Principal Component Analysis and Singular Value Decomposition

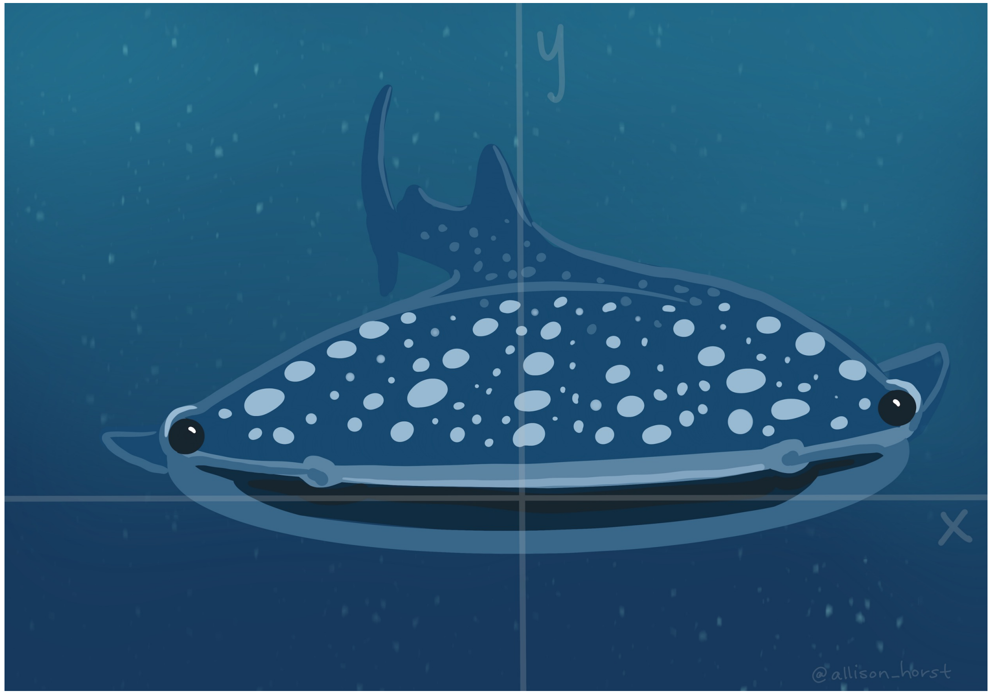
Vincent Guillemot

Mental images

Potato Chips Analysis

Cut the yummiest French fries

Whale versus krill: this is you (credit: Allison Horst)



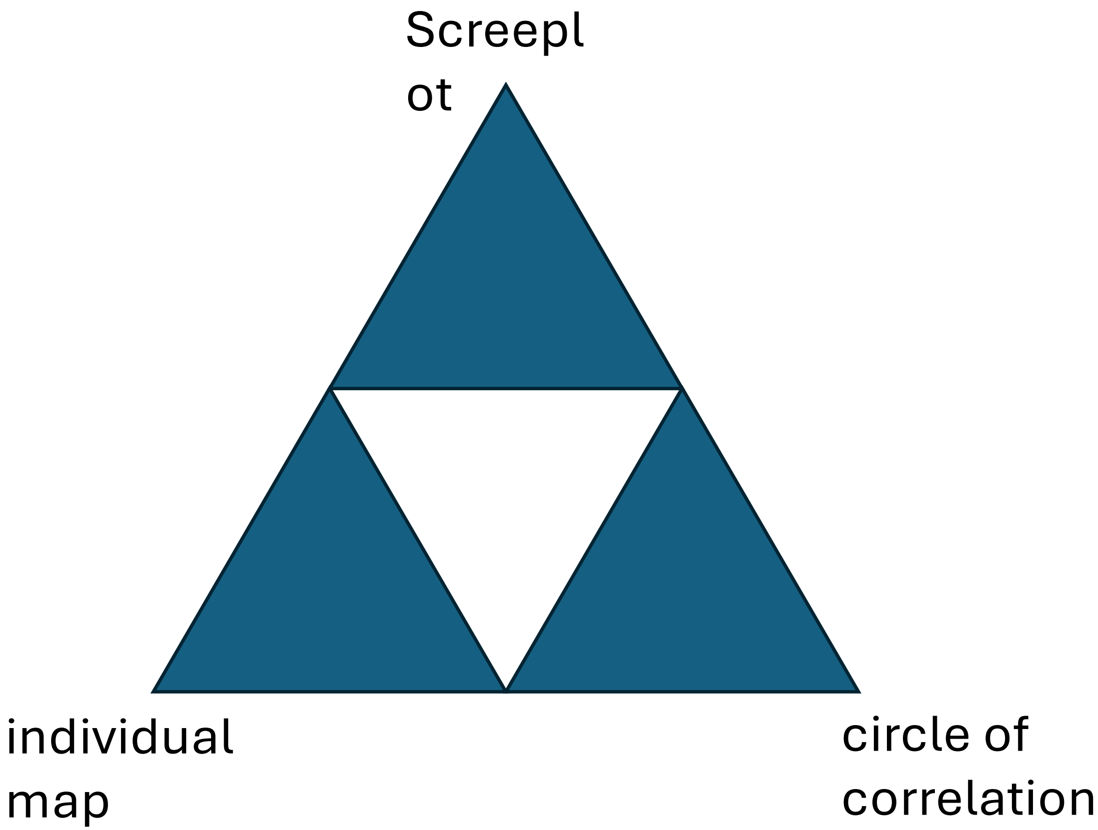
Eat the most krill (put on your 3D glasses)

Whale versus krill: this is your data (credit: Allison Horst)

Eat the most krill (put on your 3D glasses)

Artwork by @allison_hor

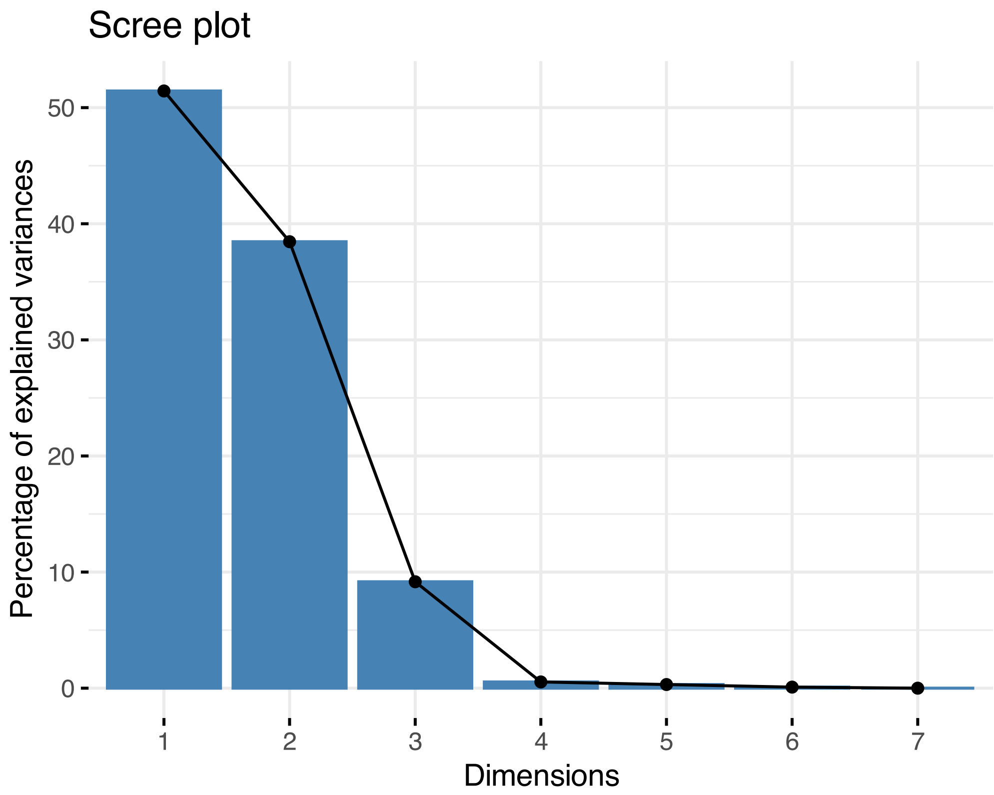
The tri-force of PCA



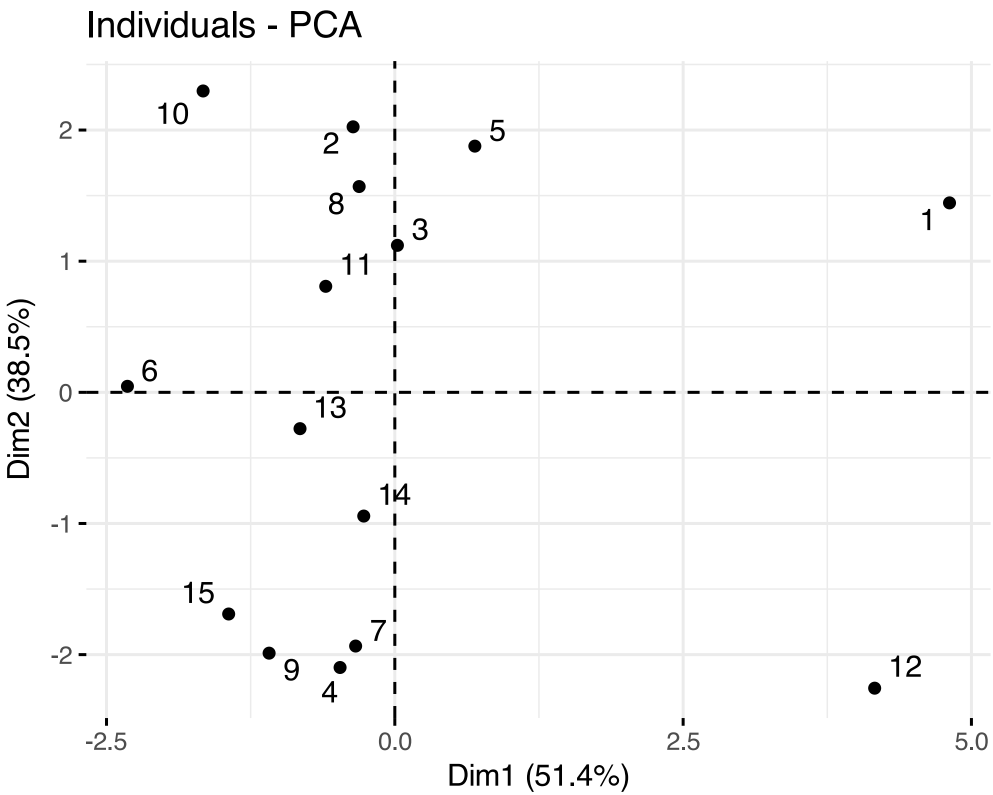
Example data

```r
n <- 15
dat.ex <- tibble(
  X1 = rnorm(n),
  X2 = rnorm(n),
  X3 = -X1,
  X4 = 2 * X2  + 0.25 * rnorm(n),
  X5 = X1 + X2 + 0.25 * rnorm(n),
  X6 = X1 - X2 + 0.25 * rnorm(n),
  X7 = rnorm(n)
)
```

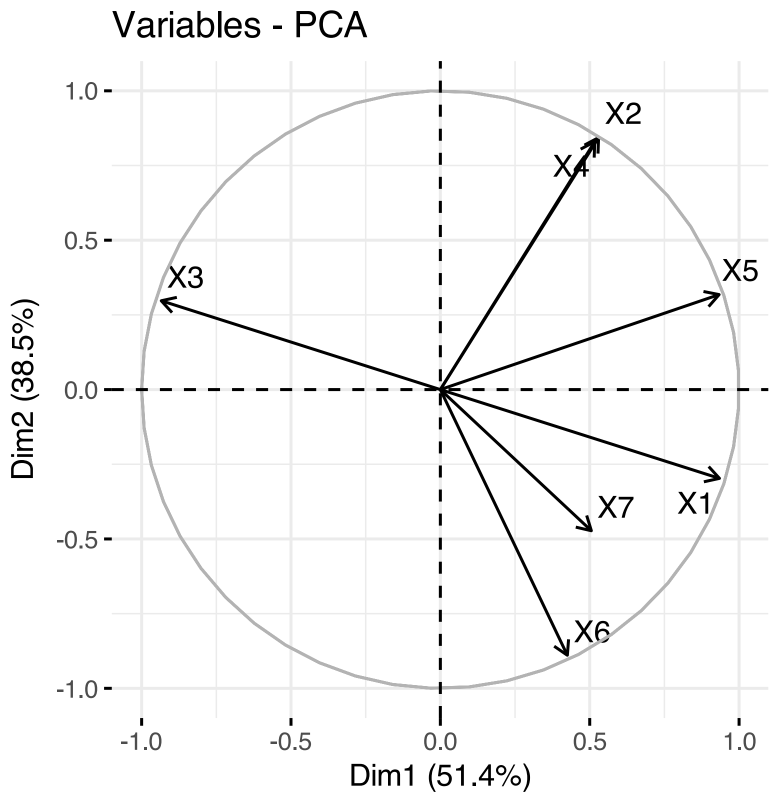
Example screeplot



Example individual map



Example circle of correlation



Vocabulary

French versus English

"Aaaaah, mais acépé en fait c'est la PCA !"

(Anonymous student, after 6 hours of teaching PCA in French)

English	French
PCA = principal component analysis	ACP = analyse en composantes principales
SVD = singular value decomposition	SVD = décomposition en valeurs singulières
EVD = eigenvalue decomposition	décomposition en éléments propres
ICA = independent component analysis	ICA = analyse en composantes indépendantes
MDS = multidimensional	MDS = multidimensional

R vocabulary

Base methods:

- `eigen` for eigenvalue decomposition, `svd` for singular value decomposition,
- `prcomp` and `princomp` for PCA,
- `biplot`

Nice packages:

- `FactoMineR`: `PCA`, `MFA`, `CA`, `MCA` and associates. In earlier versions, the graphs were “crude”…
- `factoextra`: “helper” package to make beautiful plots, and much more!
- `ade4`: more than “one block” type of analyses. Made by ecologists so ⇒ PCOA, coinertia analysis, STATIS, etc.
- `ExPosition`: made for psychometricians (they like PLS)

And a few nice books and papers

MOOC analyse de données de François Husson : https://husson.github.io/MOOC_AnaDo/index.html

(also in English)

PCA paper(s) by Hervé Abdi:

https://personal.utdallas.edu/~herve/abdi-awPCA2010.pdf

(more?)

A little bit of Math

Notations

(non-universal) Conventions: matrices and vectors are **bold**

- n = number of observations, p = number of variables (only quantitative)
- i for an individual observation, and j for a single variable
- $\mathbf{X}$ = data matrix, with n rows and p columns, sometimes already centered, and scaled, to make our life easy
- $\mathbf{X}_j$ = variable j, and jth column of $\mathbf{X}$
- $\mathbf{w}$ a set of weights

A little detour: matrix multiplication

Take a pen and paper, and do this multiplication:

$$\begin{bmatrix} 1 & -1 \\ 0 & 1 \\ 2 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 2 & 3 & 4 \\ -1 & 0 & 0 & 1 \end{bmatrix}$$

Cool video: 5 ways to see matrix multiplication

PCA

> "Find a linear combination of the columns of the data that would capture the most information."

In mathematical words, find

$$\mathbf{Xw} = w_1\mathbf{X}_1 + \cdots + w_p\mathbf{X}_p$$

that maximizes… wait a minute! What are the dimensions?

- $\mathbf{X}$: n rows and p columns,
- $\mathbf{w}$: p rows and 1 columns,
- $\mathbf{Xw}$: n rows and 1 column.

The mathematical translation of the intuitions

Most popular intuition of PCA: how does it translate?

"PCA creates a linear combination of variables that maximizes variance."

$$\arg\max_{\|\mathbf{w}\|_2^2=1} \operatorname{var}(\mathbf{Xw})$$

- Why $\| \mathbf{w} \|_2 = 1$?
- Dirty trick: $\operatorname{var}(\mathbf{Xw}) = \mathbf{w}^\top \mathbf{X}^\top \mathbf{Xw}$

Least “well-known” intuition of PCA: how does it translate?

“PCA creates a linear combination of variables that maximizes correlation.”

$$\underset{\mathbf{w}}{\operatorname{argmax}} \sum_{j=1}^{p} \operatorname{cor}\left(\mathbf{X}\mathbf{w}, \mathbf{X}_j\right)^2$$

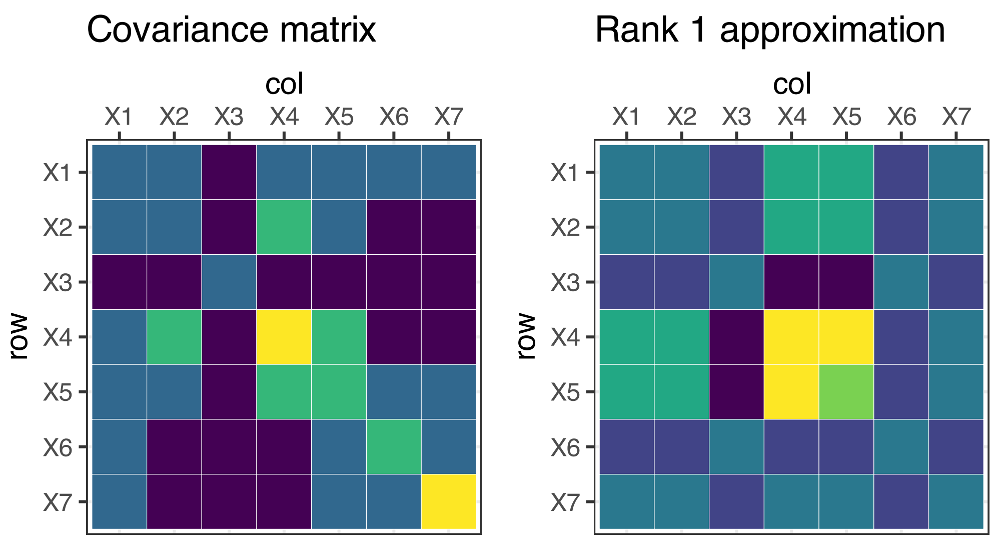
Second least "well-known" intuition of PCA: how does it translate?

"PCA creates the best lower rank approximation of the covariance matrix."

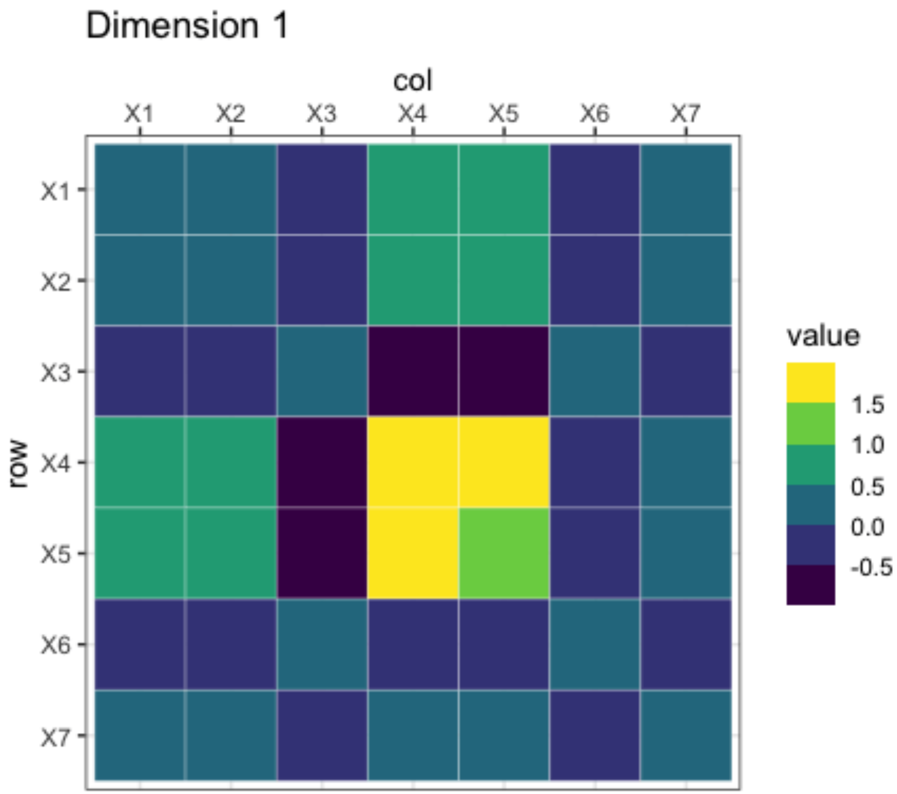
$$\arg\min_{\|w\|_2^2=1} \left\| \frac{1}{n}\mathbf{X}^\top\mathbf{X} - \lambda\mathbf{w}\mathbf{w}^\top \right\|_F^2$$

- $\frac{1}{n}\mathbf{X}^\top\mathbf{X}$
- λ: the [blank] of the covariance matrix
- $\mathbf{w}$: the [blank] of the covariance matrix

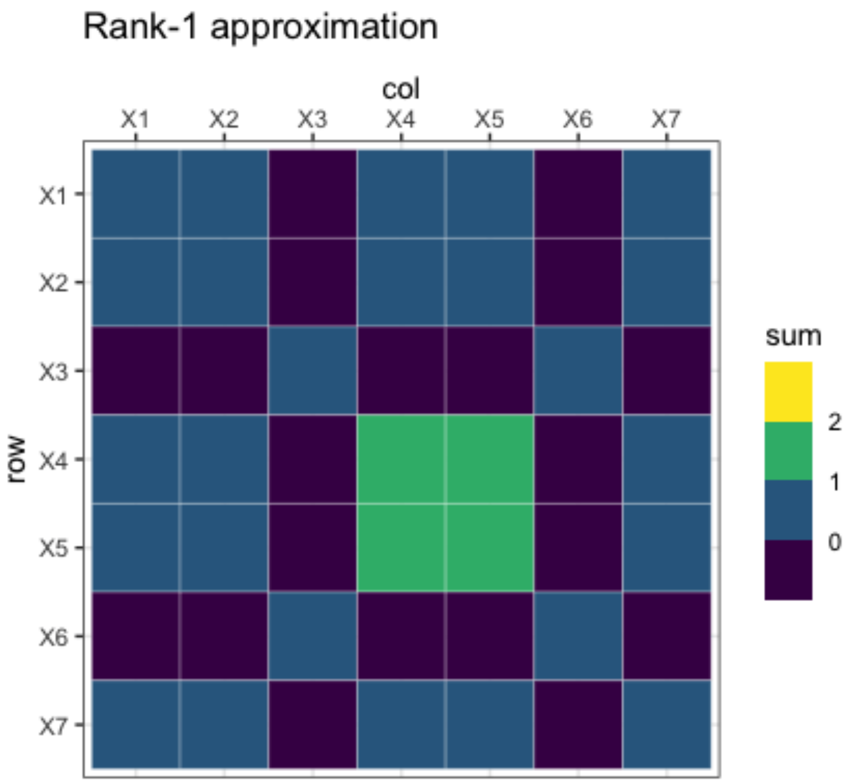
A little image



Rank-1 approximations



Increasing rank approximations



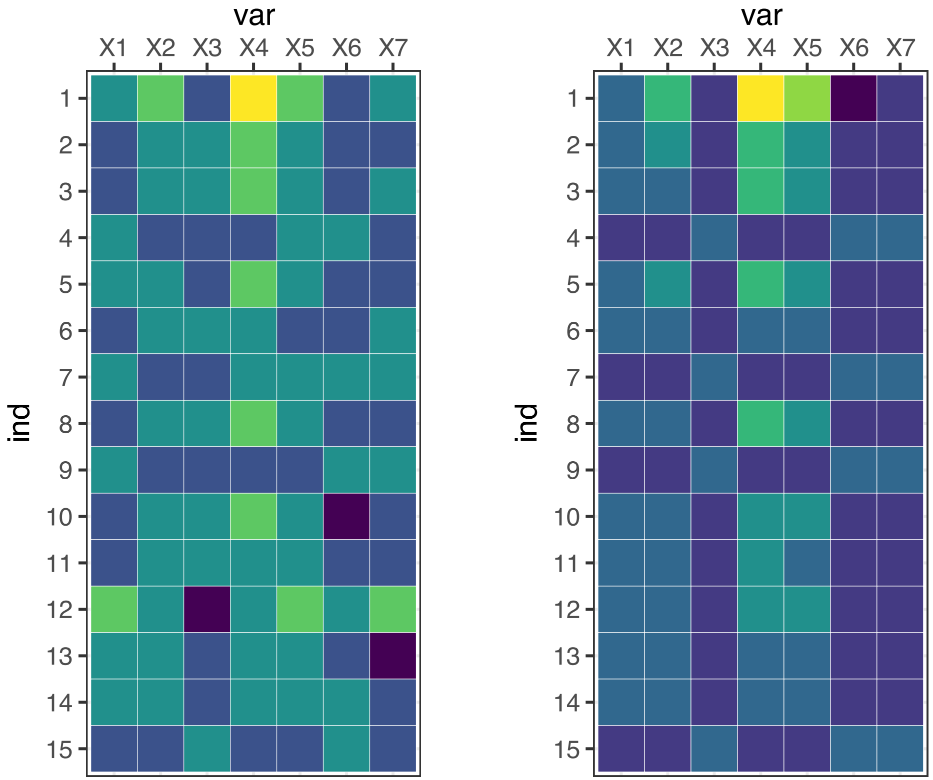
We can do the same kind of magic with the data itself

Singular value decomposition can be used to approximate a rectangular matrix with a lower ranked matrix of the same dimension

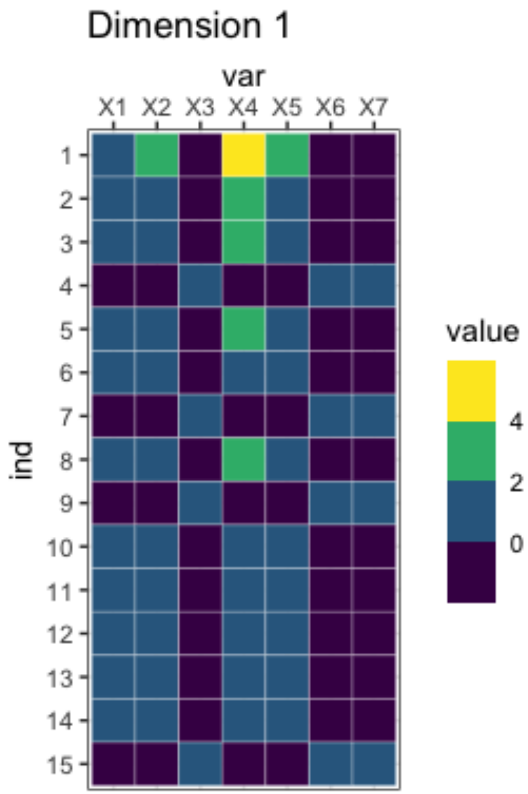
$$\arg\min_{\|\mathbf{u}\|_2^2=\|\mathbf{w}\|_2^2=1} \|\mathbf{X} - \delta\mathbf{u}\mathbf{w}^\top\|_F^2$$

- δ: singular value
- $\mathbf{u}$: left singular vector
- $\mathbf{w}$: right singular vector

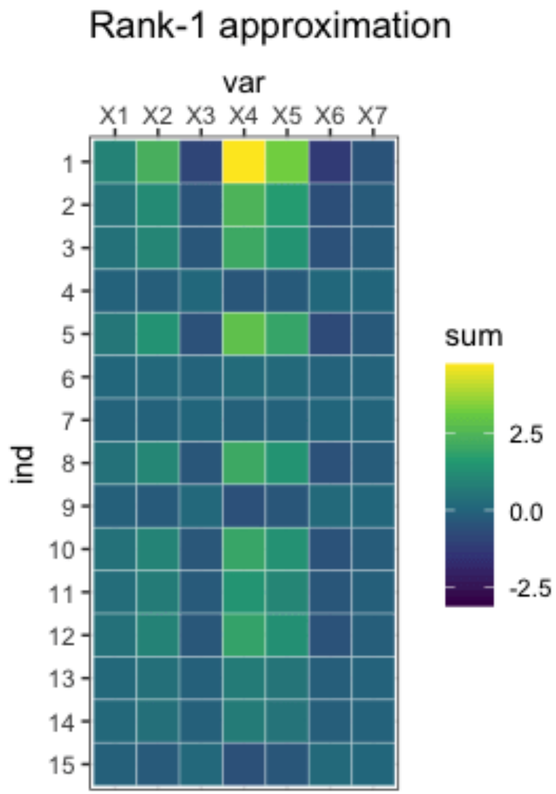
Rank 1 approximation



Rank-1 approximations



Increasing rank approximations



```
library(dplyr)
library(FactoMineR)
library(factoextra)
library(ggplot2)


n <- 15
dat.ex <- tibble(
 X1 = rnorm(n),
 X2 = rnorm(n),
 X3 = -X1,
 X4 = 2 * X2  + 0.25 * rnorm(n),
 X5 = X1 + X2 + 0.25 * rnorm(n),
 X6 = X1 - X2 + 0.25 * rnorm(n),
 X7 = rnorm(n)
)
```

```
res.pca.ex <- PCA(dat.ex, scale.unit = TRUE, graph = FALSE)
fviz_screeplot(res.pca.ex)
fviz_pca_ind(res.pca.ex, repel = TRUE)
fviz_pca_var(res.pca.ex, repel = TRUE)
```