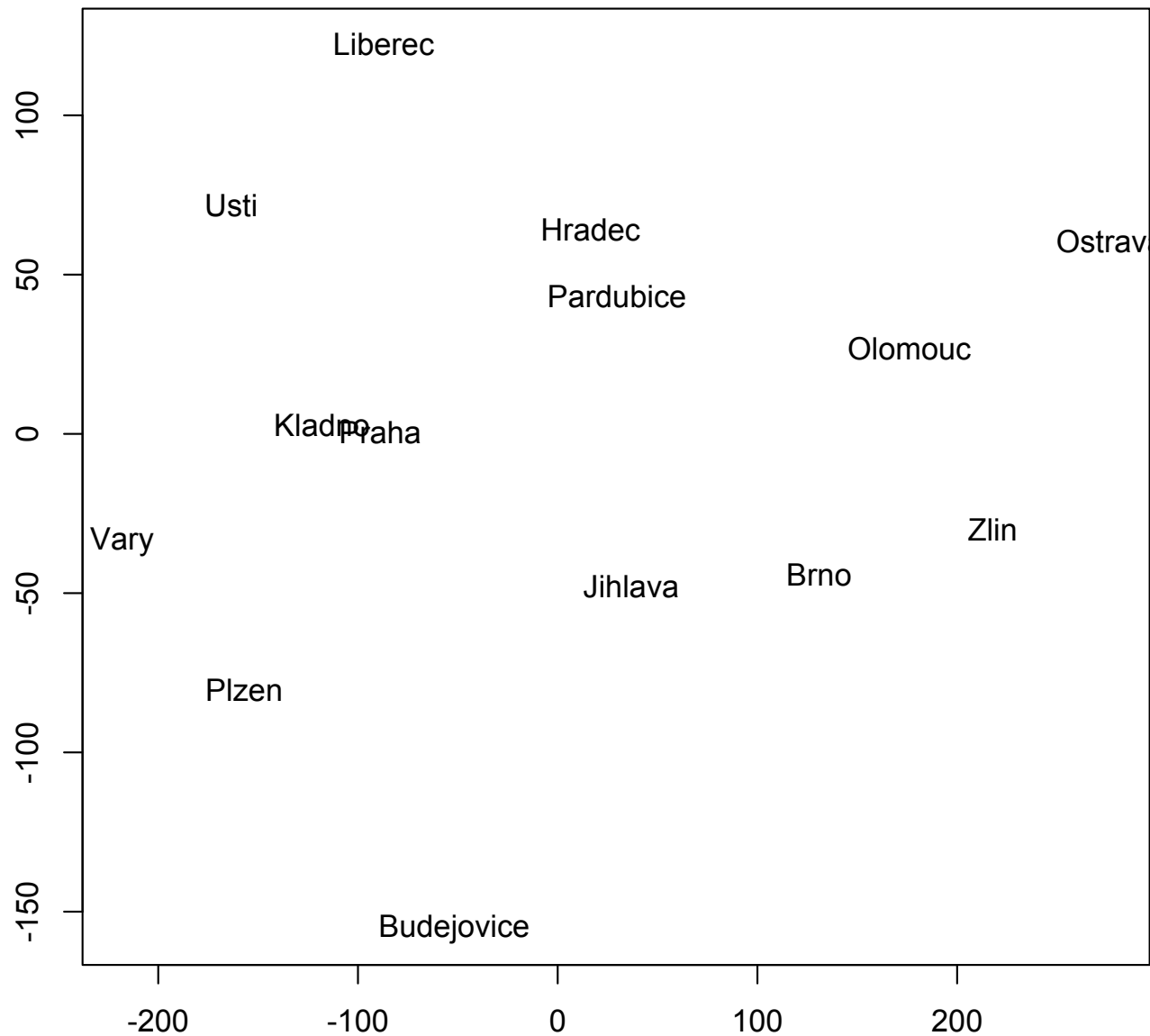
That Ostrava is maybe really far away from everything...

Brno	Plzen	Olomouc	Liberec	Budejovice
2652.0	2945.5	2949.5	2886.0	2990.0
Hradec	Usti	Pardubice	Zlin	Ostrava
2136.5	2940.5	2136.0	3426.0	4153.0
Vary	Jihlava	Praha	Kladno	
3312.0	2262.0	2135.5	2384.5	

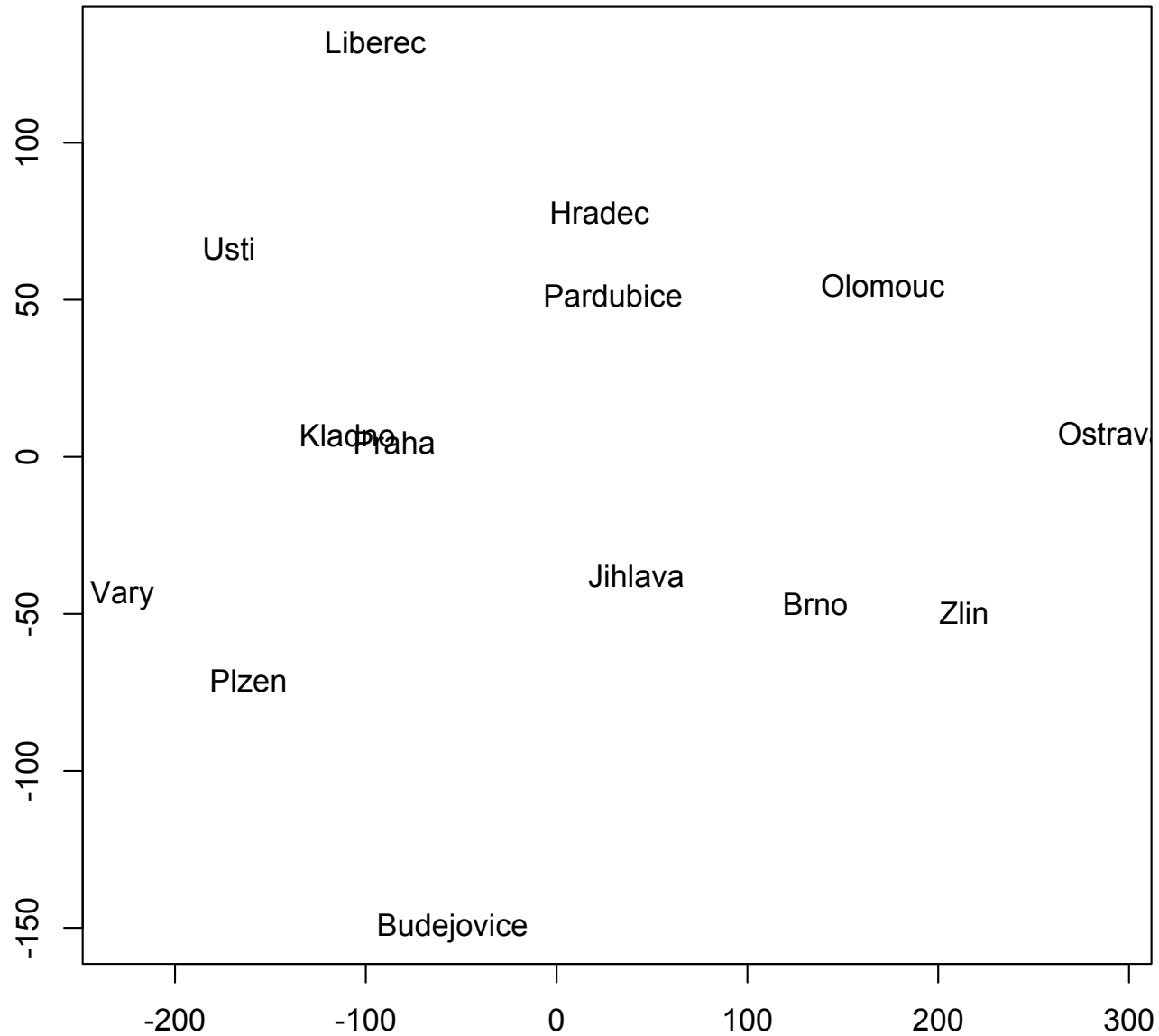
So how about...

```
> Czech.sam=sammon(Czechia)
Initial stress          : 0.01890
stress after 10 iters: 0.00528, magic = 0.500
stress after 20 iters: 0.00525, magic = 0.500
> plot(Czech.sam$points,type="n",xlab="",ylab="")
> text(Czech.sam$points,labels=rownames(Czech.sam$points))
```

Bingo? Perhaps after a bit of rotation...



...but not with Kruskal



Graves with pottery

In an archaeological study there are six graves containing five types of pottery between them

> Graves

	1	2	3	4	5
A	0	0	1	1	0
B	1	1	0	0	1
C	0	1	1	1	1
D	0	0	1	1	0
E	1	0	0	0	1
F	1	0	1	1	1

It is desired to order the graves chronologically based on the similarity/dissimilarity of the pottery found in them.

We are going to look at the dissimilarities of the rows, x_i , of the matrix shown above; note that the distance of lines A and D will be inevitably 0 in any reasonable case

Relevant dissimilarities

The Hamming distance is in this case equal to the $d_1(x_j, x_j)/5$, the ℓ^1 (“Manhattan”) distance divided by $p = 5$; the following shows the result for the ℓ^1 distance

```
> dist(Graves,method="manhattan",diag=TRUE)
```

```
  A B C D E F
```

```
A 0
```

```
B 5 0
```

```
C 2 3 0
```

```
D 0 5 2 0
```

```
E 4 1 4 4 0
```

```
F 2 3 2 2 2 0
```

Transforming similarities to dissimilarities

The book of Mardia, Kent, and Bibby champions using an ordinary matching coefficient $c(x_i, x_j)$, which counts the number of cases when both vectors are either equal to 0 or to 1, and divides them by $p = 5$: the result is

$$c(x_i, x_j) = 1 - d_1(x_i, x_j)/5.$$

In terms of the book of Mardia, Kent, and Bibby, $c(x_i, x_j)$ is a “similarity” which they convert into an euclidean dissimilarity by the transformation

$$d(x_i, x_j) = (c(x_i, x_i) - 2c(x_i, x_j) + c(x_j, x_j))^{1/2}$$

which in the present case yields

$$d(x_i, x_j) = (2 - 2c(x_i, x_j))^{1/2} = \sqrt{2d_1(x_i, x_j)/5}$$

```
> graveu <- sqrt(2*dist(Graves,method="manhattan",diag=TRUE)/5)
> eigen((diag(6)-1/6) %*% as.matrix(-graveu^2/2) %*% (diag(6)-1/6))
eigen() decomposition
$values
[1] 1.747708e+00 5.864466e-01 3.518536e-01
[3] 4.732485e-02 0.000000e+00 -9.685690e-17
...
```

Seriation: scaling into dimension one

We perform now classical multidimensional scaling into dimension $k = 1$, to obtain a possible time order of the graves

```
> gramds <- cmdscale(graveu,k=1)
> gramds
      [,1]
A  0.600019876
B -0.765783233
C  0.194649330
D  0.600019876
E -0.635067161
F  0.006161312
```

This suggests an order (A and D), C, F, E, B - or the reverse one; note that time orientation cannot be determined from the method

Seriation without euclidization

Of course, we could apply the algorithm directly to the ℓ^1 distance
- as we are scaling into dimension one, we need just the maximal eigenvalue to be positive

```
> cmdscale(dist(Graves,method="manhattan",diag=TRUE)/5,k=1)
      [,1]
```

```
A  0.414792257
```

```
B -0.566671301
```

```
C  0.136621560
```

```
D  0.414792257
```

```
E -0.408900852
```

```
F  0.009366079
```

```
> cmdscale(dist(Graves,method="manhattan",diag=TRUE),k=1)
      [,1]
```

```
A  2.0739613
```

```
B -2.8333565
```

```
C  0.6831078
```

```
D  2.0739613
```

```
E -2.0445043
```

```
F  0.0468304
```

The resulting orders are the same: (A and D), C, F, E, B

Something else

Finally, note that the application of the nonlinear methods is hampered by the fact that lines A and D have zero distance. Nonetheless, after omitting the line A, we obtain

```
> sammon(dist(Graves[-1,],method="manhattan",diag=TRUE)/5,k=1)
```

```
...
```

```
      [,1]
```

```
B  0.49885561
```

```
C -0.27272060
```

```
D -0.53060611
```

```
E  0.34010348
```

```
F -0.03563238
```

which yields the same order: D (and A), C, F, E, B

Something else

Only the Kruskal method yields somewhat different result - but note that the scores are very close there, suggesting that while the groups (A, D, C, F) and (B, E) may be really apart, the ordering within the groups may be a bit questionable

```
> isoMDS(dist(Graves[-1,],method="manhattan",diag=TRUE)/5,k=1)
...
      [,1]
B  0.5048145
C -0.3365613
D -0.3365814
E  0.5048155
F -0.3364872
...
```

Finding groups in data: cluster analysis

Two main approaches

Cluster analysis finds groups in the data - groups are formed by those items (datapoints) that have small distances (dissimilarities)

Dissimilarities - we have seen many of them, some are metrics ($d_{ij} \leq d_{ik} + d_{kj}$), some are more general; hierarchical clustering (in fact) involves *ultrametrics* ($d_{ij} \leq \max\{d_{ik}, d_{kj}\}$ - tree distance, see below).

The objective is to divide items into k groups so that the members of the same group are more alike than members of the other group: *clusters*.

The number k may be preassigned: **partitioning methods**

or not preassigned: **hierarchical clustering**.

A lot of clustering methods (a majority?) are based on distances between the items; so cluster analysis is often viewed as a distance-base method.

Methods: computational (rather than “statistical”).

R

Earlier packages:

`kmeans`: classical k-means routine, base R

`hclust`: some hierarchical clustering, but also still graphical routines in use, for instance more customizable plotting of dendrograms via `as.dendrogram(as.hclust())`

`plclust`: *deprecated*, use `pltree` (or `plot`) from the package `cluster`

Benchmark:

`cluster`, functions `agnes` (AGglomerative NESTing, agglomerative hierarchical clustering), `clara` (Clustering LARge Applications, partitioning method), `daisy` (Dissimilarity matrix calculation), `diana` (DIVisive ANALysis clustering, divisive hierarchical clustering), `fanny`, (Fuzzy ANALysis clustering), `mona` (MONothetic clustering of binary variables, hierarchical clustering), `pam` (Partitioning Around Medoids, partitioning method)

Kaufman, L. and Rousseeuw, P. J. (1990): Finding Groups in Data: An Introduction to Cluster Analysis. Wiley, New York.

Partitioning methods: k-means

The number of clusters, k , is given in advance. The clusters themselves are determined by minimizing a criterion.

k-means: minimize the sum of squared distances, within clusters, from the centers of clusters - which are subject to minimization too

The minimized criterion is the minimum

over the selection of clusters and over the selection of \mathbf{m}_i 's,

$$\sum_{i=1}^k \sum_{j \in C_i} \|\mathbf{x}_{ij} - \mathbf{m}_i\|^2$$

which is equal to the minimum over the selection of clusters, of

$$\sum_{i=1}^k \sum_{j \in C_i} \|\mathbf{x}_{ij} - \bar{\mathbf{x}}_i\|^2$$

where $\bar{\mathbf{x}}_i$ is the mean of i -th cluster C_i .

We are looking for that partition to clusters C_1, C_2, \dots, C_k that makes these sums minimal

Partitioning methods: k-medoids

The number of clusters, k , is given in advance. The cluster themselves are determined by minimizing a criterion.

k-medoids: the sum of distances, within clusters, from the centers of clusters - which are subject of minimization too; here it is also required that the center of the group is a data point itself (then general dissimilarities may be used)

The minimized criterion is the minimum, over the selection of clusters and over the selection of \mathbf{m}_i 's,

$$\sum_{i=1}^k \sum_{j \in C_i} \|\mathbf{x}_{ij} - \mathbf{m}_i\|$$

In analogy to k-means, we could take \mathbf{m}_i 's to be the spatial medians of the i -th cluster - we only have the additional requirement that *they should be one of the datapoints*, which makes computation easier

Let us try it

```
> kmeal=kmeans(trackmen,3)
```

```
> kmeal
```

```
...
```

Clustering vector:

argentin	australi	austria	belgium	bermuda	brazil	burma	canada
3	1	3	1	3	1	3	1
chile	china	columbia	cookis	costa	czech	denmark	domrep
1	1	1	2	3	1	1	2
finland	france	gdr	frg	gbni	greece	guatemal	hungary
1	1	1	1	1	1	3	1
india	indonesi	ireland	israel	italy	japan	kenya	korea
1	2	1	3	1	1	1	3
dprkorea	luxembou	malaysia	mauritiu	mexico	netherla	nz	norway
1	3	2	2	1	1	1	1
png	philippi	poland	portugal	rumania	singapor	spain	sweden
2	3	1	1	1	2	1	1
switzerl	taipei	thailand	turkey	usa	ussr	wsamoa	
1	3	2	1	1	1	2	

```
...
```

Is it not just clustering along the marathon records?

We could check it out

```
> kmea2=kmeans(trackmen[,8],3)
> kmea2
...
Clustering vector:
 [1] 1 3 1 3 1 3 1 3 3 3 3 2 1 3 3 2 3 3 3 3 3 1 3 3 2 3 1
[29] 3 3 3 1 3 1 2 2 3 3 3 3 2 1 3 3 3 2 3 3 3 1 2 3 3 3 2
...
> as.vector(kmea1$cluster)
 [1] 3 1 3 1 3 1 3 1 1 1 1 2 3 1 1 2 1 1 1 1 1 3 1 1 2 1 3
[29] 1 1 1 3 1 3 2 2 1 1 1 1 2 3 1 1 1 2 1 1 1 3 2 1 1 1 2

Are they not the same? Indeed

> c(3,2,1)[kmea2$cluster]-as.vector(kmea1$cluster)
 [1] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[29] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

So, scaling once again

```
> kmea3=kmeans(scale(trackmen),3)
```

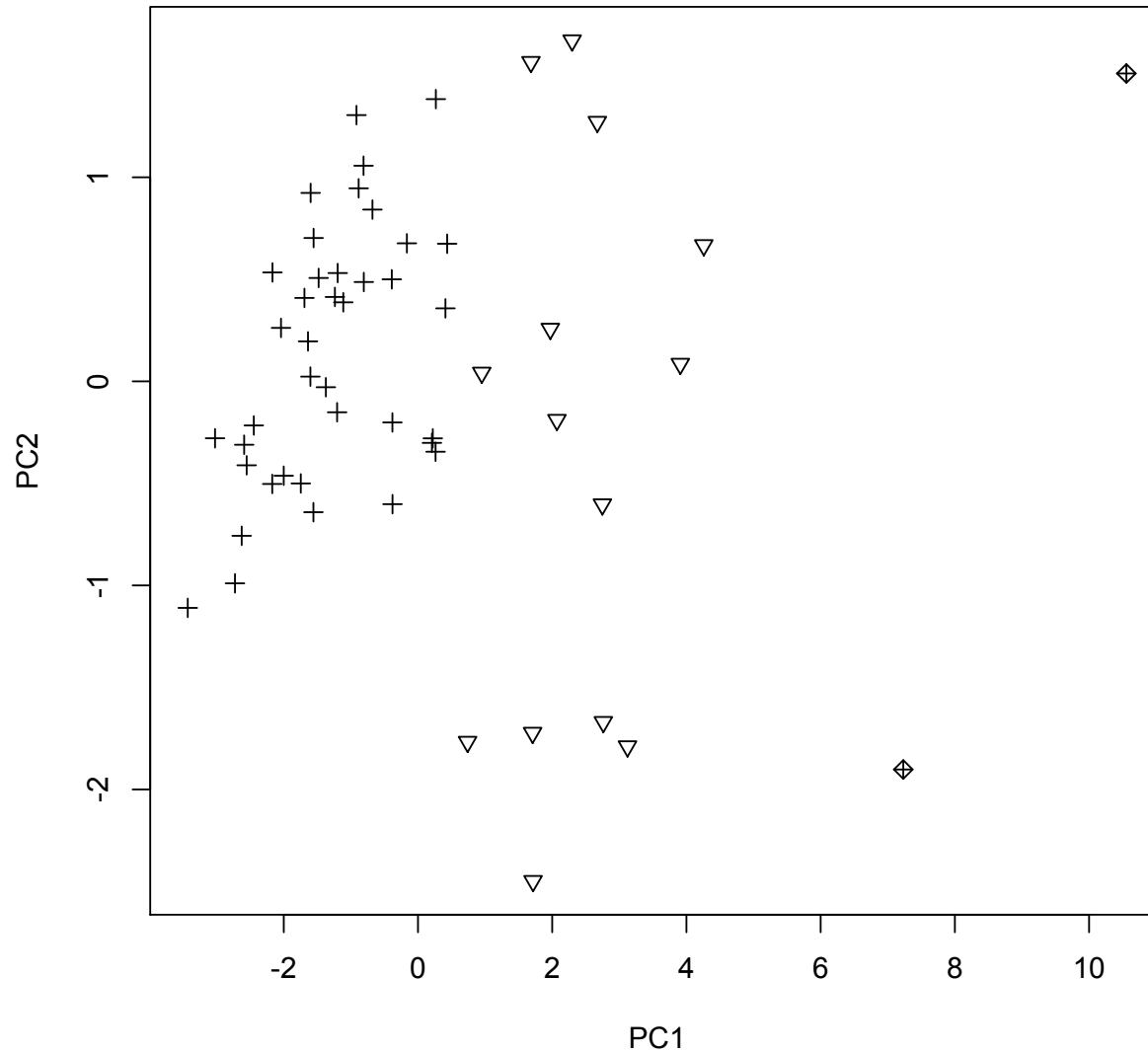
```
> kmea3
```

```
...
```

```
Clustering vector:
```

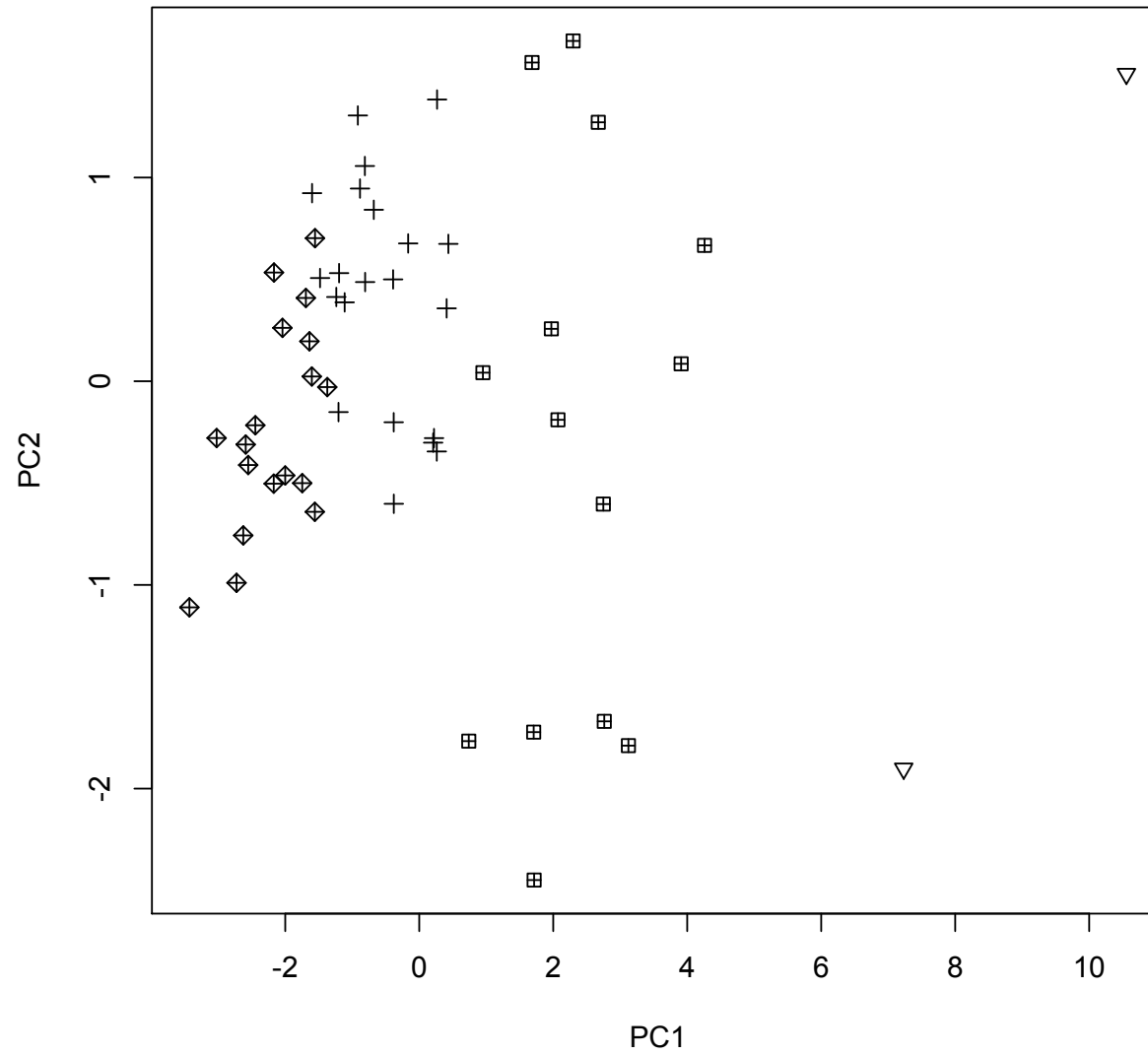
argentin	australi	austria	belgium	bermuda	brazil	burma
1	1	1	1	2	1	2
canada	chile	china	columbia	cookis	costa	czech
1	1	1	1	3	2	1
denmark	domrep	finland	france	gdr	frg	gbni
1	2	1	1	1	1	1
greece	guatemal	hungary	india	indonesi	ireland	israel
1	2	1	1	2	1	1
italy	japan	kenya	korea	dprkorea	luxembou	malaysia
1	1	1	1	2	1	2
mauritiu	mexico	netherla	nz	norway	png	philippi
2	1	1	1	1	2	2
poland	portugal	rumania	singapor	spain	sweden	switzerl
1	1	1	2	1	1	1
taipei	thailand	turkey	usa	ussr	wsamoa	
2	2	1	1	1	3	

A cautious picture



```
plot(predict(prcomp(trackmen,scale=T)),pch=3*kmea3$cluster)
```

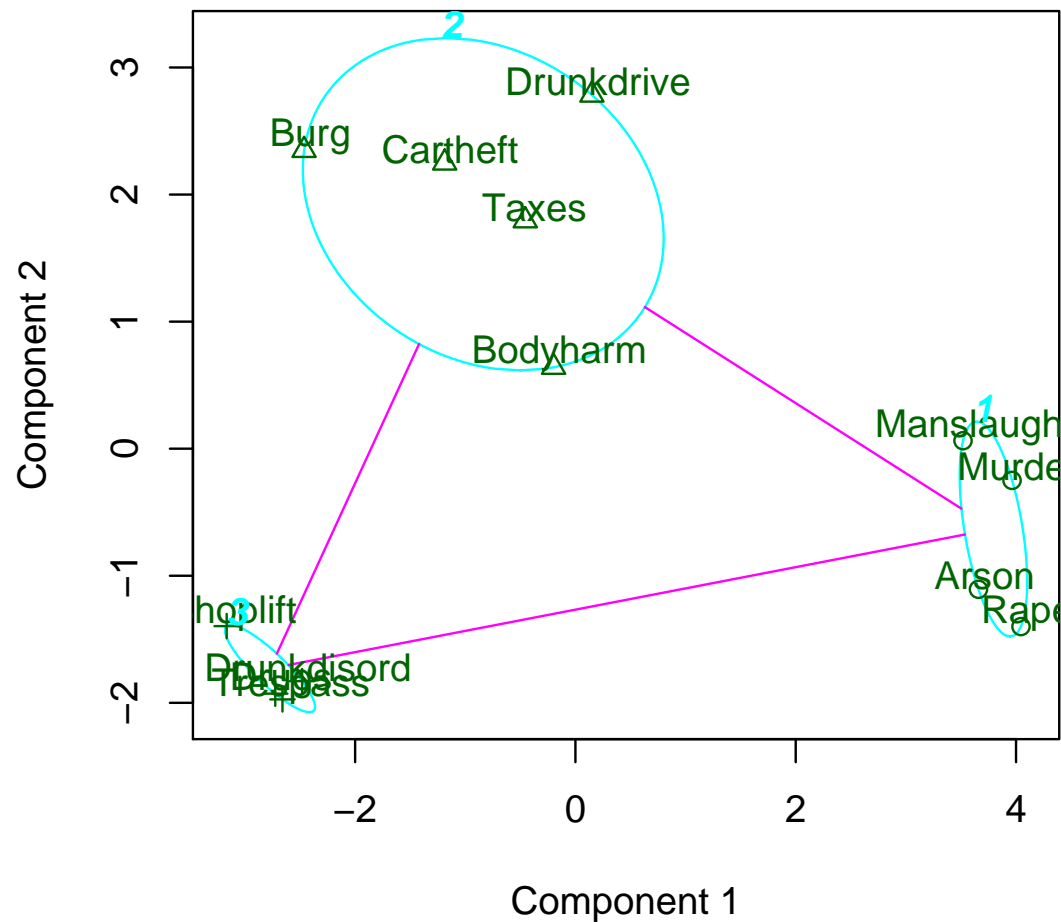
4-means?



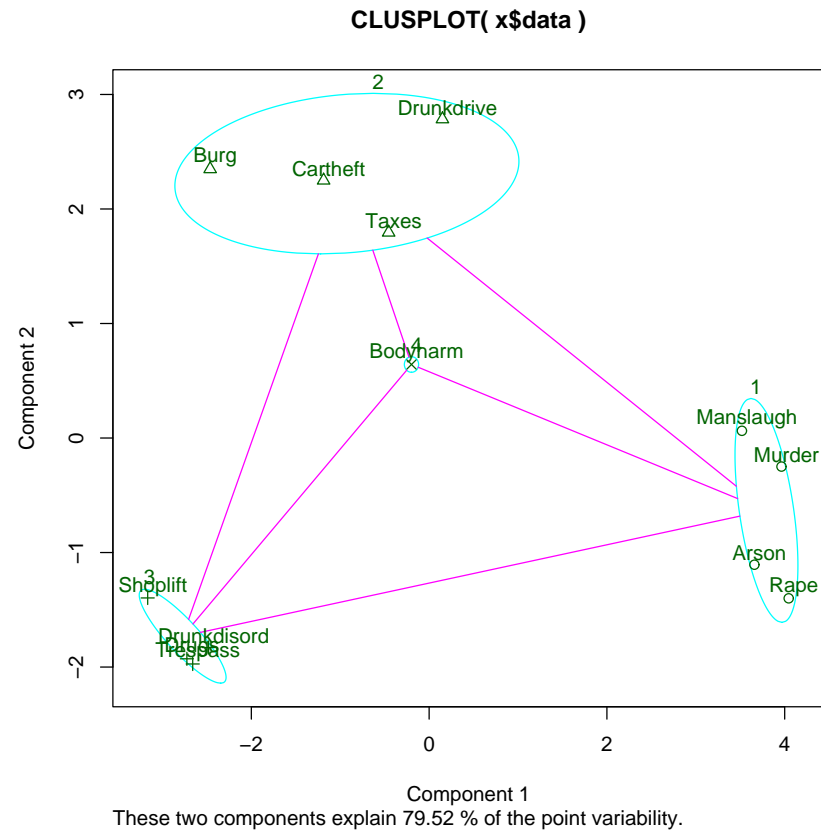
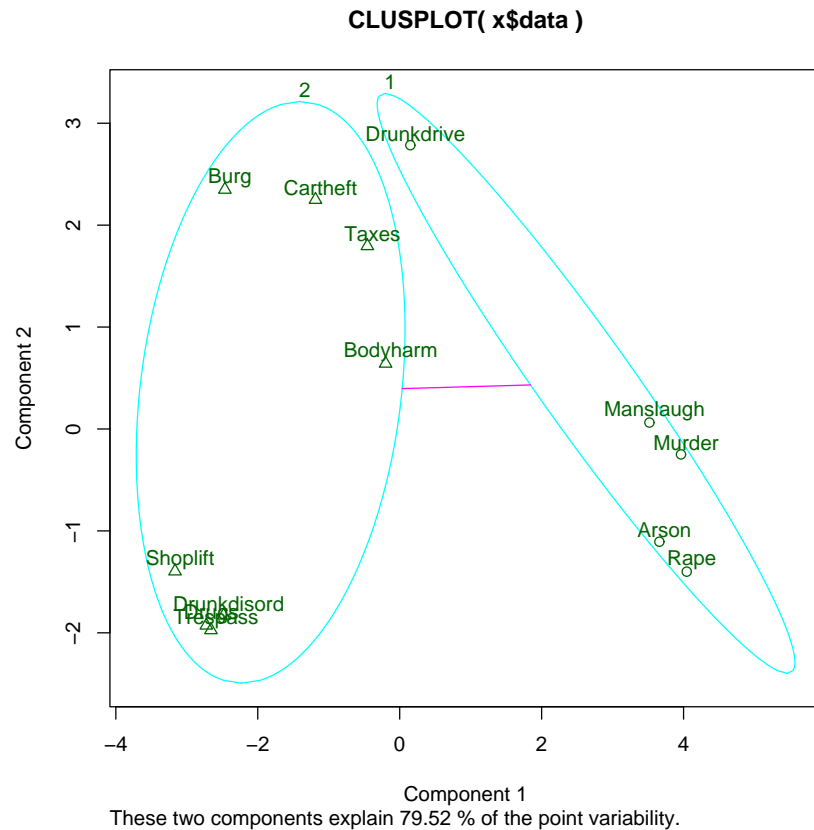
Crimes: 3-medoids

```
> library(cluster)
> clusplot(pam(Crime,3),labels=2,sub='')
```

clusplot(pam(x = Crime, k = 3))



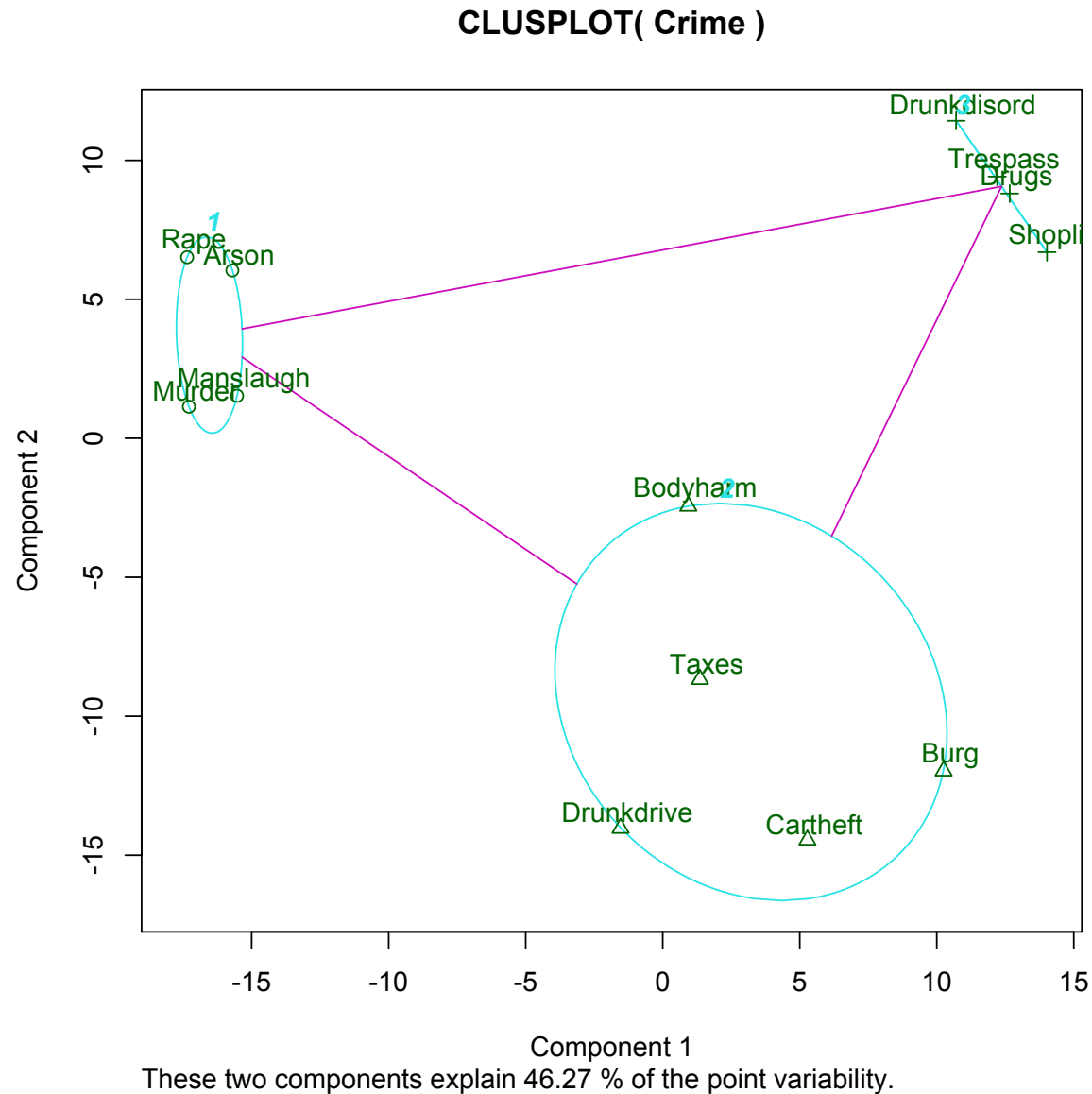
Crimes: k-medoids with different k



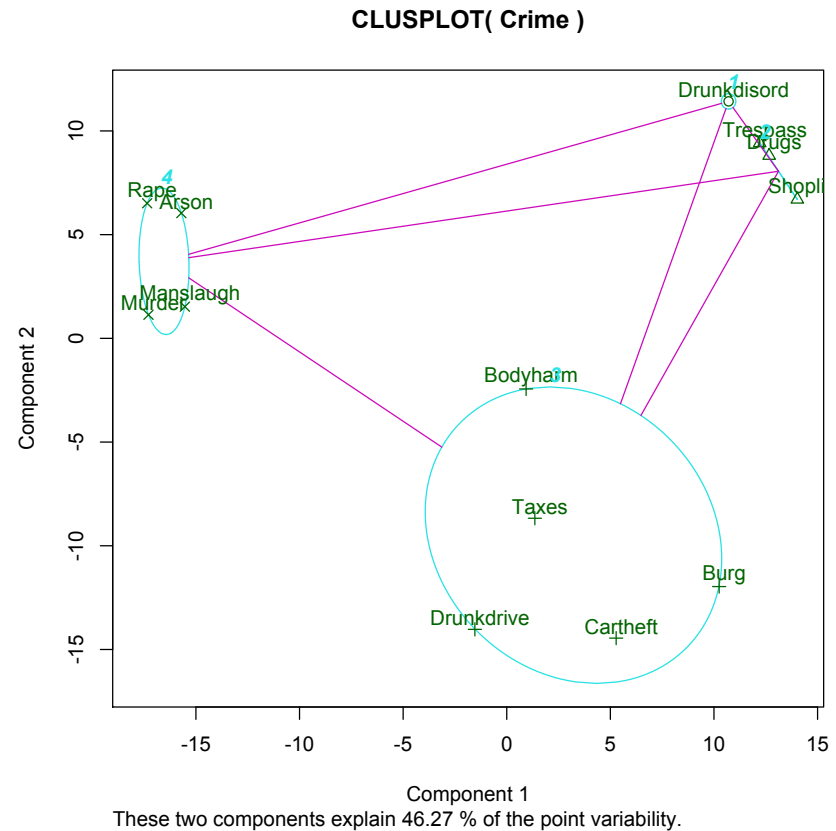
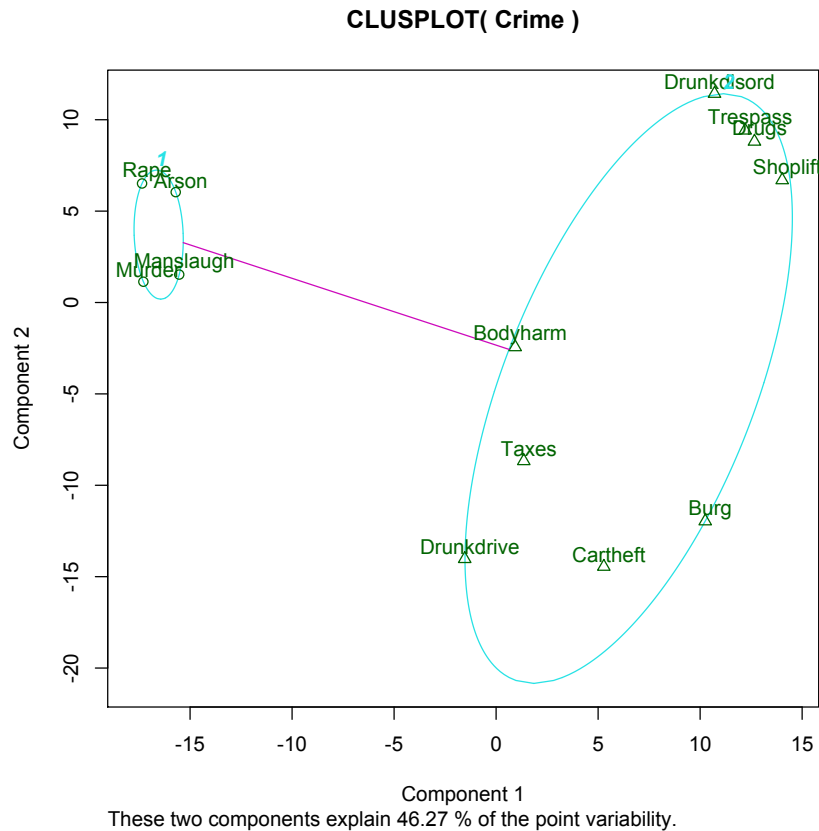
k-means give Cartheft to the other when $k = 2$;
 $k = 4$: Bodyharm extra

Crimes: 3-means

```
> clusplot(Crime,kmeans(Crime,3)$cluster,diss=T,labels=2)
```



Crimes: k-means with different k



$k = 2$: different from 2-medoids

$k = 4$: Drunkdisord is extra

Hierarchical clustering

We may:

- start with clusters containing 1 item and end up with all items in one cluster: **agglomerative** clustering
- or other way round: divide and divide: **divisive** clustering

At every step, we are trying to join some two clusters (agglomerative) or divide some cluster (divisive). A criterion for that may be

- **single linkage**: clusters are close if each contains one element such that the two are close (*take min of distances*)
- **complete linkage**: clusters are close if each element of the first is close to each element of the second (*max of distances*)
- **average linkage**: clusters are close if the elements are close on average (each to each) (*average of distances*)

Divisive methods

An example of divisive method is the algorithm of MacNaughton and Smith: the item is put into a new cluster if the average dissimilarity to the objects of that cluster is smaller than the average dissimilarity to the members of its old cluster.

At each stage, the cluster with the largest diameter is selected. (The diameter of a cluster is the largest dissimilarity between any two of its observations.) To divide the selected cluster, the algorithm first looks for its most disparate observation (i.e., which has the largest average dissimilarity to the other observations of the selected cluster). This observation initiates the "splinter group". In subsequent steps, the algorithm reassigns observations that are closer to the "splinter group" than to the "old party". The result is a division of the selected cluster into two new clusters.

(Implemented in function `diana` from the package `cluster`.)

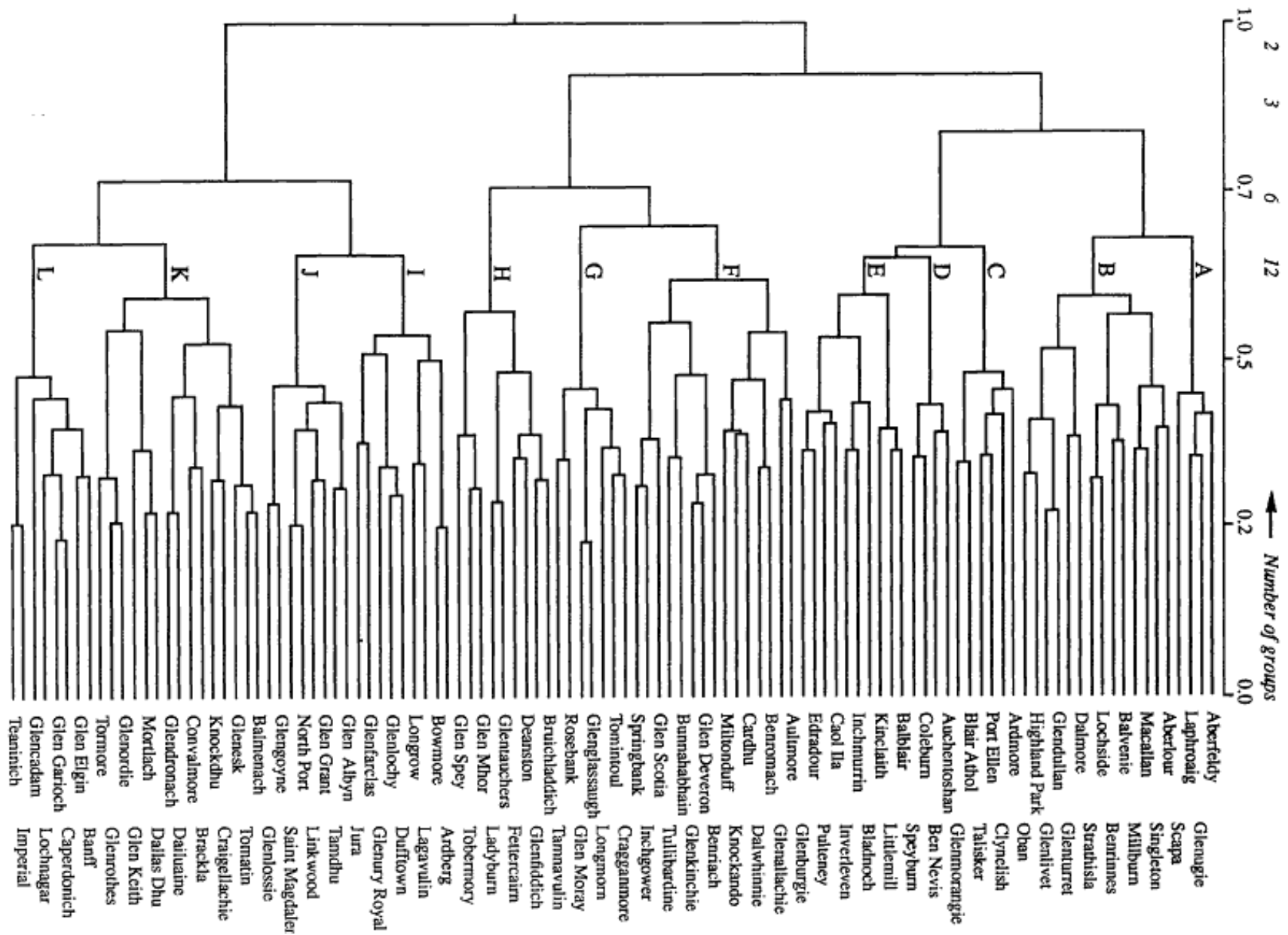
Dendrogram

The specific plot for cluster analysis: **dendrogram** (in principle, can be used also for partitioning methods, we just vary k). From the graph theory perspective, it is a tree: a connected graph with no cycles

The dissimilarity that can be read from the dendrogram is the *tree distance* (of cases and clusters): the value of this distance is the maximum *height* we have to get to on the dendrogram when traveling from one cluster or object to another connecting the two clusters or objects, the value of the distance in the moment they enter the common cluster. This dissimilarity is an ultrametric

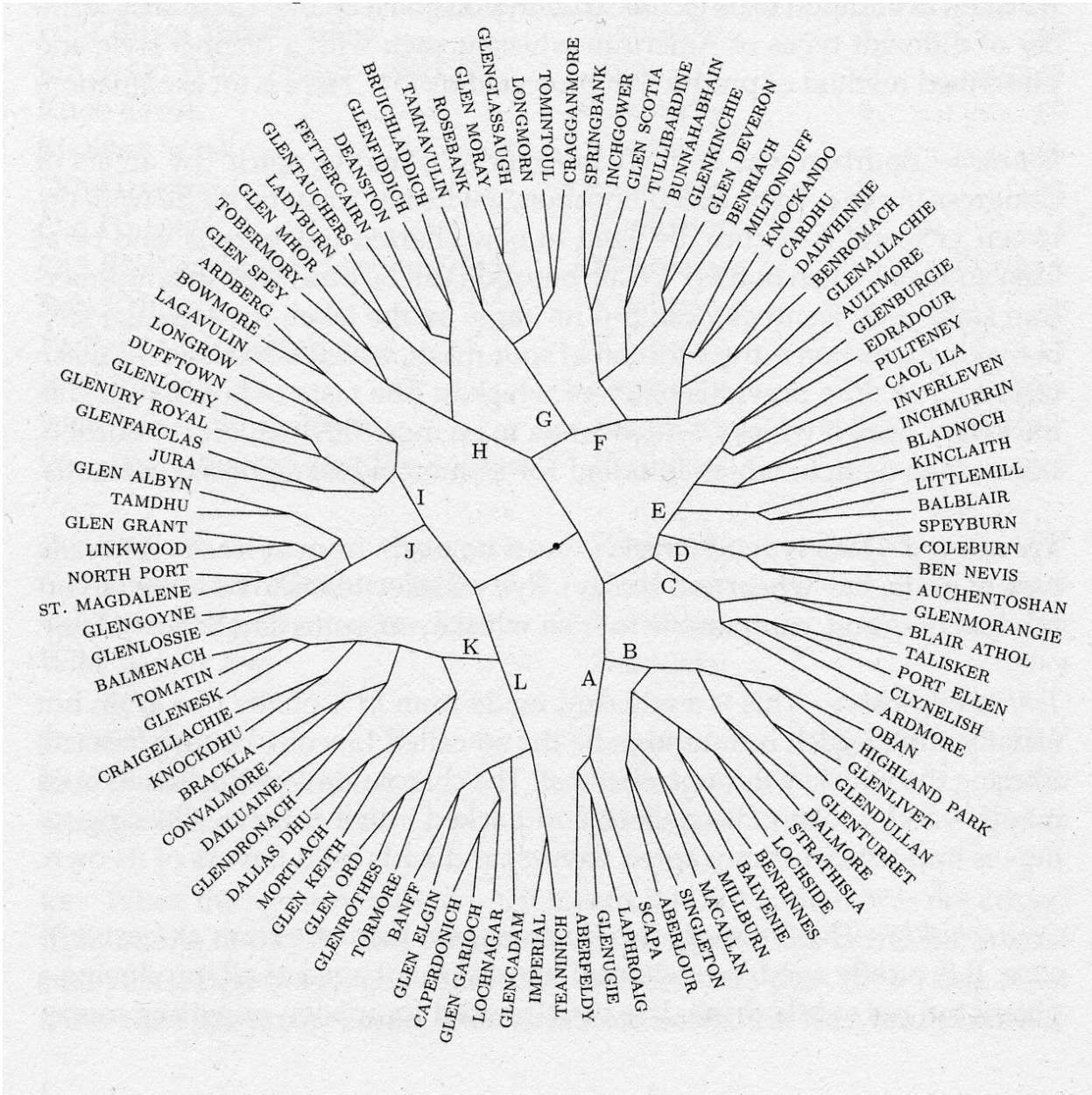
For two original objects, however, their tree distance is not necessarily equal to their original dissimilarity - this is true only when the original dissimilarity is itself an ultrametric, and also not true for every type of linkage. From this aspect, the dendrogram should be viewed rather as an approximation

A Scotch example



F. J. Lapointe & P. Legendre, Applied Statistics 43, 237-257 (1994)

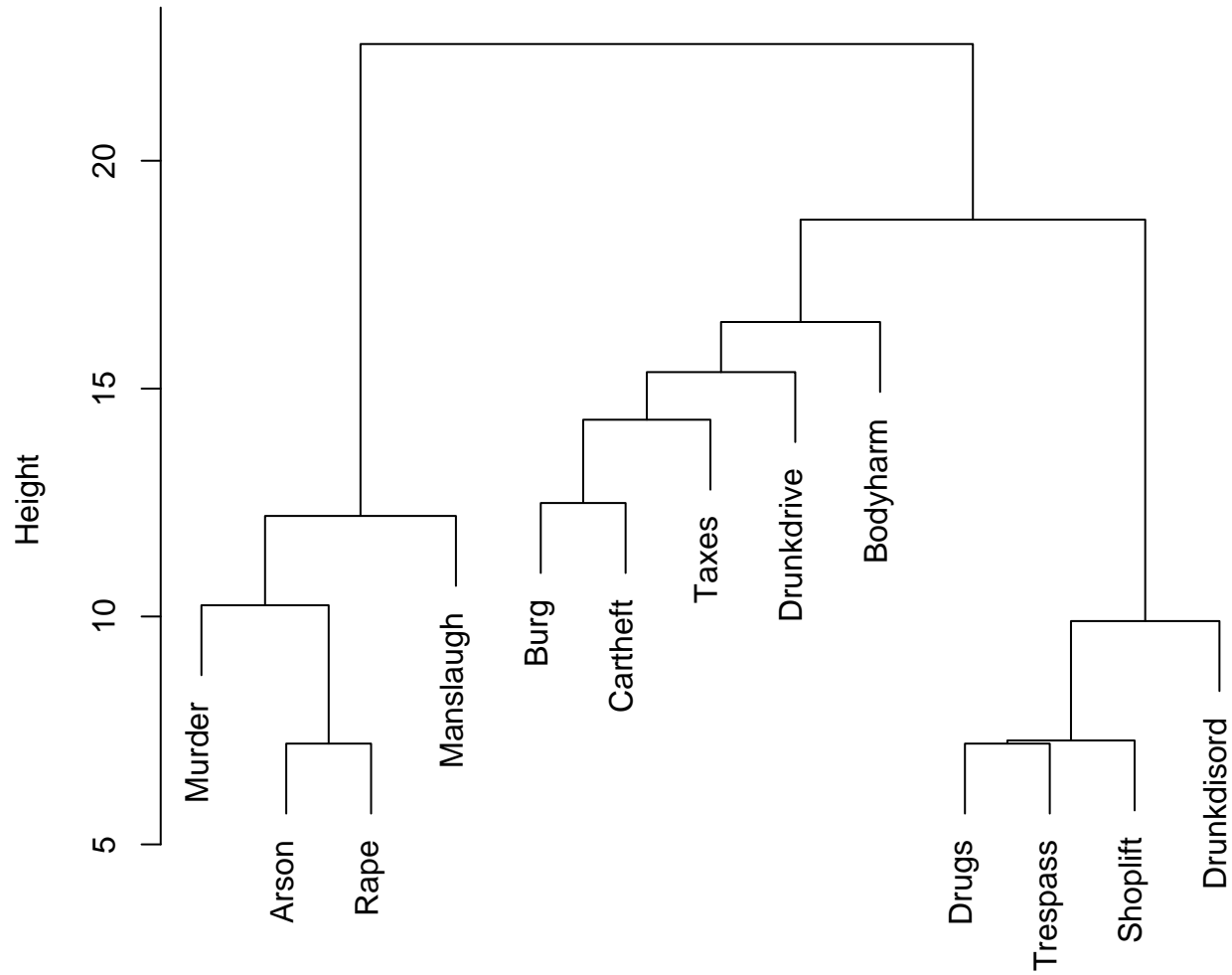
The Scotch revisited



(Thomas Fink, *The Man's Book*, Little, Brown, and Company, New York, 2009)

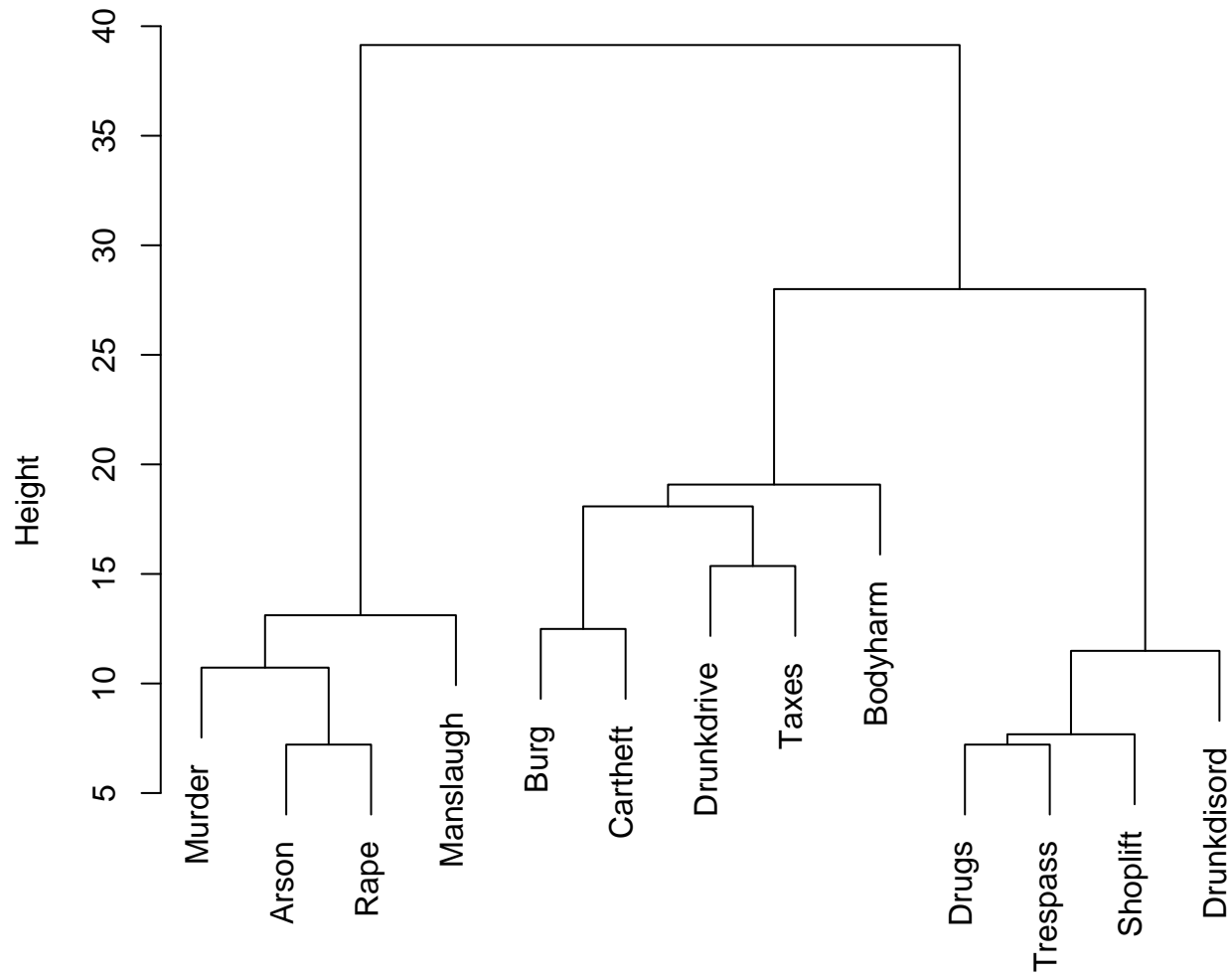
Crimes, hierarchical: single

Dendrogram of `agnes(x = crime, method = "single")`



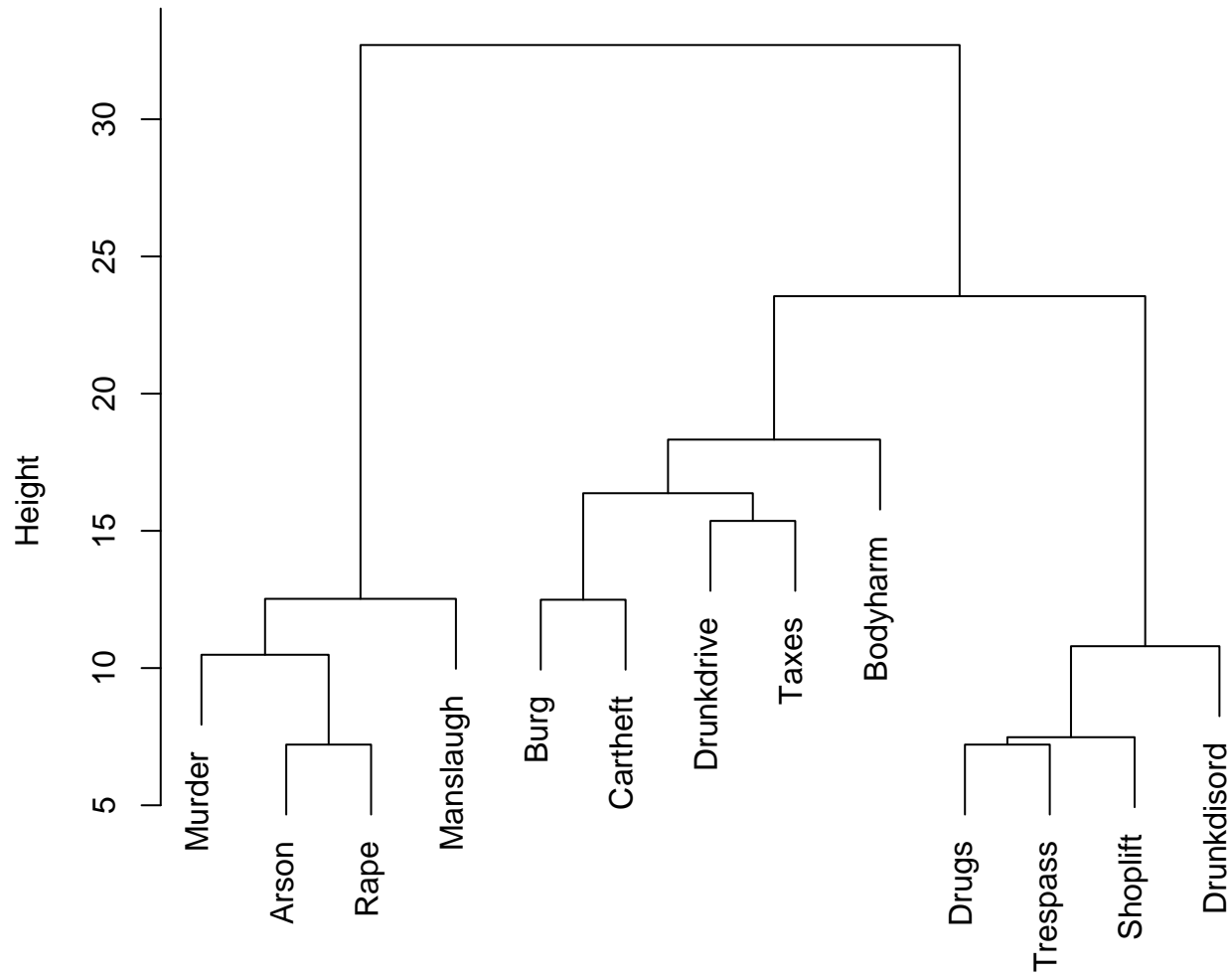
Crimes, hierarchical: complete

Dendrogram of `agnes(x = crime, method = "complete")`



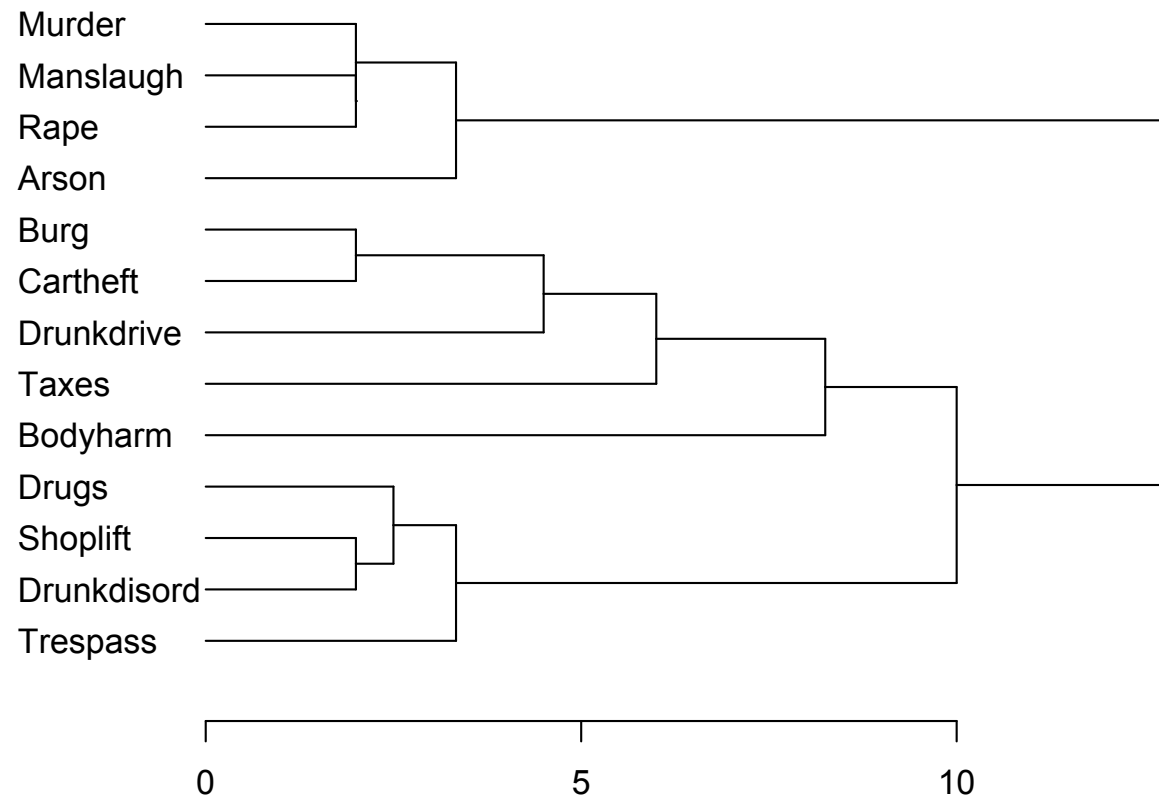
Crimes, hierarchical: average

Dendrogram of `agnes(x = crime, method = "average")`



Two styles of dendrogram plots: I

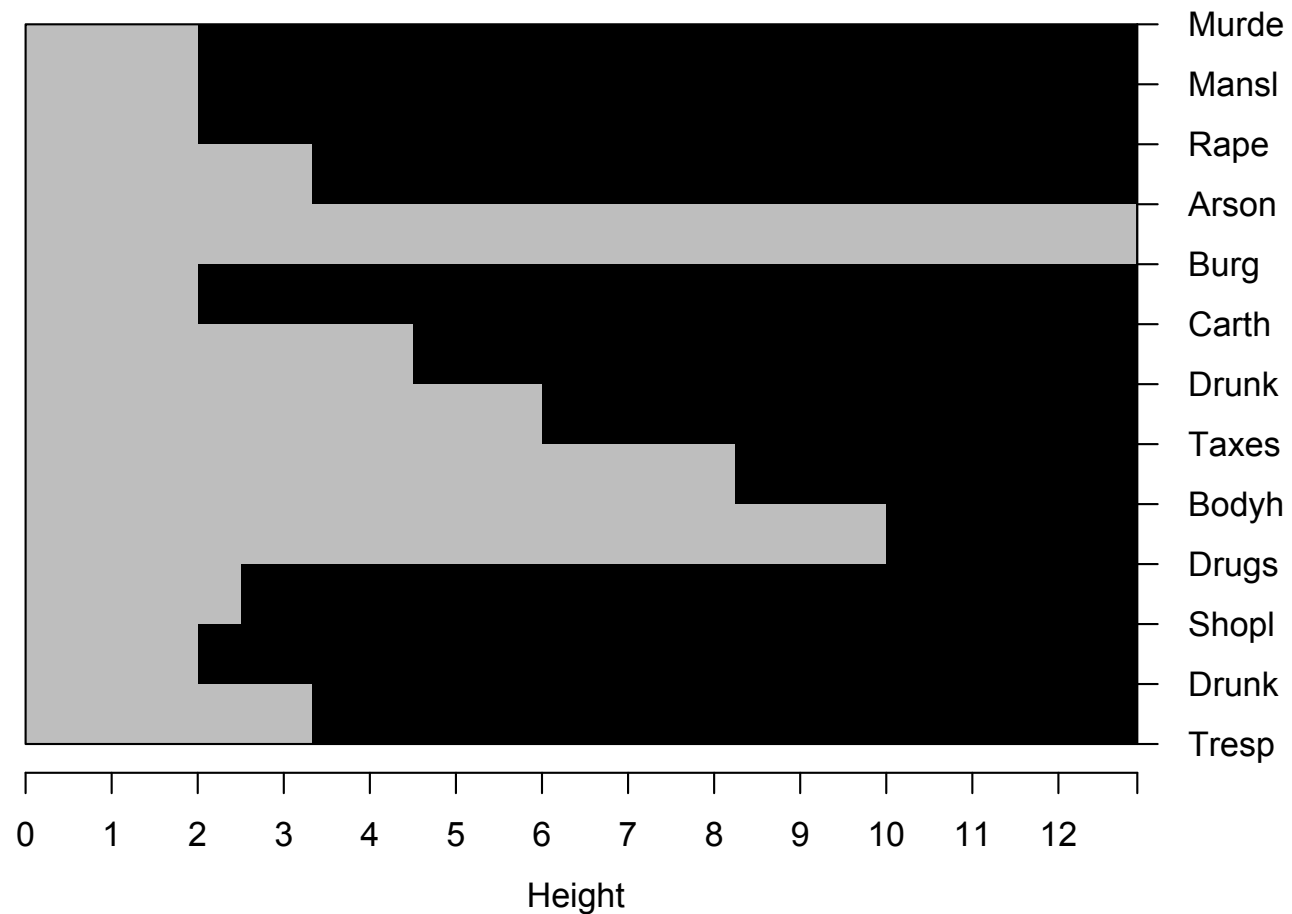
```
> plot(as.dendrogram(as.hclust(agnes(Crime))),horiz=T,  
+ xlim=c(-2,13),ylim=c(14,0),dLeaf=-2.5)
```



Two styles of dendrogram plots: II

```
> plot(agnes(Crime), which=1, col=c(8,1))
```

Banner of agnes(x = Crime)



Agglomerative Coefficient = 0.75

Silhouette plot

For the observation with index i , define the silhouette width s_i

First, let a_i - average dissimilarity between i -th object and all other points of the cluster to which i belongs; if i -th object is the only one in its cluster, $s_i = 0$ without further calculations.

Then, for all other clusters C , let $d(i, C)$ be average dissimilarity of i -th object to all observations of C ; the smallest of these $d(i, C)$ is $b_i = \min_C d(i, C)$, and can be seen as the dissimilarity between i -th object and its “neighbor” cluster, the nearest one to which it does not belong; and then

$$s_i = \frac{b_i - a_i}{\max\{a_i, b_i\}}$$

Observations with a large s_i (almost 1) are very well clustered, a small s_i (around 0) means that the observation lies between two clusters, and observations with a negative s_i are probably placed in the wrong cluster.

Silhouette plot is primarily designed for partitioning methods, but may be used also for the hierarchical ones - which is facilitated by function `cutree`

So

```
> plot(silhouette(pam(Crime,3)))
```

This would not work that nice:

```
> plot(silhouette(cutree(agnes(Crime),3),dist=Crime))
```

But this makes it up:

```
> sil <- silhouette(cutree(agnes(Crime),3),dist=Crime)
> row.names(sil) <- labels(Crime)
> plot(sil)
```

The silhouette plots come up as same - why?

Silhouette for 3 medoids

Silhouette plot of pam(x = Crime, k = 3)

n = 13

3 clusters C_j

$j : n_j \mid \text{ave}_{i \in C_j} s_i$

Rape

Mansl

Murde

Arson

Drunk

Burg

Carth

Taxes

Bodyh

Drunk

Drugs

Shopl

Tresp

1 : 4 | 0.77

2 : 5 | 0.36

3 : 4 | 0.72

0.0

0.2

0.4

0.6

0.8

1.0

Silhouette width s_i

Average silhouette width : 0.6

Silhouette for 3 agglomerative clusters (same)

Silhouette plot of (x = cutree(agnes(Crime), 3), dist = Crime)

n = 13

3 clusters C_j

$j : n_j \mid \text{ave}_{i \in C_j} s_i$

Rape

Mansl

Murde

Arson

Drunk

Burg

Carth

Taxes

Bodyh

Drunk

Drugs

Shopl

Tresp

1 : 4 | 0.77

2 : 5 | 0.36

3 : 4 | 0.72

0.0

0.2

0.4

0.6

0.8

1.0

Silhouette width s_i

Average silhouette width : 0.6

A possible twist of mind: clustering of variables

We can cluster variables in the same way as objects - once we can find a measure of dissimilarity for them

And the handy ones are those based on (various versions of) correlation coefficients

Of course, rather than ρ itself it is $1 - \rho^2$ that qualifies as a dissimilarity

Or perhaps $1 - |\rho|$, or $1/(1 - \rho^2) - 1$, or $1/(1 - |\rho|) - 1$

But others may argue also for $1 - \rho$, or $1/(1 - \rho) - 1/2$

Maclean's 2004

	StudentBodyAverageEnteringGrade	StudentProportionWith75PercOrHigher	StudentProportionWhoGraduate	
Toronto	86.5	99.78	92.6	
Queens	89.0	100.00	91.6	
McGill	89.3	99.77	92.5	
UBC	88.5	99.55	88.1	
McMaster	85.0	99.98	89.2	
Dalhousie	84.4	96.85	87.9	
Western	88.1	99.96	91.8	
Alberta	85.9	96.31	82.3	
Ottawa	83.7	91.74	90.3	
Sask	86.5	93.59	86.8	
Sherbrooke	86.5	97.89	90.5	
Montreal	87.6	99.30	91.6	
Laval	86.1	97.02	79.4	
Manitoba	83.1	82.31	84.8	
Calgary	82.6	91.20	78.6	
	StudentOutOffProvince1stYear	StudentInternationalGraduate	StudentInternational1stYear	StudentRetentionRate
Toronto	3.8	16.6	6.2	95.8
Queens	14.2	24.9	2.2	95.5
McGill	30.0	22.8	17.9	92.4
UBC	13.4	23.6	8.6	90.9
McMaster	1.7	21.0	6.8	90.1
Dalhousie	52.6	20.9	6.1	83.9
Western	4.6	14.5	4.8	94.9
Alberta	15.2	26.4	3.4	84.7
Ottawa	13.5	20.9	5.8	89.8
Sask	5.8	29.3	0.8	84.4
Sherbrooke	3.6	17.5	1.4	93.8
Montreal	7.9	20.8	12.8	90.0
Laval	2.4	20.3	11.5	95.2
Manitoba	9.1	17.4	5.1	85.1
Calgary	12.9	17.0	1.9	84.3

	StudentAwards	ClassesClassSizes1stAnd2ndYearLevel	Classes1stAnd2ndYearLevel1To25
Toronto	7.7	3.18	6.03
Queens	8.5	3.34	4.91
McGill	9.9	3.54	9.07
UBC	7.8	3.73	9.82
McMaster	5.8	3.19	3.23
Dalhousie	6.9	3.80	7.53
Western	4.8	4.06	16.65
Alberta	7.1	3.66	7.75
Ottawa	4.6	3.90	10.36
Sask	3.1	4.19	16.51
Sherbrooke	4.1	4.74	19.55
Montreal	6.0	4.24	14.26
Laval	5.7	4.25	20.82
Manitoba	5.2	3.79	7.40
Calgary	5.1	3.70	6.75

	Classes1stAnd2ndYearLevel26To50	Classes1stAnd2ndYearLevel51To100	Classes1stAnd2ndYearLevel101To250
Toronto	9.37	19.86	35.25
Queens	9.46	24.51	38.00
McGill	13.43	25.91	32.72
UBC	15.62	22.96	42.31
McMaster	11.29	14.19	44.43
Dalhousie	19.71	29.70	33.15
Western	19.72	32.00	18.69
Alberta	15.61	26.68	34.43
Ottawa	17.08	29.24	38.90
Sask	25.10	25.58	26.80
Sherbrooke	41.59	32.10	6.76
Montreal	19.70	44.71	18.45
Laval	16.89	31.25	28.89
Manitoba	17.54	28.03	41.02
Calgary	15.22	27.96	41.48

	Classes1stAnd2ndYearLevel251To500	Classes1stAnd2ndYearLevelMore500	ClassesClassSizes3rdAnd4thYearLevel
Toronto	20.23	9.25	4.55
Queens	21.80	1.33	4.60
McGill	11.34	7.52	4.93

UBC	8.21	1.09	4.30
McMaster	25.98	0.88	4.29
Dalhousie	8.32	1.59	4.95
Western	10.56	2.38	5.08
Alberta	15.54	0.00	4.62
Ottawa	4.42	0.00	4.76
Sask	6.01	0.00	5.09
Sherbrooke	0.00	0.00	4.98
Montreal	2.88	0.00	4.83
Laval	2.16	0.00	4.91
Manitoba	5.99	0.00	4.85
Calgary	8.60	0.00	4.84
Classes3rdAnd4thYearLevel1To25 Classes3rdAnd4thYearLevel126To50 Classes3rdAnd4thYearLevel151To100			
Toronto	22.25	30.12	30.74
Queens	24.71	30.94	25.46
McGill	33.07	36.49	23.04
UBC	15.14	28.78	32.29
McMaster	19.87	21.84	28.87
Dalhousie	34.92	32.68	25.11
Western	39.69	35.30	17.96
Alberta	26.32	27.74	28.43
Ottawa	26.55	31.36	33.42
Sask	35.97	41.83	17.67
Sherbrooke	24.36	50.92	22.74
Montreal	26.57	35.90	31.56
Laval	36.51	28.17	24.76
Manitoba	30.95	29.27	33.39
Calgary	25.77	40.73	24.85
Classes3rdAnd4thYearLevel101To250 Classes3rdAnd4thYearLevel1251To500 Classes3rdAnd4thYearLevelMore500			
Toronto	14.53	2.37	0
Queens	17.54	1.35	0
McGill	5.65	1.75	0
UBC	18.37	5.42	0
McMaster	26.11	3.31	0
Dalhousie	7.29	0.00	0
Western	7.05	0.00	0

Alberta	16.32	1.19	0
Ottawa	8.66	0.00	0
Sask	4.53	0.00	0
Sherbrooke	1.98	0.00	0
Montreal	5.98	0.00	0
Laval	10.56	0.00	0
Manitoba	6.38	0.00	0
Calgary	8.65	0.00	0

	ClassesTaughtByTenuredFaculty	FacultyFacultyWithPhD	AwardsPerFullTimeFaculty
Toronto	68.90	98.6	10.8
Queens	62.10	95.3	13.7
McGill	49.50	94.3	8.9
UBC	52.90	98.9	8.8
McMaster	57.90	96.9	4.8
Dalhousie	54.40	92.7	2.2
Western	73.00	98.3	4.0
Alberta	45.90	98.9	6.4
Ottawa	58.70	97.2	5.6
Sask	61.10	93.7	3.4
Sherbrooke	66.80	92.7	3.5
Montreal	60.10	94.4	5.9
Laval	68.00	97.8	4.2
Manitoba	44.30	95.9	1.8
Calgary	61.39	91.9	3.6

	HumanitiesAverageGrantSizePerFaculty	HumanitiesNumberOfGrantsPerFaculty
Toronto	20719	57.17
Queens	8902	29.79
McGill	19506	61.96
UBC	15105	47.99
McMaster	9706	31.62
Dalhousie	7819	27.90
Western	8311	25.53
Alberta	10464	32.80
Ottawa	11396	33.48
Sask	7295	18.40
Sherbrooke	5891	14.50

Montreal	15629	37.30
Laval	8531	25.48
Manitoba	6289	20.45
Calgary	5510	19.89
MedicalScienceGrantsAverageGrantSizePerFaculty MedicalScienceNumberOfGrantsPerFaculty		
Toronto	126520	218.25
Queens	81948	103.21
McGill	111852	161.38
UBC	92459	152.14
McMaster	78282	130.10
Dalhousie	43649	88.35
Western	84162	152.01
Alberta	84031	168.12
Ottawa	72827	126.93
Sask	37278	74.60
Sherbrooke	55142	99.42
Montreal	90428	133.57
Laval	74439	126.15
Manitoba	44526	82.80
Calgary	72167	118.49
FinancesOperatingBudget FinancesScholarshipsBursariesPercOfBudget FinancesStudentServicesPercOfBudget		
Toronto	9878	13.29 7.37
Queens	8053	14.00 4.60
McGill	8860	11.34 5.46
UBC	7110	12.14 8.05
McMaster	8451	11.53 6.53
Dalhousie	8472	10.16 4.04
Western	8500	15.88 5.16
Alberta	9467	12.47 4.77
Ottawa	9532	10.53 5.72
Sask	9611	5.11 3.66
Sherbrooke	7836	11.81 4.33
Montreal	9490	10.20 4.34
Laval	8628	7.94 4.42
Manitoba	8108	5.42 3.93
Calgary	8684	10.26 5.16

	LibraryTotalLibraryHoldingsThousand	LibraryHoldingsPerStudent	LibraryAcquisitions	LibraryExpenses
Toronto	14468	258	50.66	8.30
Queens	5402	289	50.79	6.82
McGill	4919	200	47.97	7.27
UBC	8903	253	41.50	7.81
McMaster	3116	156	46.35	5.25
Dalhousie	2252	167	42.75	5.02
Western	7904	283	58.10	7.74
Alberta	10029	337	47.84	7.30
Ottawa	4279	176	46.85	5.14
Sask	4387	286	49.97	6.65
Sherbrooke	1859	138	49.54	4.63
Montreal	5202	145	40.48	5.78
Laval	4716	189	49.28	4.95
Manitoba	3211	155	41.62	7.60
Calgary	509	210	44.62	6.07
	ReputationAlumniSupport	ReputationalRanking	TotalRanking	
Toronto	26.80	99.0	1	
Queens	16.20	98.0	2	
McGill	18.80	97.9	3	
UBC	14.50	96.9	6	
McMaster	13.60	97.5	4	
Dalhousie	13.90	50.0	11	
Western	25.80	70.0	7	
Alberta	14.70	96.0	5	
Ottawa	13.50	35.0	14	
Sask	13.40	60.0	9	
Sherbrooke	18.50	60.3	8	
Montreal	15.90	55.0	10	
Laval	12.40	40.0	13	
Manitoba	14.80	30.0	15	
Calgary	14.09	45.0	12	

Maclean's condensed

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	
Toronto	86.5	99.78	92.6	3.8	16.6	6.2	95.8	7.7	3.18	6.03	9.37	19.86	35.25	20.23	9.25	4.55	22.25	30.12	30.74	
Queens	89.0	100.00	91.6	14.2	24.9	2.2	95.5	8.5	3.34	4.91	9.46	24.51	38.00	21.80	1.33	4.60	24.71	30.94	25.46	
McGill	89.3	99.77	92.5	30.0	22.8	17.9	92.4	9.9	3.54	9.07	13.43	25.91	32.72	11.34	7.52	4.93	33.07	36.49	23.04	
UBC	88.5	99.55	88.1	13.4	23.6	8.6	90.9	7.8	3.73	9.82	15.62	22.96	42.31	8.21	1.09	4.30	15.14	28.78	32.29	
McMaster	85.0	99.98	89.2	1.7	21.0	6.8	90.1	5.8	3.19	3.23	11.29	14.19	44.43	25.98	0.88	4.29	19.87	21.84	28.87	
Dalhousie	84.4	96.85	87.9	52.6	20.9	6.1	83.9	6.9	3.80	7.53	19.71	29.70	33.15	8.32	1.59	4.95	34.92	32.68	25.11	
Western	88.1	99.96	91.8	4.6	14.5	4.8	94.9	4.8	4.06	16.65	19.72	32.00	18.69	10.56	2.38	5.08	39.69	35.30	17.96	
Alberta	85.9	96.31	82.3	15.2	26.4	3.4	84.7	7.1	3.66	7.75	15.61	26.68	34.43	15.54	0.00	4.62	26.32	27.74	28.43	
Ottawa	83.7	91.74	90.3	13.5	20.9	5.8	89.8	4.6	3.90	10.36	17.08	29.24	38.90	4.42	0.00	4.76	26.55	31.36	33.42	
Sask	86.5	93.59	86.8	5.8	29.3	0.8	84.4	3.1	4.19	16.51	25.10	25.58	26.80	6.01	0.00	5.09	35.97	41.83	17.67	
Sherbrooke	86.5	97.89	90.5	3.6	17.5	1.4	93.8	4.1	4.74	19.55	41.59	32.10	6.76	0.00	0.00	4.98	24.36	50.92	22.74	
Montreal	87.6	99.30	91.6	7.9	20.8	12.8	90.0	6.0	4.24	14.26	19.70	44.71	18.45	2.88	0.00	4.83	26.57	35.90	31.56	
Laval	86.1	97.02	79.4	2.4	20.3	11.5	95.2	5.7	4.25	20.82	16.89	31.25	28.89	2.16	0.00	4.91	36.51	28.17	24.76	
Manitoba	83.1	82.31	84.8	9.1	17.4	5.1	85.1	5.2	3.79	7.40	17.54	28.03	41.02	5.99	0.00	4.85	30.95	29.27	33.39	
Calgary	82.6	91.20	78.6	12.9	17.0	1.9	84.3	5.1	3.70	6.75	15.22	27.96	41.48	8.60	0.00	4.84	25.77	40.73	24.85	
	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39
Toronto	14.53	2.37	0	68.90	98.6	10.8	20719	57.17	126520	218.25	9878	13.29	7.37	14468	258	50.66	8.30	26.80	99.0	1
Queens	17.54	1.35	0	62.10	95.3	13.7	8902	29.79	81948	103.21	8053	14.00	4.60	5402	289	50.79	6.82	16.20	98.0	2
McGill	5.65	1.75	0	49.50	94.3	8.9	19506	61.96	111852	161.38	8860	11.34	5.46	4919	200	47.97	7.27	18.80	97.9	3
UBC	18.37	5.42	0	52.90	98.9	8.8	15105	47.99	92459	152.14	7110	12.14	8.05	8903	253	41.50	7.81	14.50	96.9	6
McMaster	26.11	3.31	0	57.90	96.9	4.8	9706	31.62	78282	130.10	8451	11.53	6.53	3116	156	46.35	5.25	13.60	97.5	4
Dalhousie	7.29	0.00	0	54.40	92.7	2.2	7819	27.90	43649	88.35	8472	10.16	4.04	2252	167	42.75	5.02	13.90	50.0	11
Western	7.05	0.00	0	73.00	98.3	4.0	8311	25.53	84162	152.01	8500	15.88	5.16	7904	283	58.10	7.74	25.80	70.0	7
Alberta	16.32	1.19	0	45.90	98.9	6.4	10464	32.80	84031	168.12	9467	12.47	4.77	10029	337	47.84	7.30	14.70	96.0	5
Ottawa	8.66	0.00	0	58.70	97.2	5.6	11396	33.48	72827	126.93	9532	10.53	5.72	4279	176	46.85	5.14	13.50	35.0	14
Sask	4.53	0.00	0	61.10	93.7	3.4	7295	18.40	37278	74.60	9611	5.11	3.66	4387	286	49.97	6.65	13.40	60.0	9
Sherbrooke	1.98	0.00	0	66.80	92.7	3.5	5891	14.50	55142	99.42	7836	11.81	4.33	1859	138	49.54	4.63	18.50	60.3	8
Montreal	5.98	0.00	0	60.10	94.4	5.9	15629	37.30	90428	133.57	9490	10.20	4.34	5202	145	40.48	5.78	15.90	55.0	10
Laval	10.56	0.00	0	68.00	97.8	4.2	8531	25.48	74439	126.15	8628	7.94	4.42	4716	189	49.28	4.95	12.40	40.0	13
Manitoba	6.38	0.00	0	44.30	95.9	1.8	6289	20.45	44526	82.80	8108	5.42	3.93	3211	155	41.62	7.60	14.80	30.0	15
Calgary	8.65	0.00	0	61.39	91.9	3.6	5510	19.89	72167	118.49	8684	10.26	5.16	509	210	44.62	6.07	14.09	45.0	12

Universities and variables

```
> row.names(Macleans)
[1] "Toronto"      "Queens"      "McGill"      "UBC"         "McMaster"
[6] "Dalhousie"    "Western"     "Alberta"     "Ottawa"      "Sask"
[11] "Sherbrooke"   "Montreal"    "Laval"       "Manitoba"    "Calgary"

> names(Macleans)
[1] "StudentBodyAverageEnteringGrade"      "StudentProportionWith75PercOrHigher"
[3] "StudentProportionWhoGraduate"         "StudentOutOffProvince1stYear"
[5] "StudentInternationalGraduate"         "StudentInternational1stYear"
[7] "StudentRetentionRate"                 "StudentAwards"
[9] "ClassesClassSizes1stAnd2ndYearLevel"  "Classes1stAnd2ndYearLevel1To25"
[11] "Classes1stAnd2ndYearLevel26To50"      "Classes1stAnd2ndYearLevel51To100"
[13] "Classes1stAnd2ndYearLevel101To250"    "Classes1stAnd2ndYearLevel251To500"
[15] "Classes1stAnd2ndYearLevelMore500"     "ClassesClassSizes3rdAnd4thYearLevel"
[17] "Classes3rdAnd4thYearLevel1To25"       "Classes3rdAnd4thYearLevel26To50"
[19] "Classes3rdAnd4thYearLevel51To100"     "Classes3rdAnd4thYearLevel101To250"
[21] "Classes3rdAnd4thYearLevel251To500"    "Classes3rdAnd4thYearLevelMore500"
[23] "ClassesTaughtByTenuredFaculty"        "FacultyFacultyWithPhD"
[25] "AwardsPerFullTimeFaculty"             "HumanitiesAverageGrantSizePerFaculty"
[27] "HumanitiesNumberOfGrantsPerFaculty"    "MedicalScienceGrantsAverageGrantSizePerFaculty"
[29] "MedicalScienceNumberOfGrantsPerFaculty" "FinancesOperatingBudget"
[31] "FinancesScholarshipsBursariesPercOfBudget" "FinancesStudentServicesPercOfBudget"
[33] "LibraryTotalLibraryHoldingsThousand"  "LibraryHoldingsPerStudent"
[35] "LibraryAcquisitions"                  "LibraryExpenses"
[37] "ReputationAlumniSupport"              "ReputationalRanking"
[39] "TotalRanking"
```


Variables omitted from the analysis

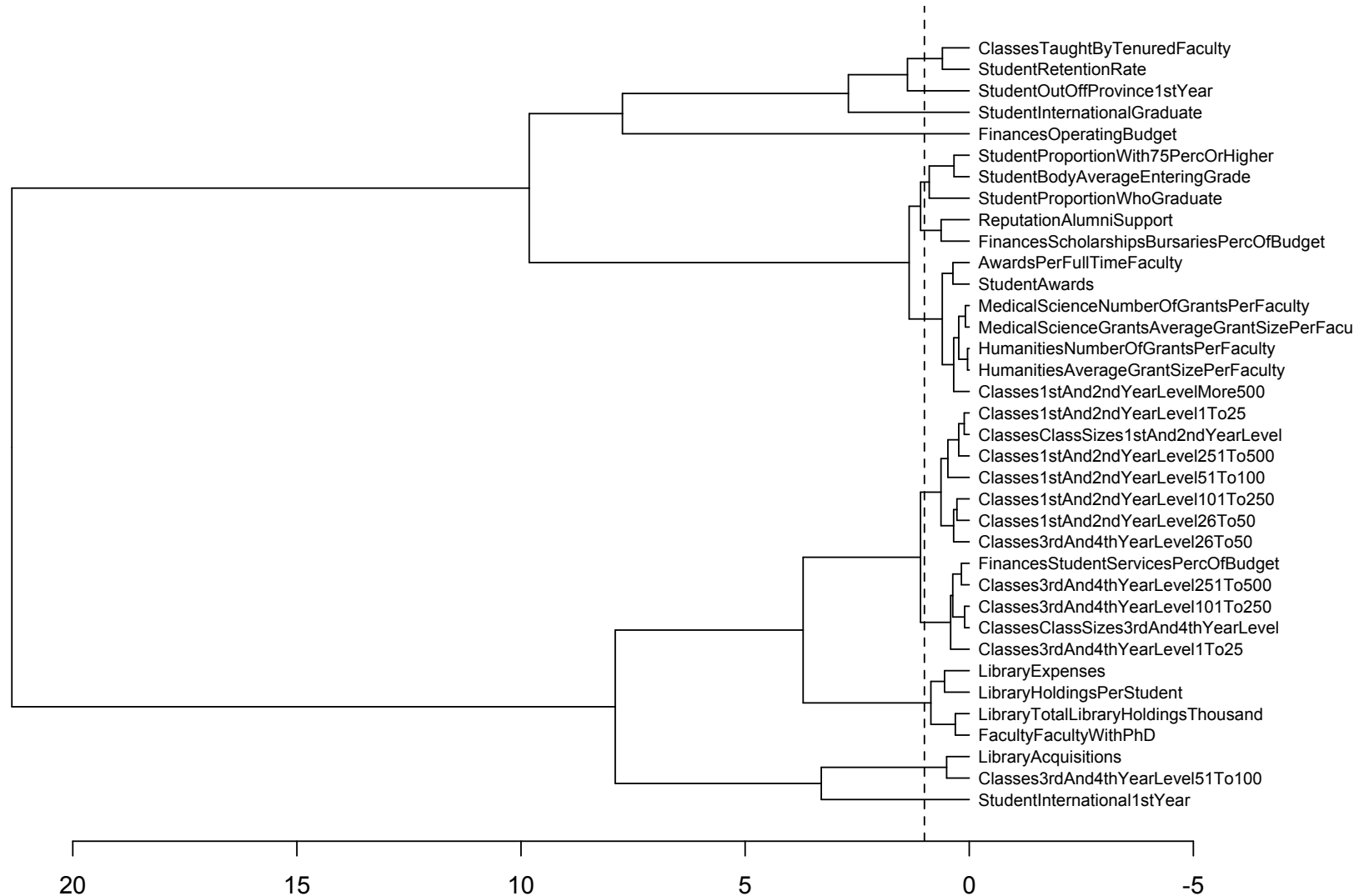
```
> Macleans[order(Macleans[,38],decreasing=TRUE),c(22,38,39)]
```

	Classes3rdAnd4thYearLevelMore500	ReputationalRanking	TotalRanking
Toronto	0	99.0	1
Queens	0	98.0	2
McGill	0	97.9	3
McMaster	0	97.5	4
UBC	0	96.9	6
Alberta	0	96.0	5
Western	0	70.0	7
Sherbrooke	0	60.3	8
Sask	0	60.0	9
Montreal	0	55.0	10
Dalhousie	0	50.0	11
Calgary	0	45.0	12
Laval	0	40.0	13
Ottawa	0	35.0	14
Manitoba	0	30.0	15

```
> Mcleans=Macleans[,-c(22,38,39)]
```

Hierarchical clustering with $1/|\rho| - 1$

`agnes(as.dist(1/abs(cor(Mcleans)))-1,diss=TRUE)`



12 clusters, perhaps

Silhouette plot of (x = cutree(Macvag, 12), dist = as.dist(1/abs(cor(Mcleans)) - 1)) -
Silhouette plot of 1))

n = 36

12 clusters C_j

$j : n_j \mid \text{ave}_{i \in C_j} s_i$

1 : 3 | 0.29

2 : 1 | 0.00

3 : 1 | 0.00

4 : 1 | 0.00

5 : 2 | 0.27

6 : 7 | 0.40

7 : 7 | 0.49

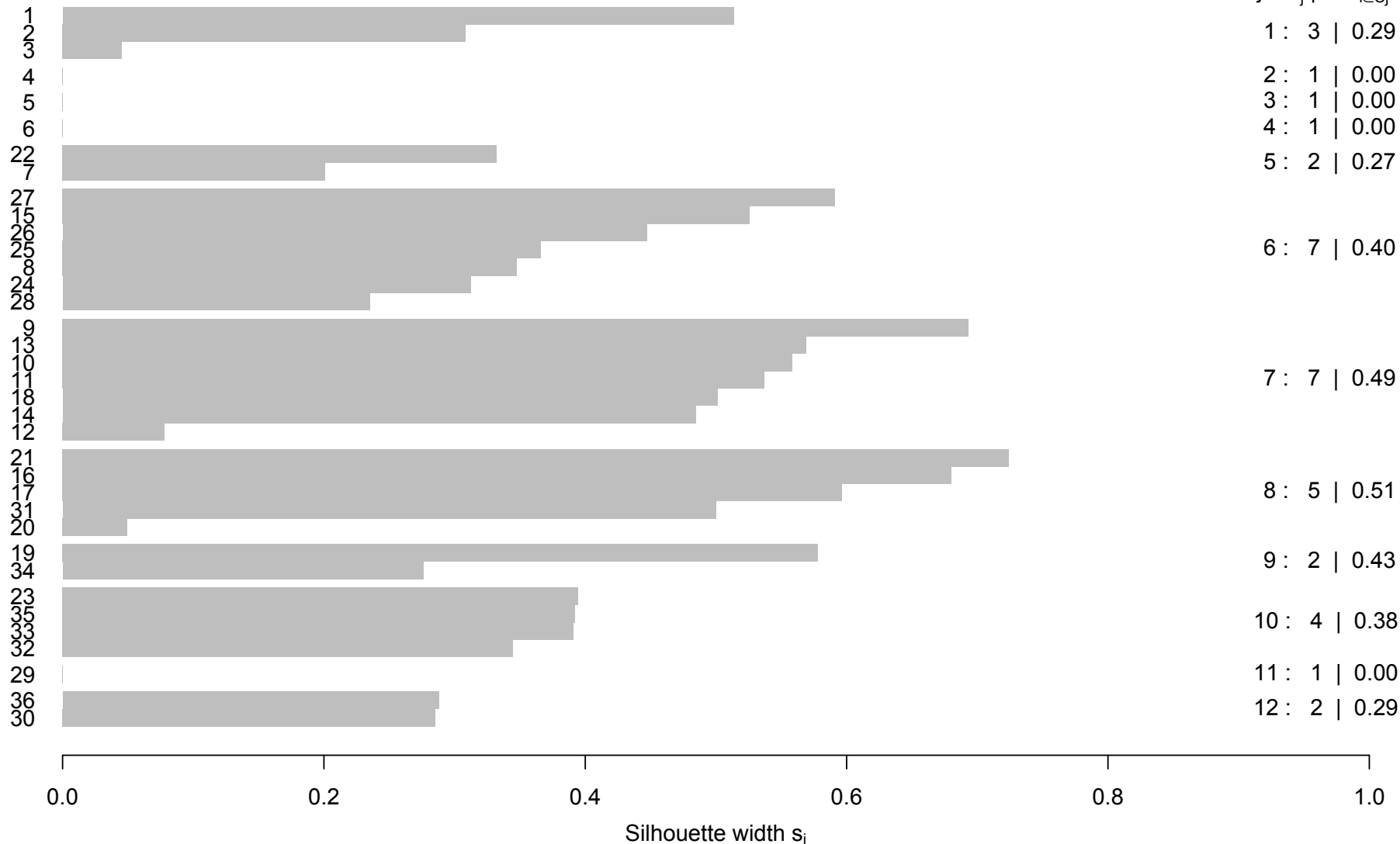
8 : 5 | 0.51

9 : 2 | 0.43

10 : 4 | 0.38

11 : 1 | 0.00

12 : 2 | 0.29



Average silhouette width : 0.37

The clusters

1	"StudentBodyAverageEnteringGrade"	"StudentProportionWith75PercOrHigher"
	"StudentProportionWhoGraduate"	
2	"StudentOutOffProvince1stYear"	
3	"StudentInternationalGraduate"	
4	"StudentInternational1stYear"	
5	"StudentRetentionRate"	"ClassesTaughtByTenuredFaculty"
6	"StudentAwards"	"Classes1stAnd2ndYearLevelMore500"
	"AwardsPerFullTimeFaculty"	"HumanitiesAverageGrantSizePerFaculty"
	"HumanitiesNumberOfGrantsPerFaculty"	"MedicalScienceGrantsAverageGrantSizePerFaculty"
	"MedicalScienceNumberOfGrantsPerFaculty"	
7	"ClassesClassSizes1stAnd2ndYearLevel"	"Classes1stAnd2ndYearLevel1To25"
	"Classes1stAnd2ndYearLevel26To50"	"Classes1stAnd2ndYearLevel51To100"
	"Classes1stAnd2ndYearLevel101To250"	"Classes1stAnd2ndYearLevel251To500"
	"Classes3rdAnd4thYearLevel26To50"	
8	"ClassesClassSizes3rdAnd4thYearLevel"	"Classes3rdAnd4thYearLevel1To25"
	"Classes3rdAnd4thYearLevel101To250"	"Classes3rdAnd4thYearLevel251To500"
	"FinancesStudentServicesPercOfBudget"	
9	"Classes3rdAnd4thYearLevel51To100"	"LibraryAcquisitions"
10	"FacultyFacultyWithPhD"	"LibraryTotalLibraryHoldingsThousand"
	"LibraryHoldingsPerStudent"	"LibraryExpenses"
11	"FinancesOperatingBudget"	
12	"FinancesScholarshipsBursariesPercOfBudget"	"ReputationAlumniSupport"

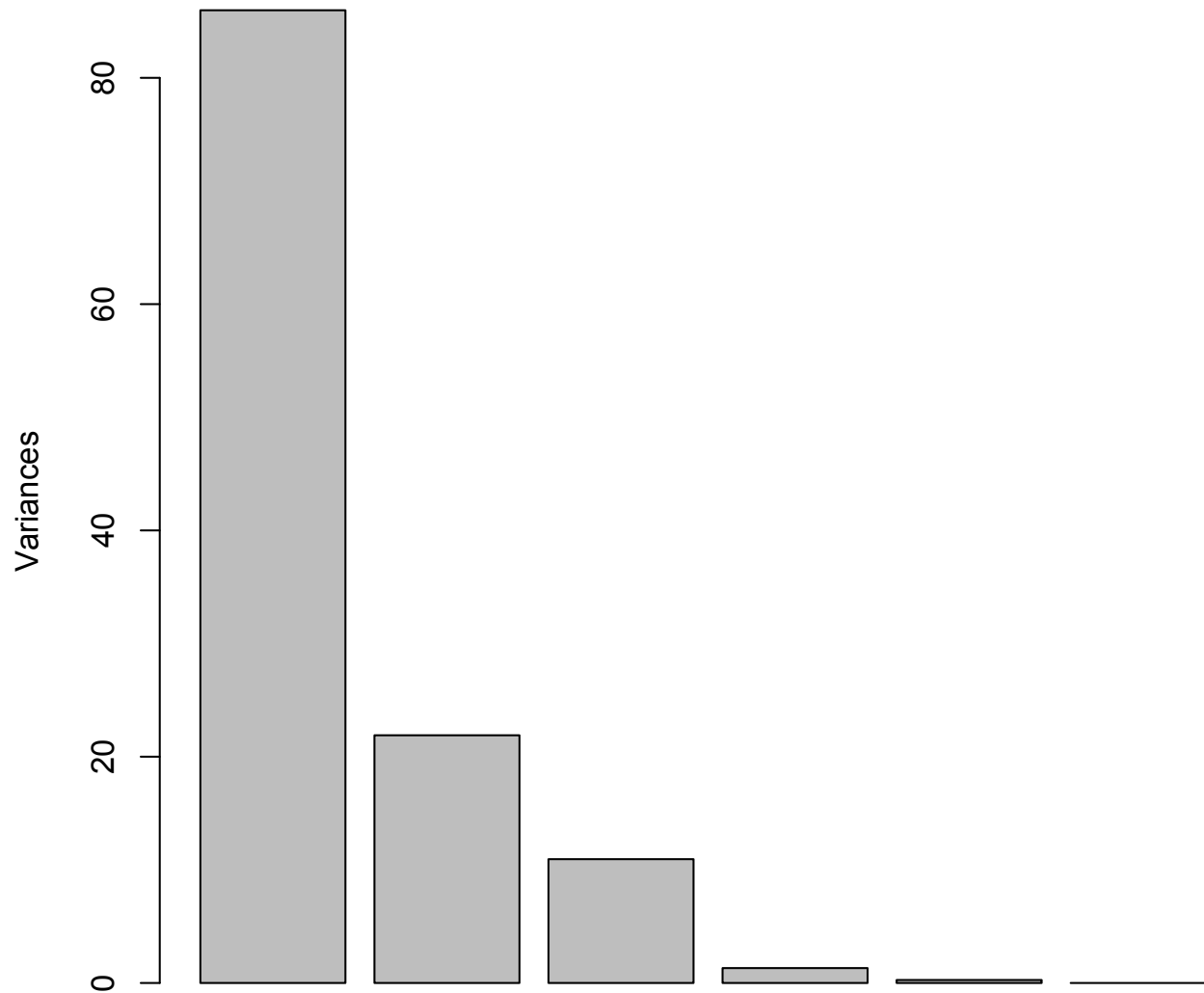
Class size variables

```
[1] "ClassesClassSizes1stAnd2ndYearLevel" "Classes1stAnd2ndYearLevel11To25"
[3] "Classes1stAnd2ndYearLevel26To50"      "Classes1stAnd2ndYearLevel51To100"
[5] "Classes1stAnd2ndYearLevel101To250"     "Classes1stAnd2ndYearLevel251To500"
[7] "ClassesClassSizes3rdAnd4thYearLevel"  "Classes3rdAnd4thYearLevel11To25"
[9] "Classes3rdAnd4thYearLevel26To50"       "Classes3rdAnd4thYearLevel101To250"
[11] "Classes3rdAnd4thYearLevel251To500"     "FinancesStudentServicesPercOfBudget"

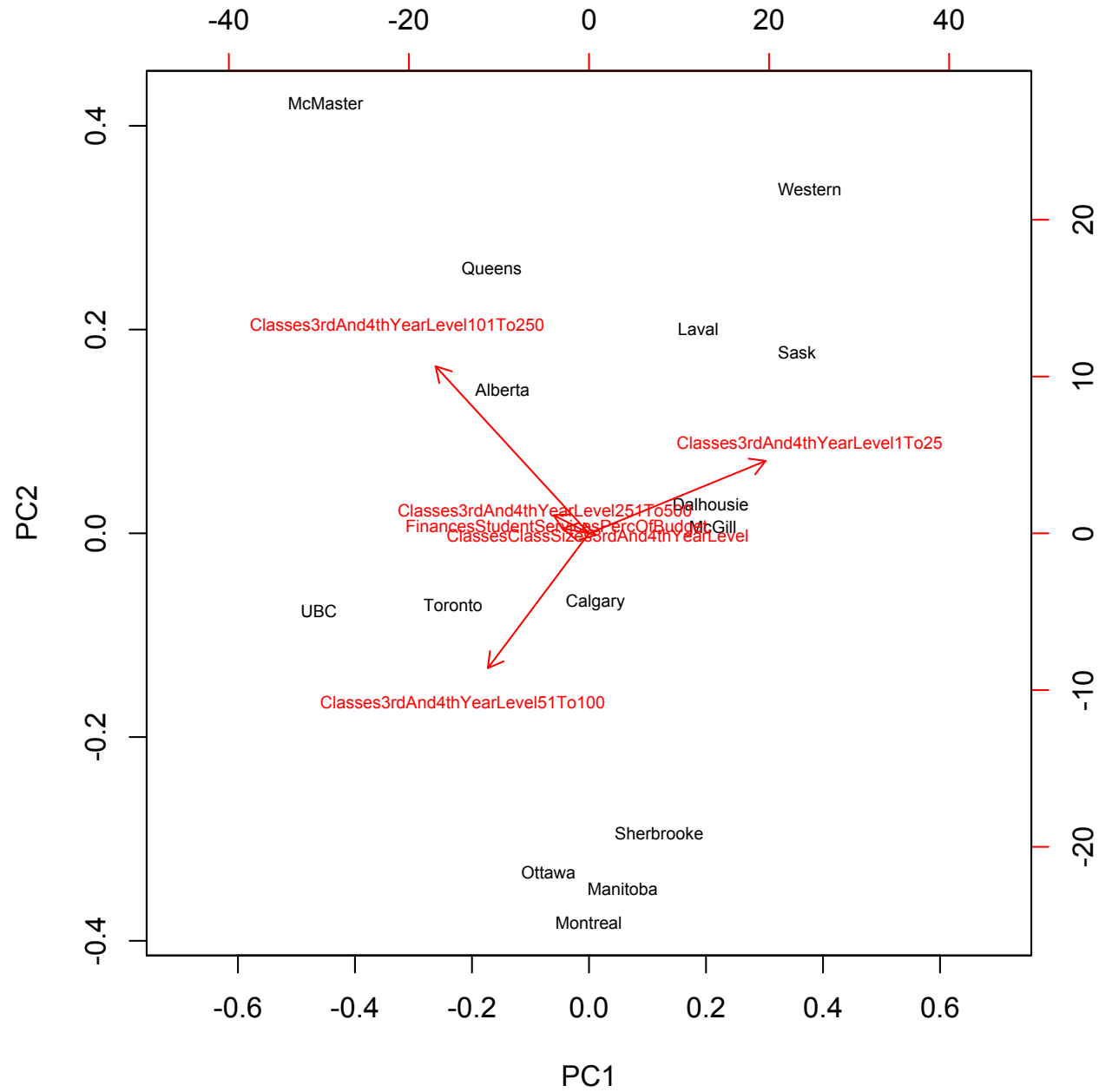
> plot(prcomp(Mcleans[,cutree(Mcvag,12) %in% (7:8)]))
> biplot(prcomp(Mcleans[,cutree(Mcvag,12) %in% (7:8)]),
+ cex=0.6,xlim=c(-.7,.7))
```

Variances

`prcomp(Mcleans[, cutree(Mcvag, 12) %in% (7:8)])`

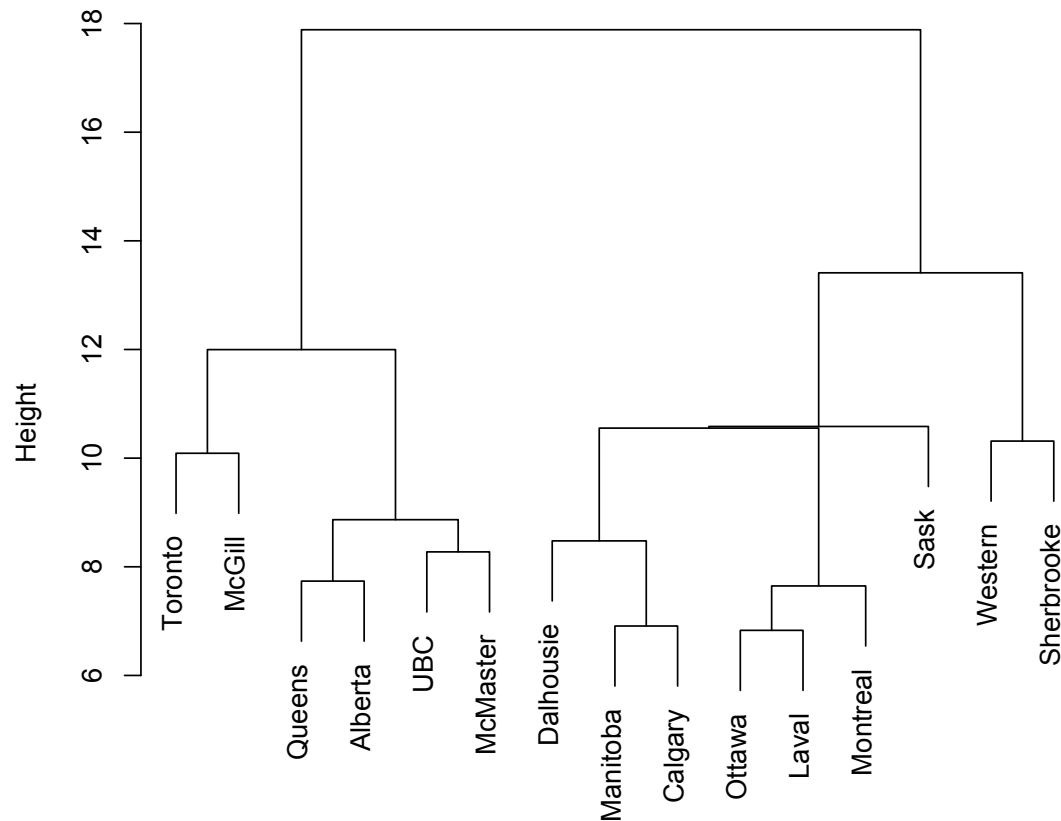


Biplot



How about universities?

Dendrogram of `diana(x = daisy(Mcleans, stand = TRUE))`



`daisy(Mcleans, stand = TRUE)`
`diana (*, "NA")`

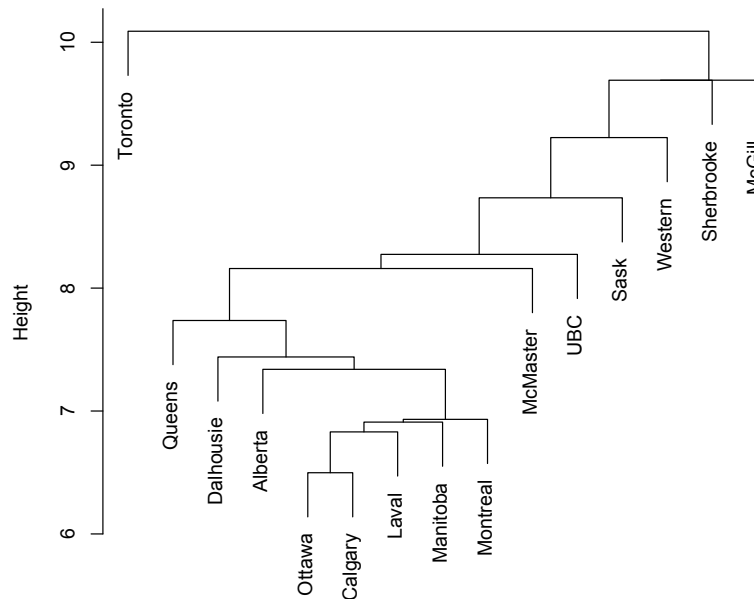
Divisive hierarchical clustering - the other versions yield similar results, except for the single linkage - see next page, also, for the explanation for the “doubled lines” in the right-hand side

Odds and ends

```
1. > diana(daisy(Mcleans,stand=TRUE))$height
[1] 10.089735 11.997787 7.736485 8.867114 8.274415
[61] 7.885711 8.476898 6.909834 10.552828 6.830103
[11] 7.647387 10.582905 13.411259 10.313927
```

2.

Dendrogram of `agnes(x = daisy(Mcleans, stand = TRUE), method = "sing`



`daisy(Mcleans, stand = TRUE)`
`agnes (*, "single")`

3. Note: standardization is a must here, otherwise we would cluster pretty much in the original variables 26, 28, 30, and 33.

Model-based clustering

Distance-base methods - work well, when distances can be trusted.

For instance, Euclidean distance can substantially depend on the scaling of the original variables.

Fitting mixtures of distributions (multivariate normal)