Principal Components

Principal Components

- Have measurements on (possibly large) number of variables on some individuals.
- Question: can we describe data using fewer variables (because original variables correlated in some way)?
- Look for direction (linear combination of original variables) in which values *most spread out*. This is *first principal component*.
- Second principal component then direction uncorrelated with this in which values then most spread out. And so on.

Principal components

- See whether small number of principal components captures most of variation in data.
- Might try to interpret principal components.
- If 2 components good, can make plot of data.
- (Like discriminant analysis, but no groups.)
- "What are important ways that these data vary?"

Packages

You might not have installed the first of these. See over for instructions.

```
library(ggbiplot) # see over
library(tidyverse)
library(ggrepel)
```

Installing ggbiplot

- ggbiplot not on CRAN, so usual install.packages will not work. This is same procedure you used for smmr in C32:
- Install package devtools first (once):

```
install.packages("devtools")
```

- Then install ggbiplot (once):

```
library(devtools)
install_github("vqv/ggbiplot")
```

Small example: 2 test scores for 8 people

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/test12.txt"
test12 <- read_table2(my_url)
test12
```

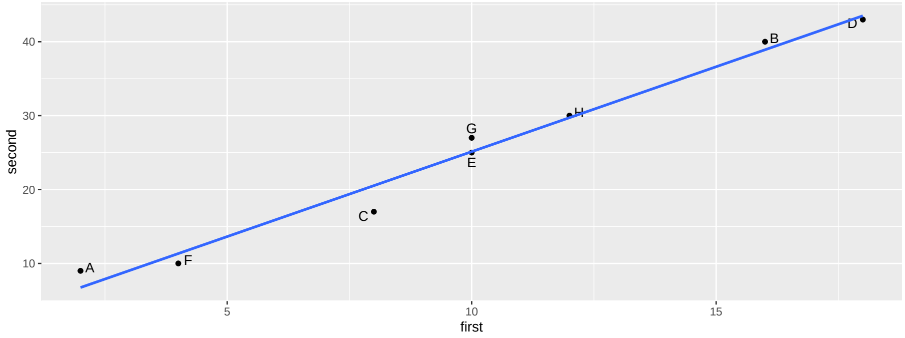
first	second	id
2	9	A
16	40	B
8	17	C
18	43	D
10	25	E
4	10	F
10	27	G
12	30	H

```
g <- ggplot(test12, aes(x = first, y = second, label = id)) +
  geom_point() + geom_text_repel()
```

The plot

```
g + geom_smooth(method = "lm", se = F)
```

```
## `geom_smooth()` using formula 'y ~ x'
```



Principal component analysis

- Grab just the numeric columns:

```
test12 %>% select_if(is.numeric) -> test12_numbers
```

- Strongly correlated, so data nearly 1-dimensional:

```
cor(test12_numbers)
```

```
##            first   second
## first  1.000000 0.989078
## second 0.989078 1.000000
```

Finding principal components

- Make a score summarizing this one dimension. Like this:

```
test12.pc <- princomp(test12_numbers, cor = T)
summary(test12.pc)
```

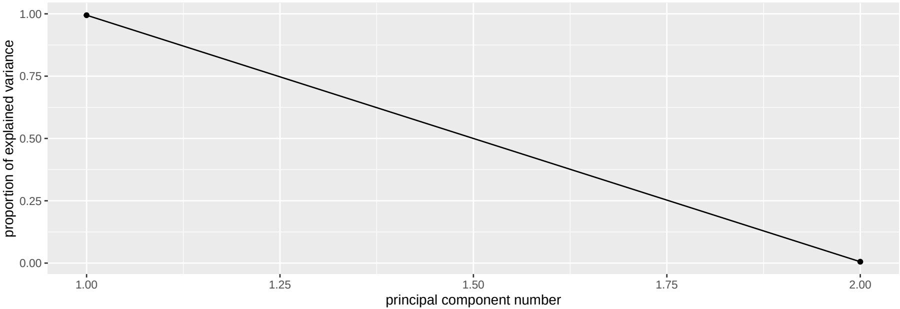
```
## Importance of components:
##                           Comp.1      Comp.2
## Standard deviation     1.410347 0.104508582
## Proportion of Variance 0.994539 0.005461022
## Cumulative Proportion  0.994539 1.000000000
```

Comments

- "Standard deviation" shows relative importance of components (as for LDs in discriminant analysis)
- Here, first one explains almost all (99.4%) of variability.
- That is, look only at first component and ignore second.
- `cor=T` standardizes all variables first. Usually wanted, because variables measured on different scales. (Only omit if variables measured on same scale and expect similar variability.)

Scree plot

```
ggscreeplot(test12.pc)
```



Imagine scree plot continues at zero, so 2 components is a *big* elbow (take one component).

Component loadings

explain how each principal component depends on (standardized) original variables (test scores):

```
test12.pc$loadings
```

```
##
## Loadings:
##        Comp.1 Comp.2
## first   0.707  0.707
## second  0.707 -0.707
##
##                Comp.1 Comp.2
## SS loadings       1.0    1.0
## Proportion Var    0.5    0.5
## Cumulative Var    0.5    1.0
```

First component basically sum of (standardized) test scores. That is, person tends to score similarly on two tests, and a composite score would summarize performance.

Component scores

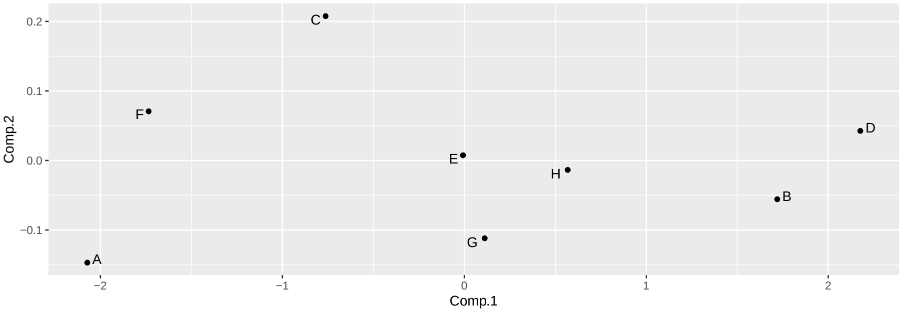
```
d <- data.frame(test12, test12.pc$scores)
d
```

first	second	id	Comp.1	Comp.2
2	9	A	-2.0718190	-0.1469818
16	40	B	1.7198628	-0.0557622
8	17	C	-0.7622897	0.2075895
18	43	D	2.1762675	0.0425333
10	25	E	-0.0074606	0.0074606
4	10	F	-1.7347840	0.0706834
10	27	G	0.1119091	-0.1119091
12	30	H	0.5683139	-0.0136137

- Person A is a low scorer, very negative `comp.1` score.
- Person D is high scorer, high positive `comp.1` score.
- Person E average scorer, near-zero `comp.1` score.

Plot of scores

```
ggplot(d, aes(x = Comp.1, y = Comp.2, label = id)) +
  geom_point() + geom_text_repel()
```



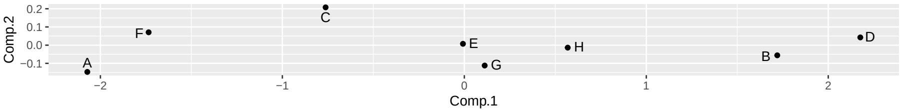
Comments

- Vertical scale exaggerates importance of `comp.2`.
- Fix up to get axes on same scale:

```
g <- ggplot(d, aes(x = Comp.1, y = Comp.2, label = id)) +
  geom_point() + geom_text_repel() +
  coord_fixed()
```

- Shows how exam scores really spread out along one dimension:

```
g
```

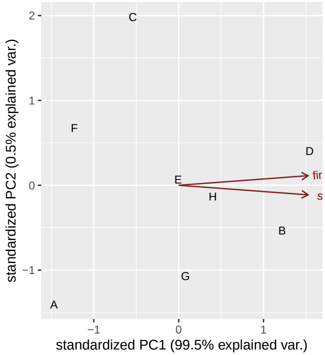


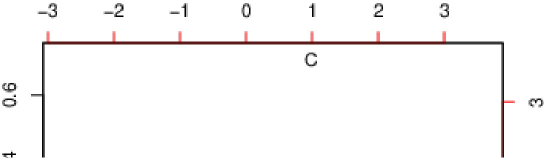
The biplot

- Plotting variables and individuals on one plot.
- Shows how components and original variables related.
- Shows how individuals score on each component, and therefore suggests how they score on each variable.
- Add `labels` option to identify individuals:

```
g <- ggbiplot(test12.pc, labels = test12$id)
```

The biplot


C
F
D
fir
E
H
s
B
G
A
2
1
0
−1
−1
0
1
standardized PC2 (0.5% explained var.)
standardized PC1 (99.5% explained var.)


−3
−2
−1
0
1
2
3
C
0.6
3

Comments

- Variables point almost same direction (left). Thus very negative value on `comp.1` goes with high scores on both tests, and test scores highly correlated.
- Position of individuals on plot according to scores on principal components, implies values on original variables. Eg.:
- D very negative on `comp.1`, high scorer on both tests.
- A and F very positive on `comp.1`, poor scorers on both tests.
- C positive on `comp.2`, high score on first test relative to second.
- A negative on `comp.2`, high score on second test relative to first.

Track running data

Track running records (1984) for distances 100m to marathon, arranged by country. Countries labelled by (mostly) Internet domain names (ISO 2-letter codes):

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/men_track_field.txt"
track <- read_table(my_url)
track %>% sample_n(10)
```

m100	m200	m400	m800	m1500	m5000	m10000	marathon	country
10.34	20.68	45.04	1.73	3.60	13.22	27.45	129.95	be
10.53	21.17	46.70	1.79	3.62	13.13	27.38	128.65	pt
10.34	20.81	45.86	1.79	3.64	13.41	27.72	128.63	jp
10.43	20.69	45.49	1.74	3.61	13.27	27.52	130.87	fi
10.44	20.81	46.82	1.79	3.60	13.26	27.72	135.90	at
10.17	20.22	45.68	1.76	3.63	13.55	28.09	130.15	ca
10.51	20.88	46.10	1.74	3.54	13.21	27.70	128.98	nz
10.35	20.65	45.64	1.76	3.58	13.42	28.19	134.32	cz
10.39	21.09	47.91	1.83	3.84	15.23	32.56	149.90	th
10.40	20.92	46.30	1.82	3.80	14.64	31.01	154.10	my

Country names

Also read in a table to look country names up in later:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/isocodes.csv"
iso <- read_csv(my_url)
iso
```

Country	ISO2	ISO3	M49
Afghanistan	af	afg	4
Aland Islands	ax	ala	248
Albania	al	alb	8
Algeria	dz	dza	12
American Samoa	as	asm	16
Andorra	ad	and	20
Angola	ao	ago	24
Anguilla	ai	aia	660
Antarctica	aq	ata	10
Antigua and Barbuda	ag	atg	28
Argentina	ar	arg	32
Armenia	am	arm	51
Aruba	aw	abw	533

Data and aims

- Times in seconds 100m–400m, in minutes for rest (800m up).
- This taken care of by standardization.
- 8 variables; can we summarize by fewer and gain some insight?
- In particular, if 2 components tell most of story, what do we see in a plot?

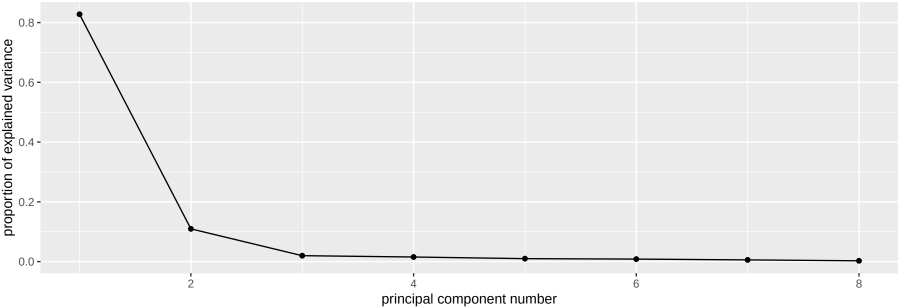
Fit and examine principal components

```
track %>% select_if(is.numeric) -> track_num
track.pc <- princomp(track_num, cor = T)
summary(track.pc)
```

```
## Importance of components:
##                           Comp.1    Comp.2
## Standard deviation     2.5733531 0.9368128
## Proportion of Variance 0.8277683 0.1097023
## Cumulative Proportion  0.8277683 0.9374706
##                            Comp.3     Comp.4
## Standard deviation     0.39915052 0.35220645
## Proportion of Variance 0.01991514 0.01550617
## Cumulative Proportion  0.95738570 0.97289187
##                             Comp.5      Comp.6
## Standard deviation     0.282630981 0.260701267
## Proportion of Variance 0.009985034 0.008495644
## Cumulative Proportion  0.982876903 0.991372547
##                             Comp.7      Comp.8
## Standard deviation     0.215451919 0.150333291
## Proportion of Variance 0.005802441 0.002825012
```

Scree plot

```
ggscreeplot(track.pc)
```



How many components?

- As for discriminant analysis, look for “elbow” in scree plot.
- See one here at 3 components; everything 3 and beyond is “scree”.
- So take 2 components.
- Note difference from discriminant analysis: want “large” rather than “small”, so go 1 step left of elbow.
- Another criterion: any component with eigenvalue bigger than about 1 is worth including. 2nd one here has eigenvalue just less than 1.
- Refer back to `summary`: cumulative proportion of variance explained for 2 components is 93.7%, pleasantly high. 2 components tell almost whole story.

How do components depend on original variables?

Loadings:

```
track.pc$loadings
```

```
##
## Loadings:
##          Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6 Comp.7 Comp.8
## m100      0.318  0.567  0.332  0.128  0.263  0.594  0.136  0.106
## m200      0.337  0.462  0.361 -0.259 -0.154 -0.656 -0.113
## m400      0.356  0.248 -0.560  0.652 -0.218 -0.157
## m800      0.369        -0.532 -0.480  0.540        -0.238
## m1500     0.373 -0.140 -0.153 -0.405 -0.488  0.158  0.610  0.139
## m5000     0.364 -0.312  0.190        -0.254  0.141 -0.591  0.547
## m10000    0.367 -0.307  0.182        -0.133  0.219 -0.177 -0.797
## marathon  0.342 -0.439  0.263  0.300  0.498 -0.315  0.399  0.158
##
##                Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6 Comp.7
## SS loadings     1.000  1.000  1.000  1.000  1.000  1.000  1.000
## Proportion Var  0.125  0.125  0.125  0.125  0.125  0.125  0.125
## Cumulative Var  0.125  0.250  0.375  0.500  0.625  0.750  0.875
```

Comments

- `comp.1` loads about equally (has equal weight) on times over all distances.
- `comp.2` has large positive loading for short distances, large negative for long ones.
- `comp.3`: large negative for middle distance, large positive especially for short distances.
- Country overall good at running will have lower than average record times at all distances, so `comp.1` *small*. Conversely, for countries bad at running, `comp.1` very positive.
- Countries relatively better at sprinting (low times) will be *negative* on `comp.2`; countries relatively better at distance running *positive* on `comp.2`.

Commands for plots

- Principal component scores (first two). Also need country IDs.

```
d <- data.frame(track.pc$scores,
  country = track$country
)
names(d)
```

```
## [1] "Comp.1"  "Comp.2"  "Comp.3"  "Comp.4"  "Comp.5"  "Comp
## [7] "Comp.7"  "Comp.8"  "country"
```

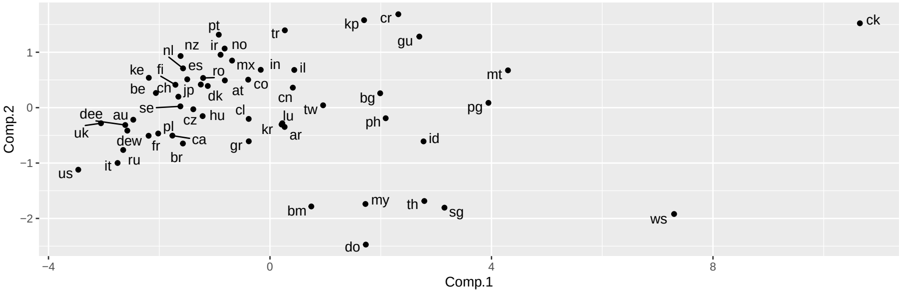
```
g1 <- ggplot(d, aes(x = Comp.1, y = Comp.2,
  label = country)) +
  geom_point() + geom_text_repel() + coord_fixed()
```

- Biplot:

```
g2 <- ggbiplot(track.pc, labels = track$country)
```

Principal components plot

g1

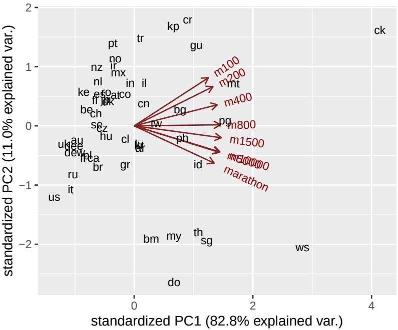


Comments on principal components plot

- Good running countries at left of plot: US, UK, Italy, Russia, East and West Germany.
- Bad running countries at right: Western Samoa, Cook Islands.
- Better sprinting countries at bottom: US, Italy, Russia, Brazil, Greece. `do` is Dominican Republic, where sprinting records relatively good, distance records very bad.
- Better distance-running countries at top: Portugal, Norway, Turkey, Ireland, New Zealand, Mexico. `ke` is Kenya.

Biplot

```
g2
```



standardized PC1 (82.8% explained var.)
standardized PC2 (11.0% explained var.)
m100
m200
m400
m800
m1500
marathon

Comments on biplot

- Had to do some pre-work to interpret PC plot. Biplot more self-contained.
- All variable arrows point right; countries on right have large (bad) record times overall, countries on left good overall.
- Imagine that variable arrows extend negatively as well. Bottom right = bad at distance running, top left = good at distance running.
- Top right = bad at sprinting, bottom left = good at sprinting.
- Doesn't require so much pre-interpretation of components.

Best 8 running countries

Need to look up two-letter abbreviations in ISO table:

```
d %>%
  arrange(Comp.1) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.1, country, Country) %>%
  slice(1:8)
```

Comp.1	country	Country
-3.462175	us	United States of America
-3.052104	uk	United Kingdom
-2.752084	it	Italy
-2.651062	ru	Russian Federation
-2.613964	dee	East Germany
-2.576272	dew	West Germany
-2.468919	au	Australia
-2.191917	fr	France

Worst 8 running countries

```
d %>%
  arrange(desc(Comp.1)) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.1, country, Country) %>%
  slice(1:8)
```

Comp.1	country	Country
10.652914	ck	Cook Islands
7.297865	ws	Samoa
4.297909	mt	Malta
3.945224	pg	Papua New Guinea
3.150886	sg	Singapore
2.787272	th	Thailand
2.773125	id	Indonesia
2.697066	gu	Guam

Better at distance running

```
d %>%
  arrange(desc(Comp.2)) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.2, country, Country) %>%
  slice(1:10)
```

Comp.2	country	Country
1.6860391	cr	Costa Rica
1.5791490	kp	Korea (North)
1.5226742	ck	Cook Islands
1.3957839	tr	Turkey
1.3167578	pt	Portugal
1.2829272	gu	Guam
1.0663756	no	Norway
0.9547437	ir	Iran, Islamic Republic of
0.9318729	nz	New Zealand
0.8495104	mx	Mexico

Better at sprinting

```
d %>%
  arrange(Comp.2) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.2, country, Country) %>%
  slice(1:10)
```

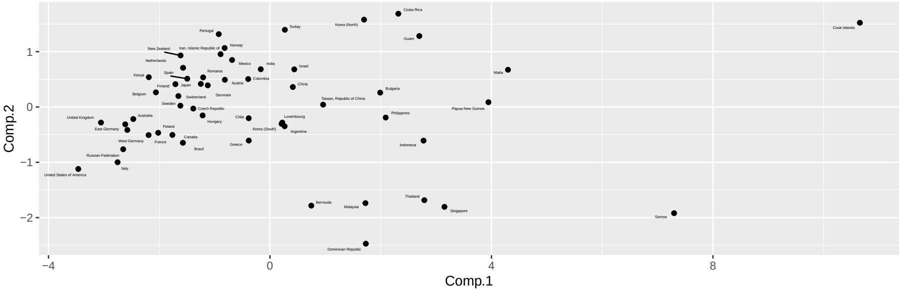
Comp.2	country	Country
-2.4715736	do	Dominican Republic
-1.9196130	ws	Samoa
-1.8055052	sg	Singapore
-1.7832229	bm	Bermuda
-1.7386063	my	Malaysia
-1.6851772	th	Thailand
-1.1204235	us	United States of America
-0.9989821	it	Italy
-0.7639385	ru	Russian Federation
-0.6470634	br	Brazil

Plot with country names

```
g <- d %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.1, Comp.2, Country) %>%
  ggplot(aes(x = Comp.1, y = Comp.2, label = Country)) +
  geom_point() + geom_text_repel(size = 1) +
  coord_fixed()
```

The plot

```
g
```



Costa Rica
Korea (North)
Cook Islands
Turkey
Portugal
Guam
Norway
New Zealand
Iran, Islamic Republic of
Netherlands
Mexico
India
Israel
Malta
Kenya
Spain
Romania
Colombia
Austria
Finland
Japan
China
Bulgaria
Belgium
Switzerland
Denmark
Taiwan, Republic of China
Sweden
Czech Republic
Papua New Guinea
United Kingdom
Australia
Chile
Luxembourg
Philippines
Hungary
East Germany
Poland
Korea (South)
Argentina
Canada
West Germany
France
Greece
Indonesia
Brazil
Russian Federation
Italy
United States of America
Thailand
Bermuda
Malaysia
Singapore
Samoa
Dominican Republic
1
0
−1
−2
Comp.2
−4
0
4
8
Comp.1

Principal components from correlation matrix

Create data file like this:

```
 1          0.9705 -0.9600
 0.9705    1       -0.9980
-0.9600   -0.9980   1
```

and read in like this:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/cov.txt"
mat <- read_table(my_url, col_names = F)
mat
```

X1	X2	X3
1.0000	0.9705	-0.960
0.9705	1.0000	-0.998
-0.9600	-0.9980	1.000

Pre-processing

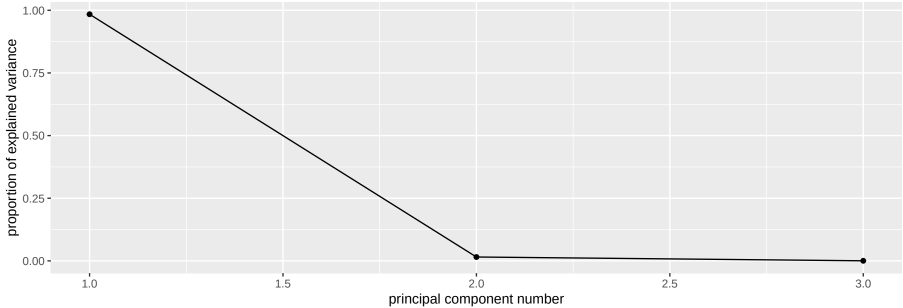
A little pre-processing required:

- Turn into matrix (from data frame)
- Feed into `princomp` as `covmat=`

```
mat.pc <- mat %>%
  as.matrix() %>%
  princomp(covmat = .)
```

Scree plot: one component fine

```
ggscreeplot(mat.pc)
```



Component loadings

Compare correlation matrix:

```
mat
```

X1	X2	X3
1.0000	0.9705	-0.960
0.9705	1.0000	-0.998
-0.9600	-0.9980	1.000

with component loadings

```
mat.pc$loadings
```

```
##
## Loadings:
##    Comp.1 Comp.2 Comp.3
## X1  0.573  0.812  0.112
## X2  0.581 -0.306 -0.755
## X3 -0.578  0.498 -0.646
##
##                Comp.1 Comp.2 Comp.3
## SS loadings     1.000  1.000  1.000
```

Comments

- When X1 large, X2 also large, X3 small.
    - Then `comp.1` *positive*.
- When X1 small, X2 small, X3 large.
    - Then `comp.1` *negative*.

No scores

- With correlation matrix rather than data, no component scores
    - So no principal component plot
    - and no biplot.