PCA: Overview

Introduction to Statistical Modelling

Prof. Joris Vankerschaver

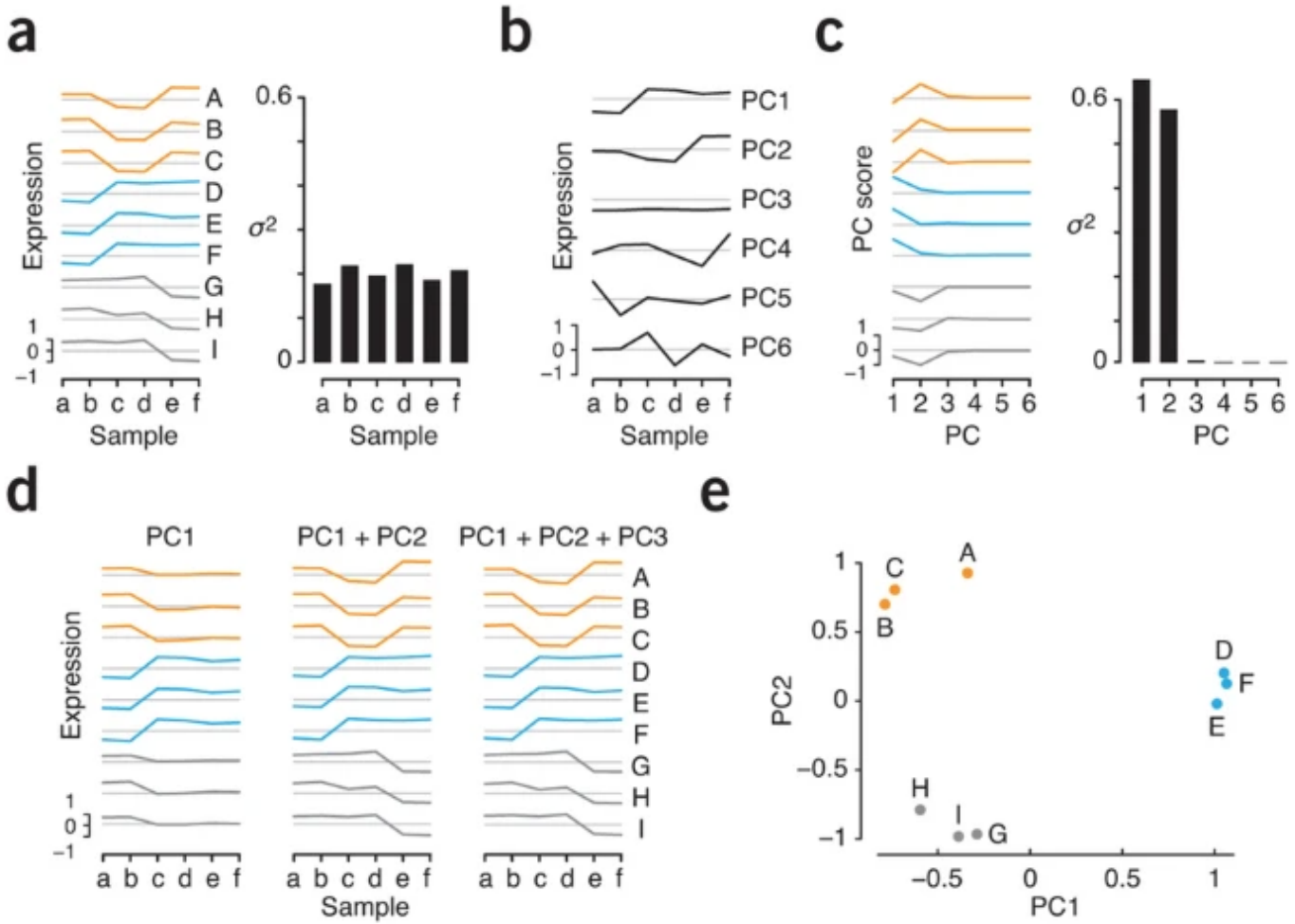
What is dimensionality reduction?

What and why

- Reduce the number of variables ("dimensionality") in a dataset **in a principled way**.
- Useful for
  - Visualization
  - Data preprocessing
  - Computational efficiency
- Many different approaches
  - Principal component analysis (this course)
  - Multidimensional scaling
  - t-SNE, UMAP, ...

Visualization

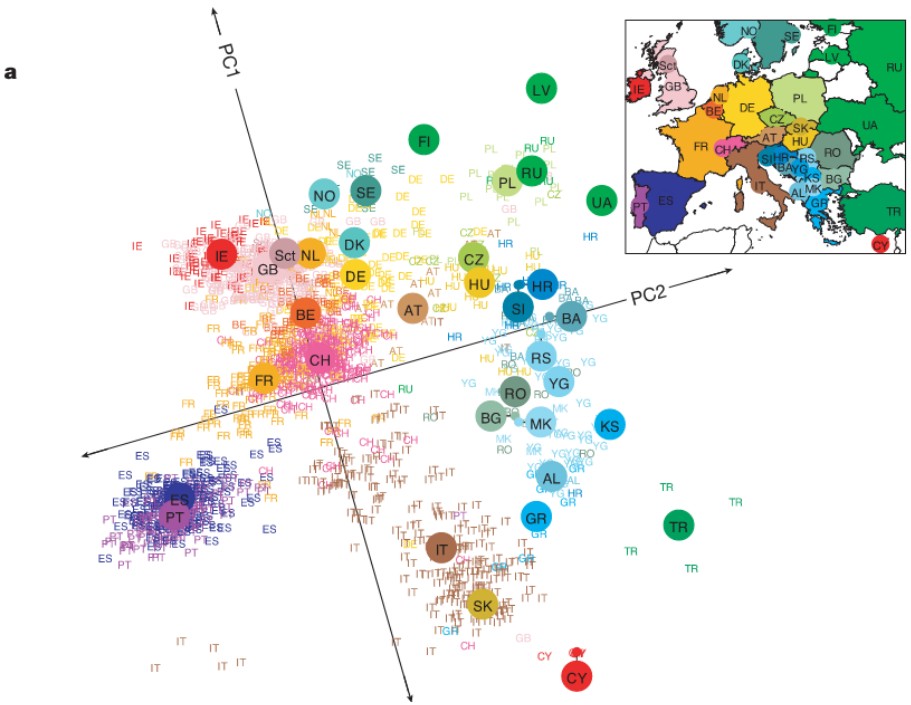
Figure 2: PCA reduction of nine expression profiles from six to two dimensions.



From: Lever et al., *Principal component analysis*, Nature Methods, Vol. 14, p. 641–642, 2017.

Visualization

Genotype data 197,146 loci in 1387 Europeans, summarized in two principal components (left) and compared to geographical origin (right).

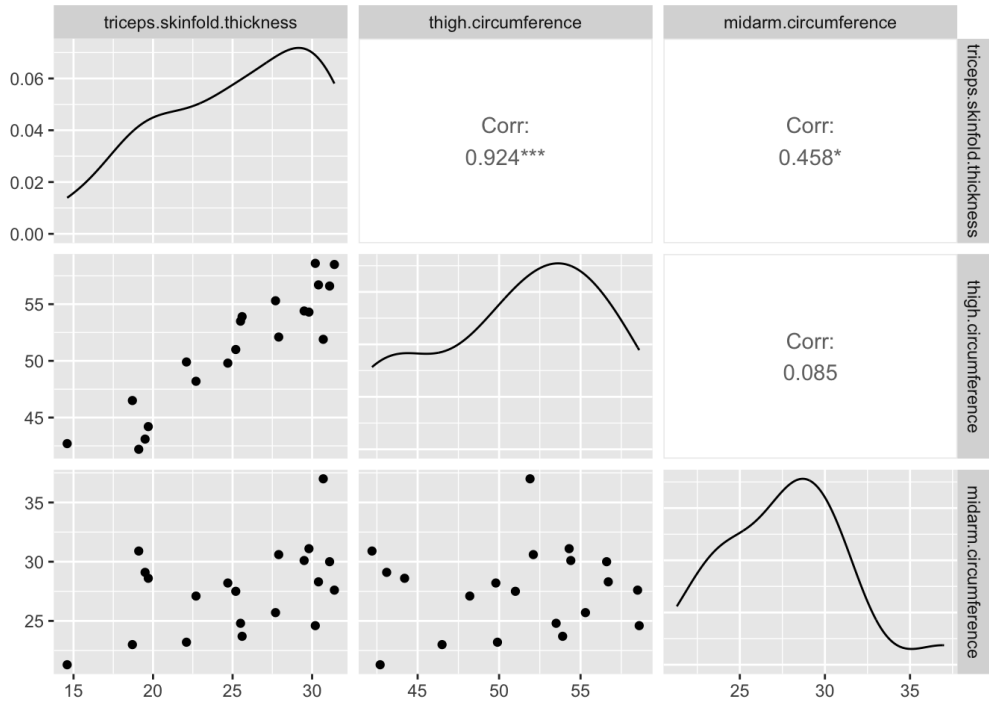


From: Novembre et al., *Genes mirror geography within Europe*, Nature, Vol. 456, 6 November 2008.

Data preprocessing

Bodyfat dataset:

- Suffered from high multicollinearity.
- Conclusions from regression model are doubtful.

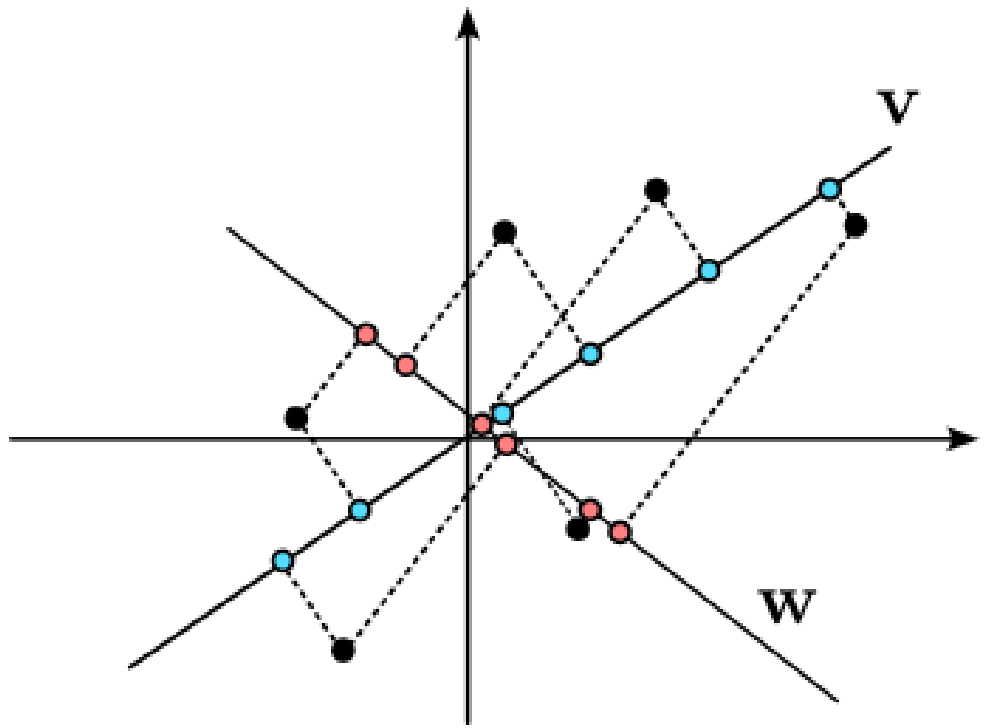


Computational efficiency

- A 250 x 250 image consists of $250^2 = 62{,}500$ pixels.
- Not all pixels are equally informative.
- Extract signal that is maximally informative, discard rest.

Principal component analysis

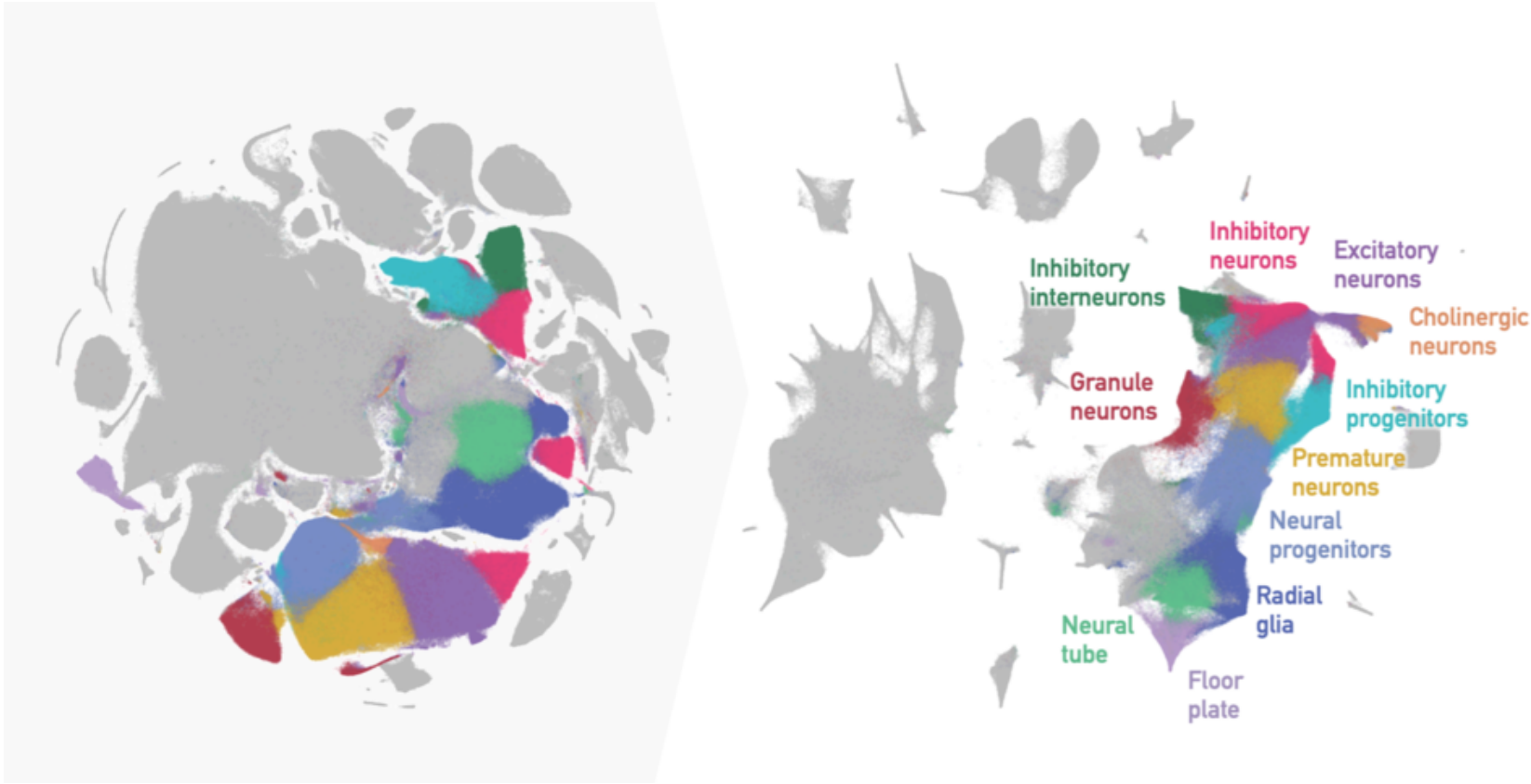
- Covered in this course.
- Works by finding directions in which **variance is maximized**.
- Good first choice, not so good if patterns are highly nonlinear.



Other dimensionality reduction methods

t-SNE, UMAP:

- Useful for highly nonlinear relations between features.
- "Deforms" data so that local structure is maintained.
- Frequently used in single-cell RNA sequencing analysis.



From https://