Visualising High-dimensional Data with R

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https://statsocaus.github.io/tutorial_highd_vis/

Session 1

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Outline

time	topic
1:00-1:20	Introduction: What is high-dimensional data, why visualise and overview of methods
1:20-1:45	Basics of linear projections, and recognising high-d structure
1:45-2:30	Effectively reducing your data dimension, in association with non-linear dimension reduction
2:30-3:00	BREAK

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Introduction

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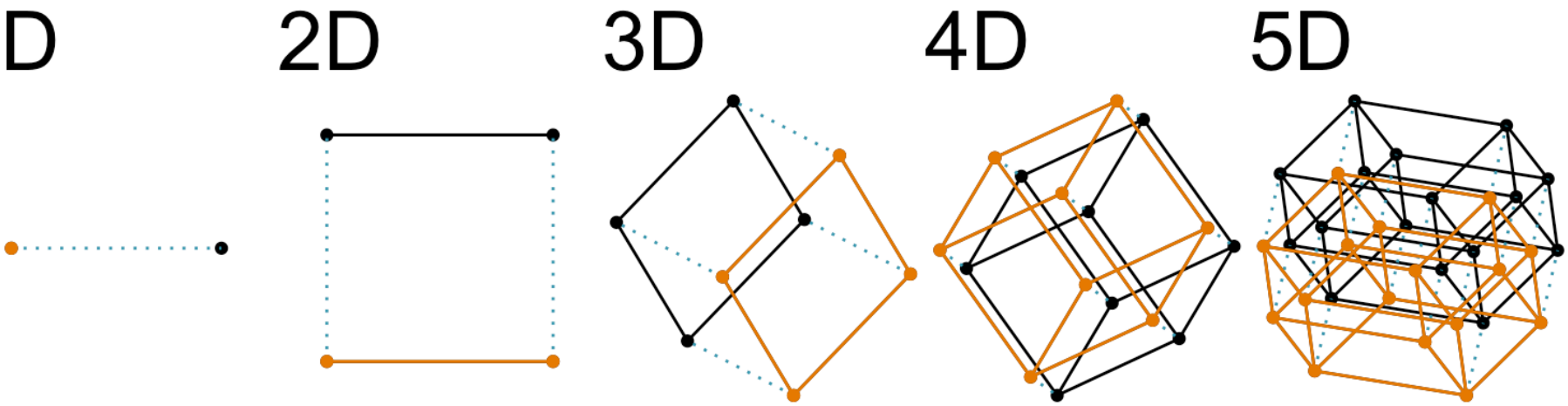
What is high-dimensional space?



Increasing dimension adds an additional orthogonal axis.

If you want more high-dimensional shapes there is an R package, geozoo, which will generate cubes, spheres, simplices, mobius strips, torii, boy surface, klein bottles, cones, various polytopes, …

And read or watch Flatland: A Romance of Many Dimensions (1884) Edwin Abbott.

Notation: Data

$$X_{n\times p} = [X_1\ X_2\ \dots\ X_p]_{n\times p} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}_{n\times}$$

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Notation: Projection

$$A_{p\times d} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1d} \\ a_{21} & a_{22} & \dots & a_{2d} \\ \vdots & \vdots & & \vdots \\ a_{p1} & a_{p2} & \dots & a_{pd} \end{bmatrix}_{p\times d}$$

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Notation: Projected data

$$Y_{n\times d} = XA = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1d} \\ y_{21} & y_{22} & \cdots & y_{2d} \\ \vdots & \vdots & & \vdots \\ y_{n1} & y_{n2} & \cdots & y_{nd} \end{bmatrix}_{n\times d}$$

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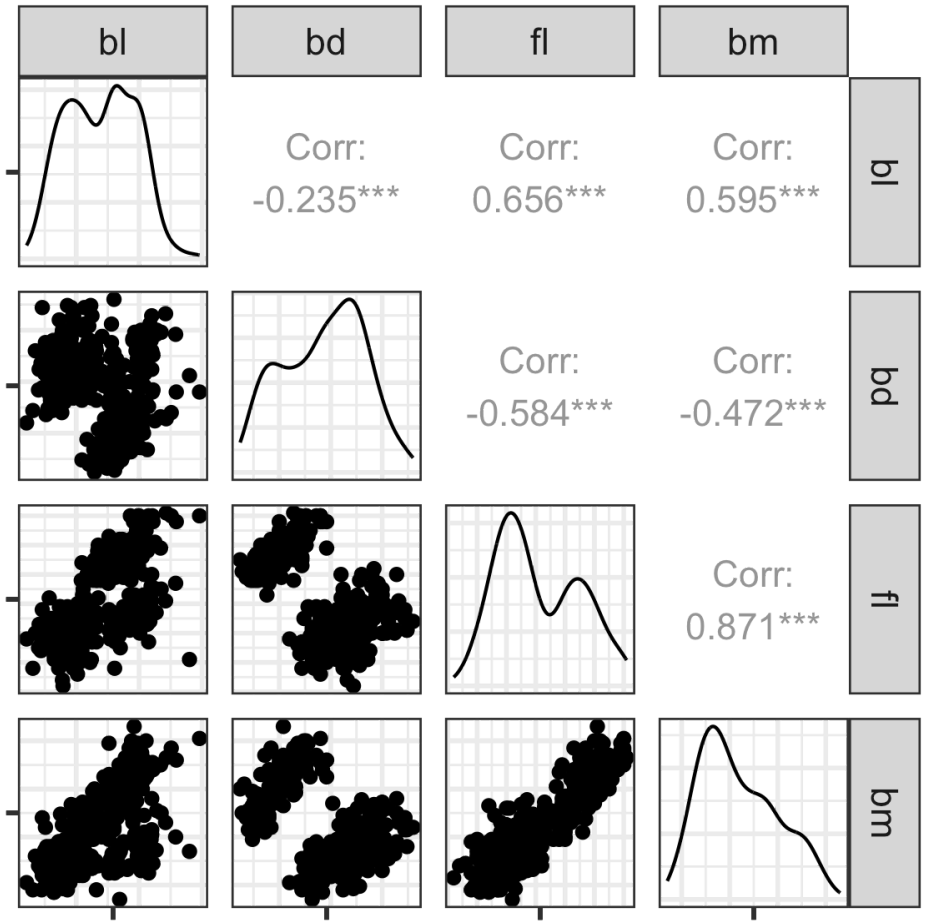
Why? (1/2)

Scatterplot matrix

Here, we see linear association, clumping and clustering, potentially some outliers.



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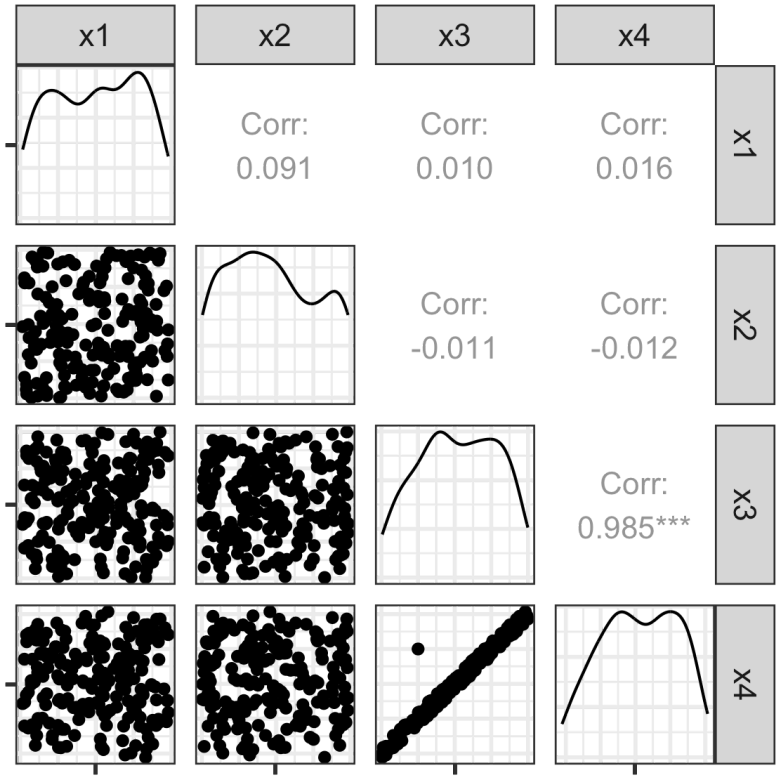
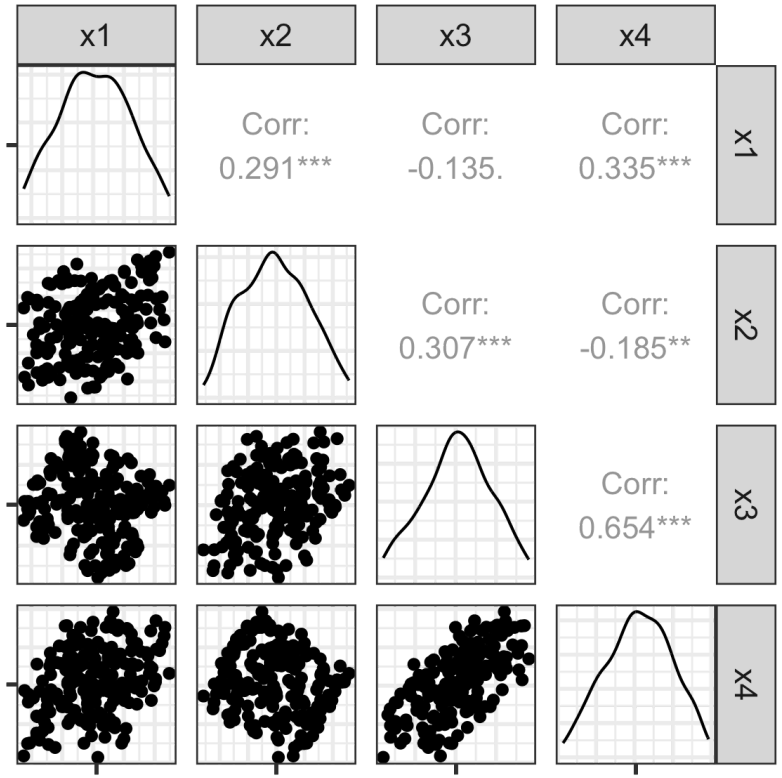
Why? (2/2)





There is an outlier in the data on the right, like the one in the left, but it is hidden in a combination of variables. It's not visible in any pair of variables.

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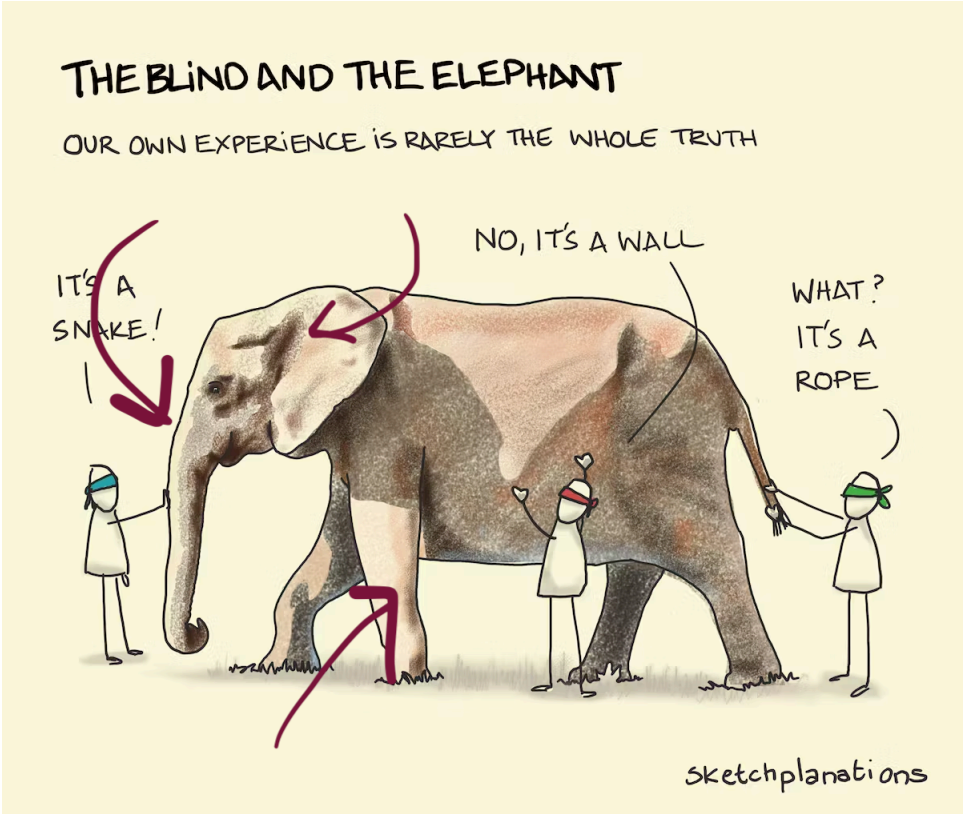
And help to see the data as a whole

To avoid misinterpretation …



… see the bigger picture!

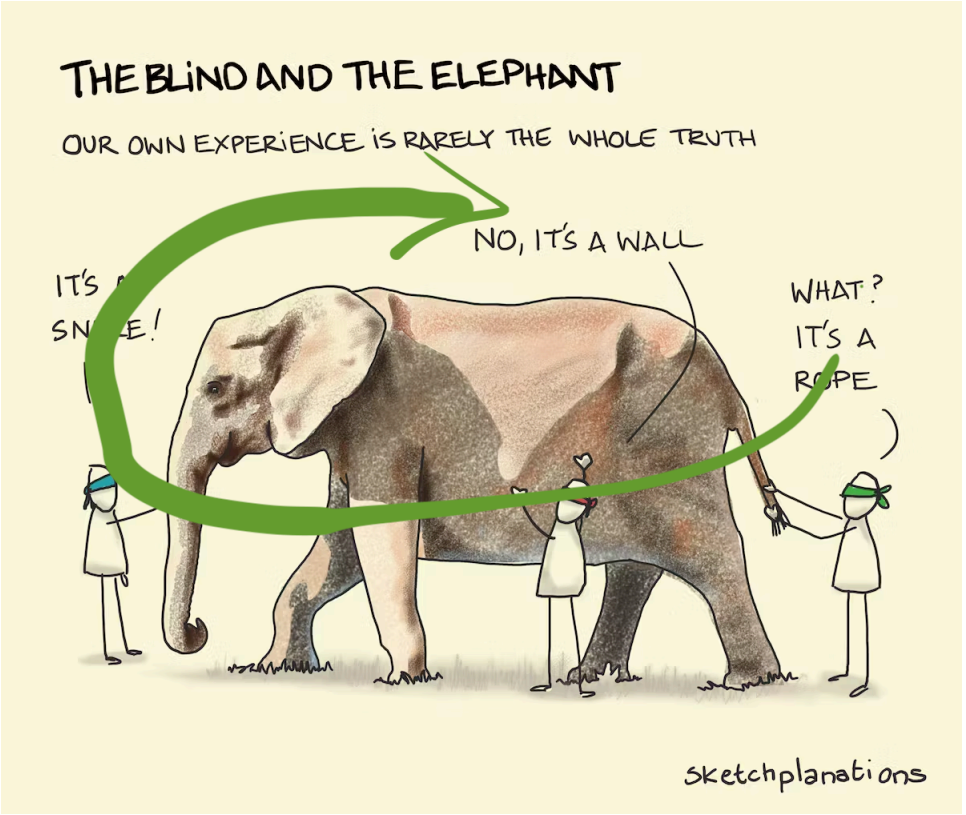


Image: Sketchplanations.

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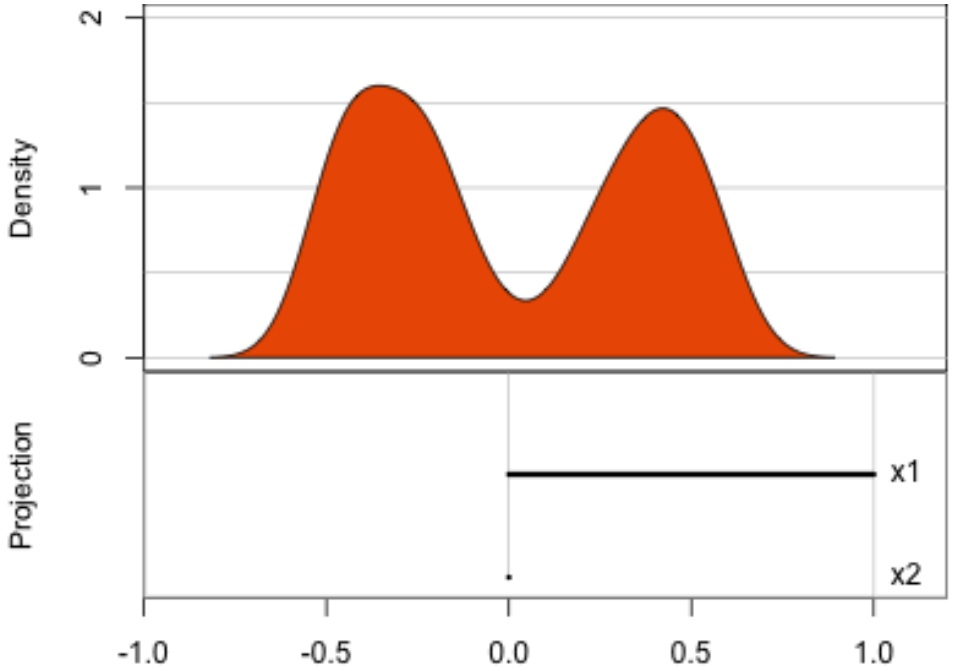
Tours of linear projections

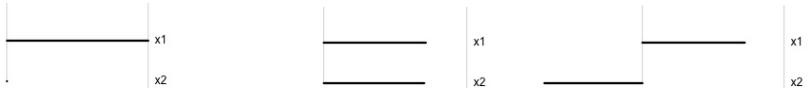


Data is 2D: $p = 2$

Projection is 1D: $d = 1$

$$A_{2\times1} = \begin{bmatrix} a_{11} \\ a_{21} \end{bmatrix}_{2\times1}$$

Notice that the values of A change between (-1, 1). All possible values being shown during the tour.



$$A = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad A = \begin{bmatrix} 0.7 \\ 0.7 \end{bmatrix} \qquad A = \begin{bmatrix} 0.7 \\ -0.7 \end{bmatrix}$$

watching the 1D shadows we can see:

- unimodality
- bimodality, there are two clusters.

What does the 2D data look like? Can you sketch it?

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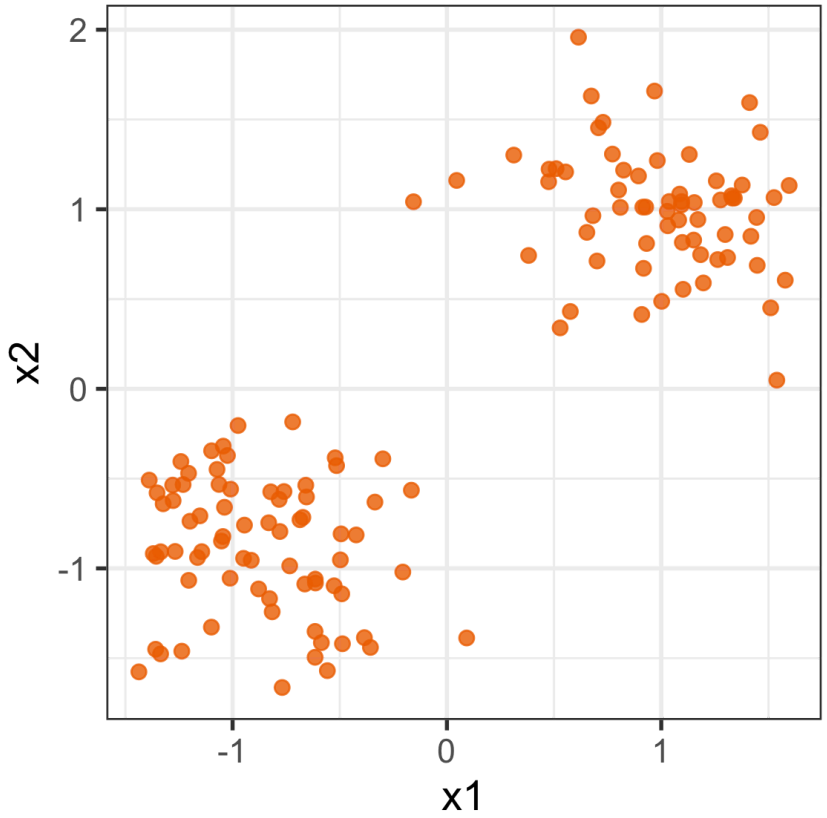
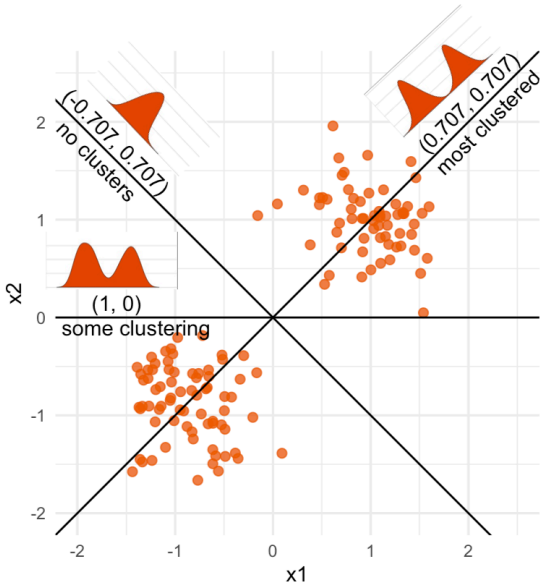
Tours of linear projections



←

The 2D data



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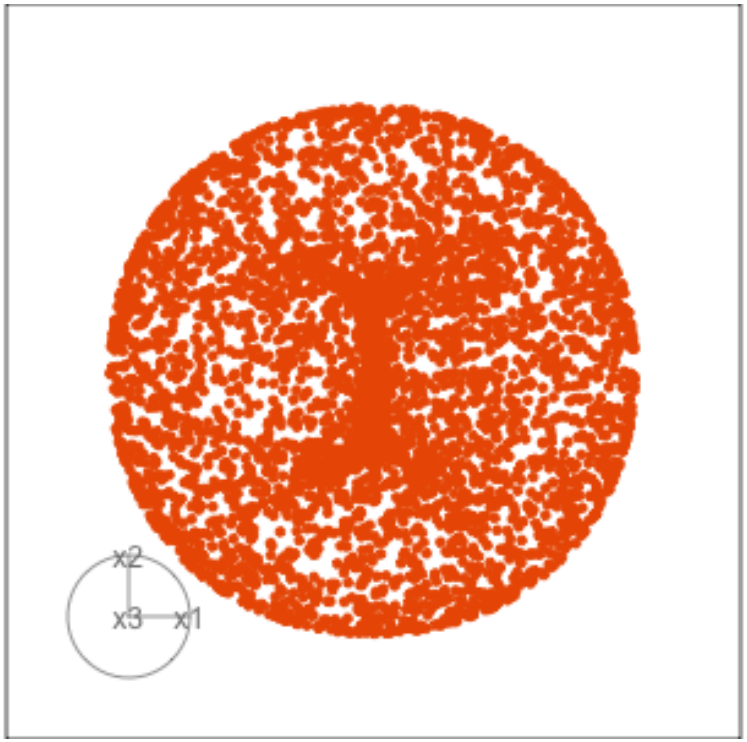
Tours of linear projections



Data is 3D: $p = 3$

Projection is 2D: $d = 2$

$$A_{3\times2} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}_{3\times2}$$

Notice that the values of A change between (-1, 1). All possible values being shown during the tour.

See:

- circular shapes
- some transparency, reveals middle
- hole in in some projections
- no clustering

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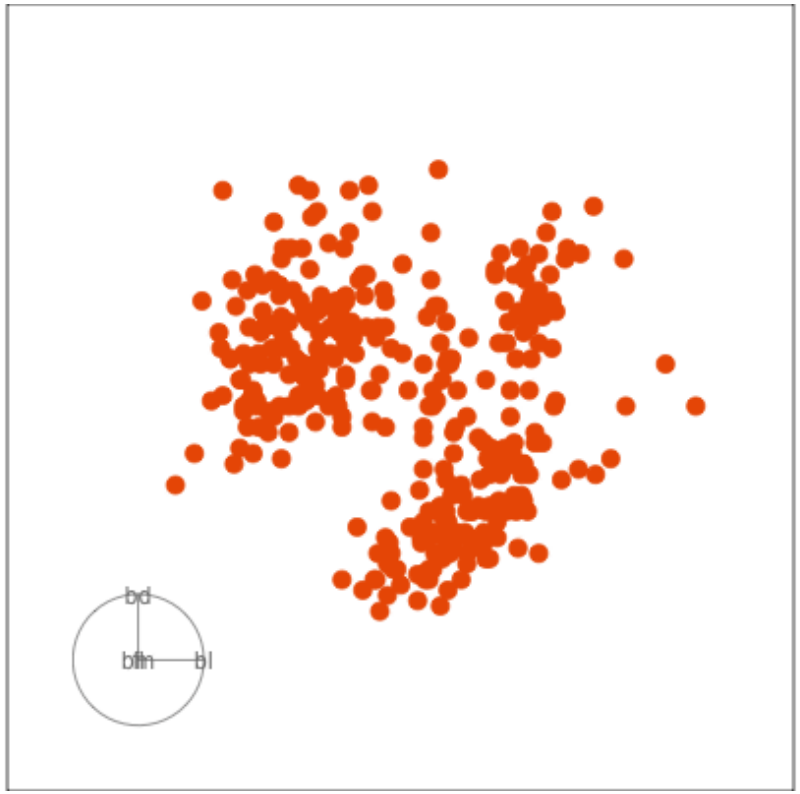
Tours of linear projections



How many clusters do you see?

- three, right?
- one separated, and two very close,
- and they each have an elliptical shape.

- do you also see an outlier or two?

Data is 4D: $p = 4$

Projection is 2D: $d = 2$

$$A_{4\times2} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \\ a_{41} & a_{42} \end{bmatrix}_{4\times2}$$

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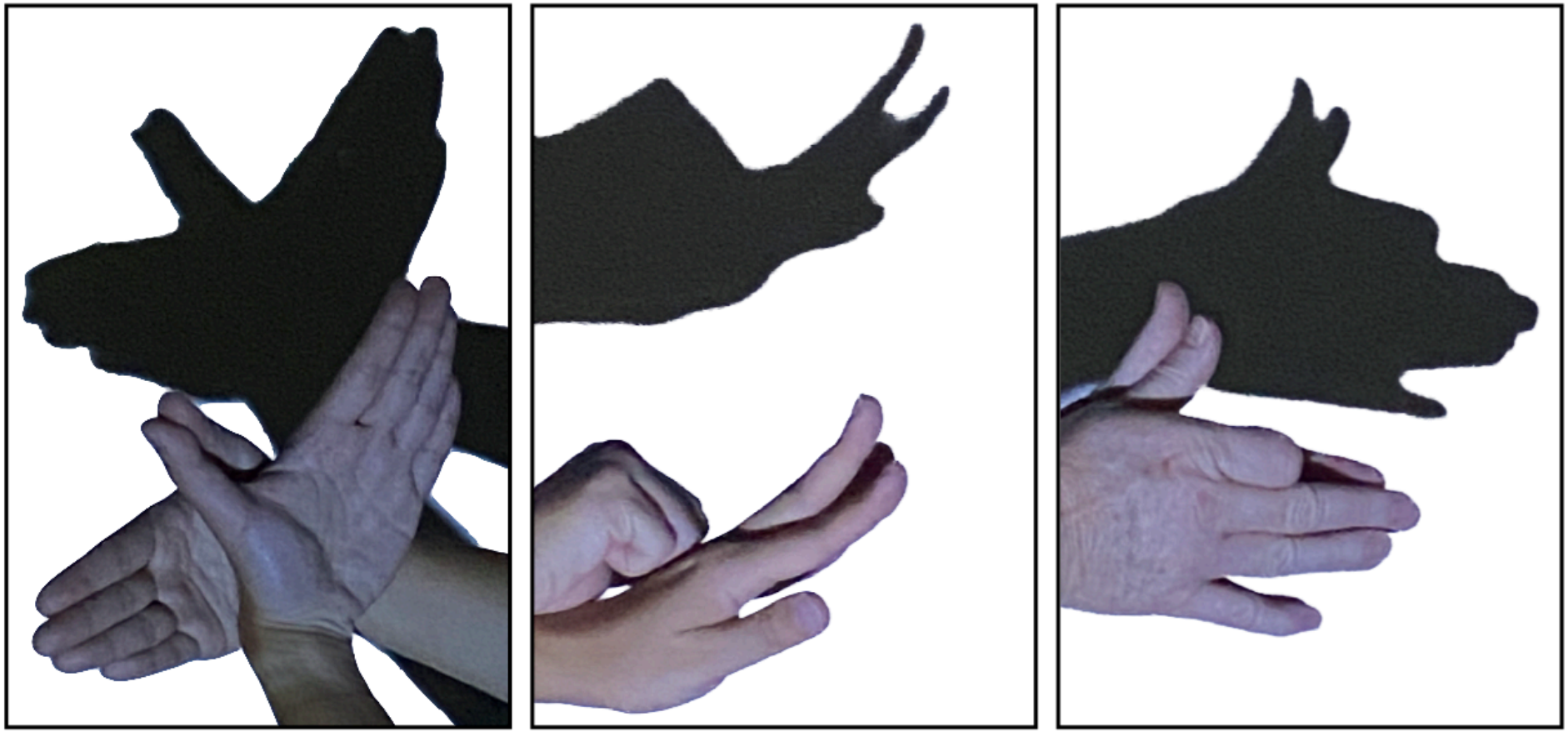
Intuitively, tours are like …



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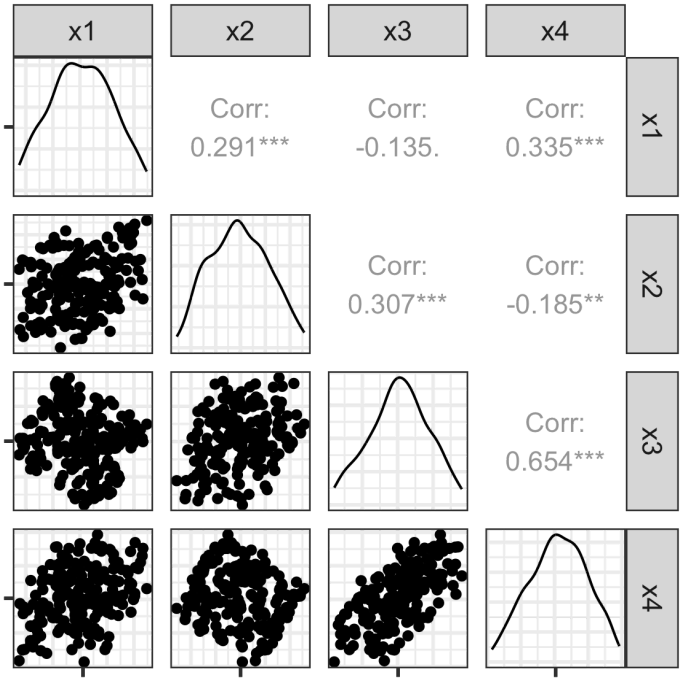
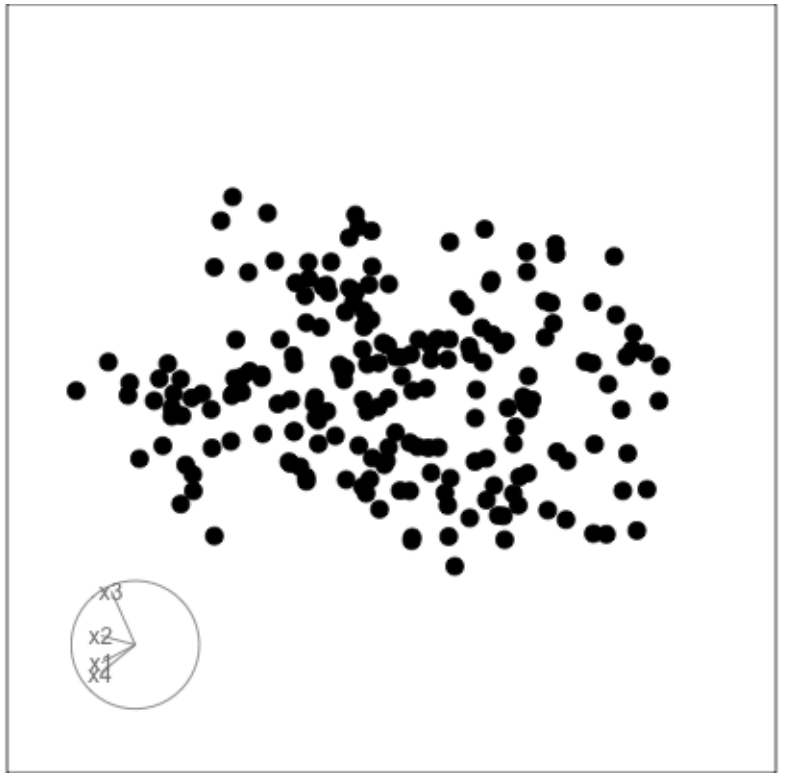
Anomaly is no longer hidden





Wait for it!

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How to use a tour in R

This is a basic tour, which will run in your RStudio plot window.

```
library(tourr)
animate_xy(flea[, 1:6], rescale=TRUE)
```

This data has a class variable, `species`.

```
flea |> slice_head(n=3)
```

```
   species tars1 tars2 head aede1 aede2 aede3
1 Concinna   191   131   53   150    15   104
2 Concinna   185   134   50   147    13   105
3 Concinna   200   137   52   144    14   102
```

Use this to colour points with:

```
animate_xy(flea[, 1:6],
           col = flea$species,
           rescale=TRUE)
```

You can specifically guide the tour choice of projections using

```
animate_xy(flea[, 1:6],
           tour_path = guided_tour(hole
           col = flea$species,
           rescale = TRUE,
           sphere = TRUE)
```

and you can manually choose a variable to control with:

```
set.seed(915)
animate_xy(flea[, 1:6],
           radial_tour(basis_random(6,
                       mvar = 6),
           rescale = TRUE,
           col = flea$species)
```

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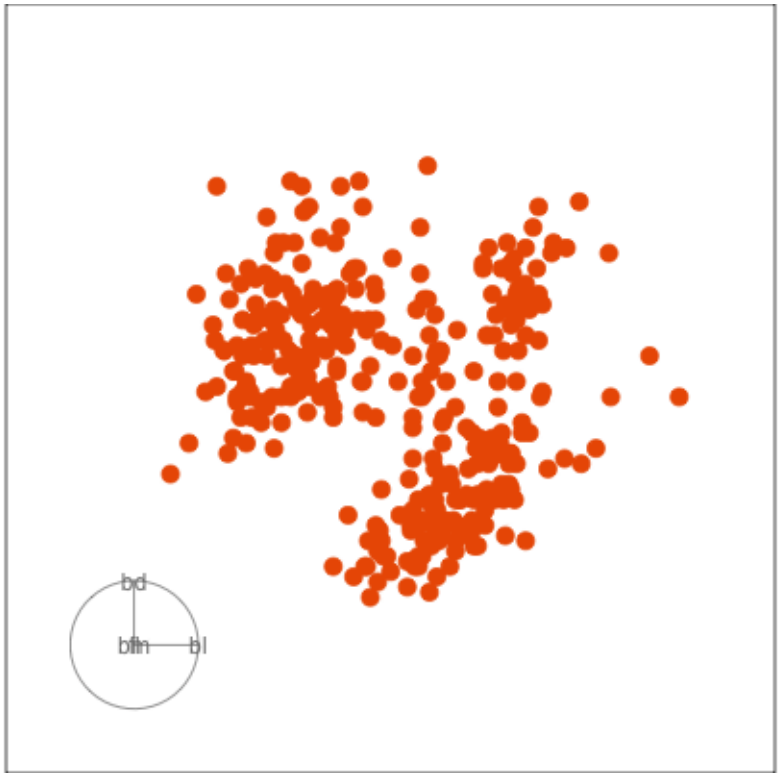
How to save a tour



To save as an animated gif:

```
set.seed(645)
render_gif(penguins_sub[,1:4]
           grand_tour(),
           display_xy(col="#E
             half_range=3.8,
             axes="bottomleft
           gif_file = "gifs/p
           apf = 1/60,
           frames = 1500,
           width = 500,
           height = 400)
```

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Your turn

Use a grand tour on the data set `c1` in the `mulgar` package. What shapes do you see?

```
library(tourr)
library(mulgar)
animate_xy(c1)
```

Have a look at `c3` or `c7` also. How are the structures different.

Dimension reduction

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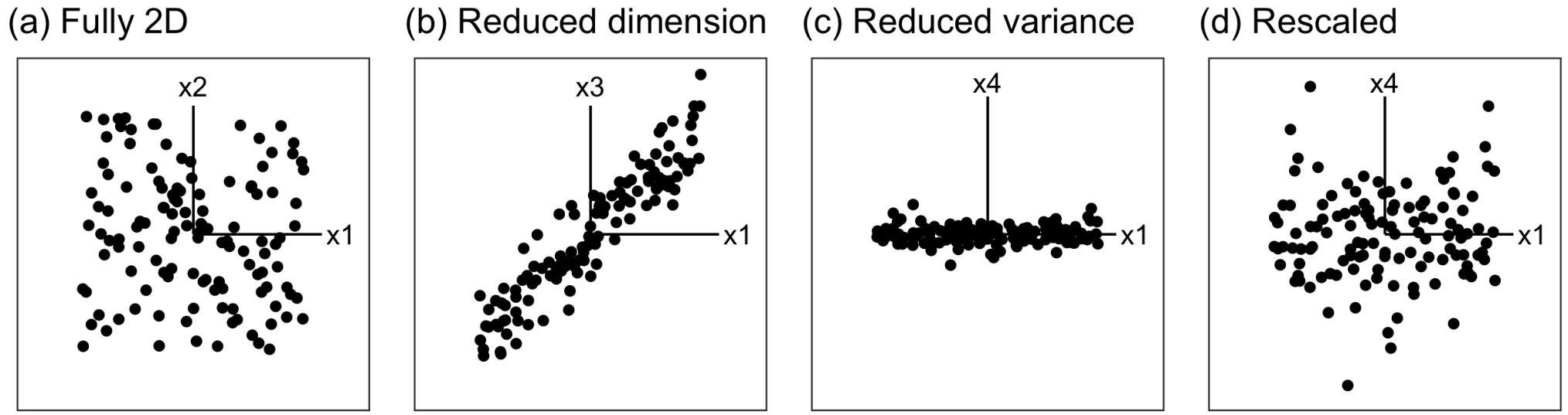
What is dimensionality?



When an axis extends out of a direction where the points are collapsed, it means that this variable is partially responsible for the reduced dimension.

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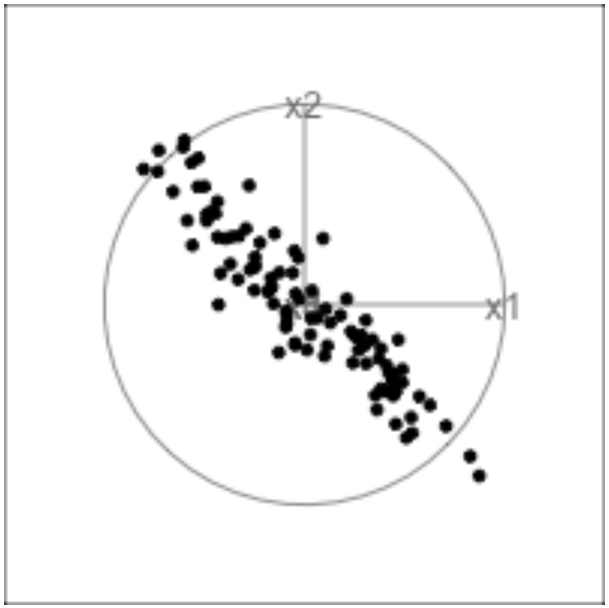
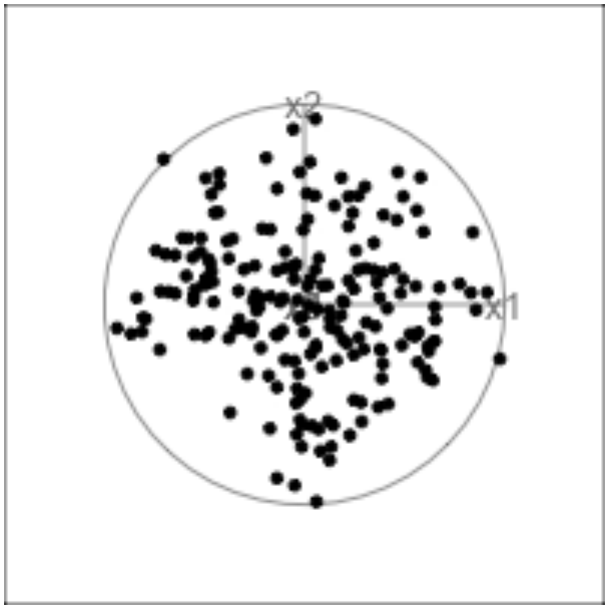
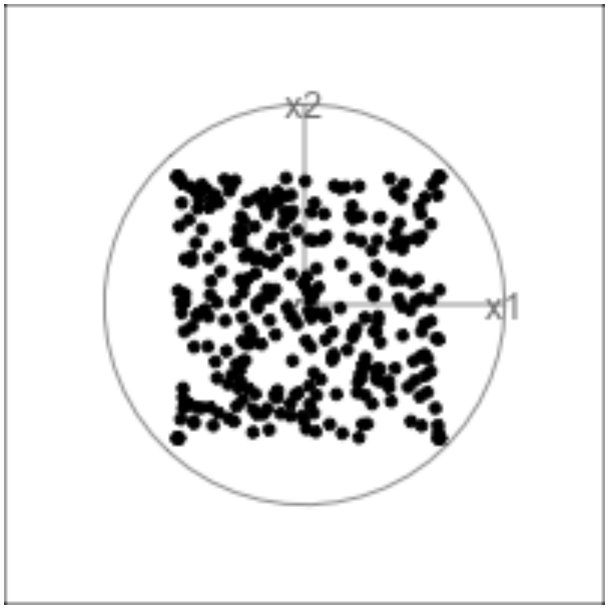
In high-dimensions



2D plane in 5D



3D plane in 5D



5D plane in 5D

Principal component analysis (PCA) will detect these dimensionalities.

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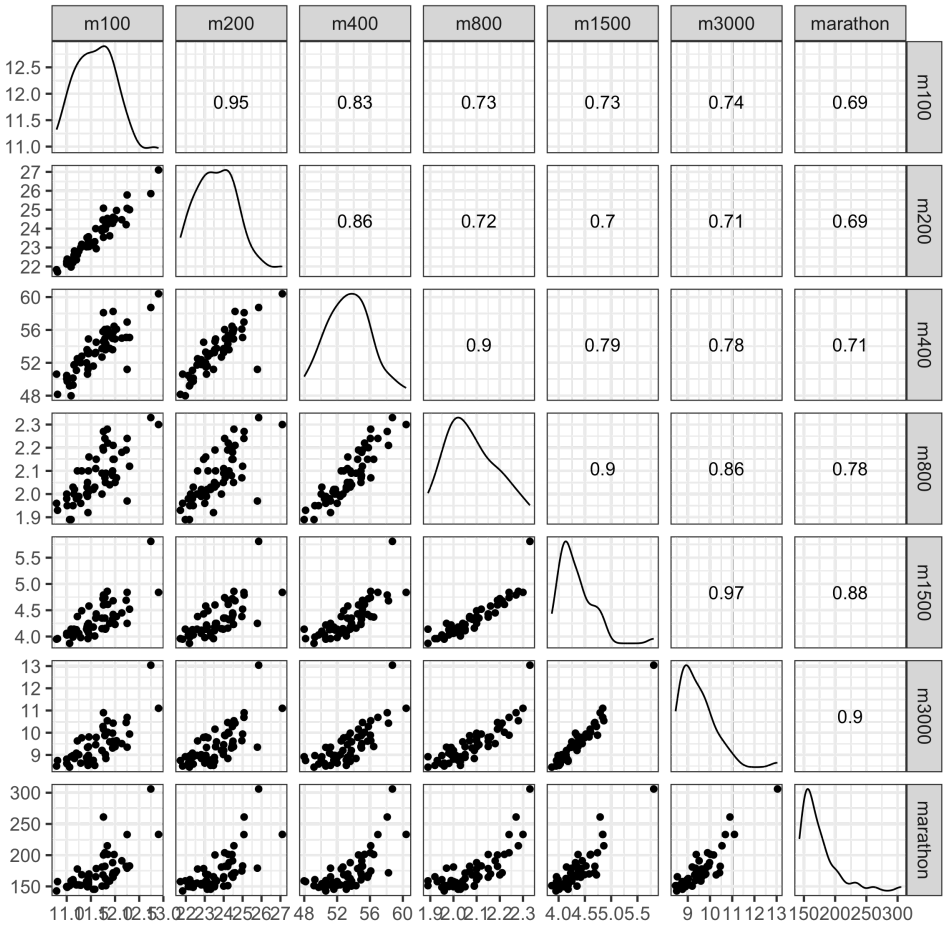
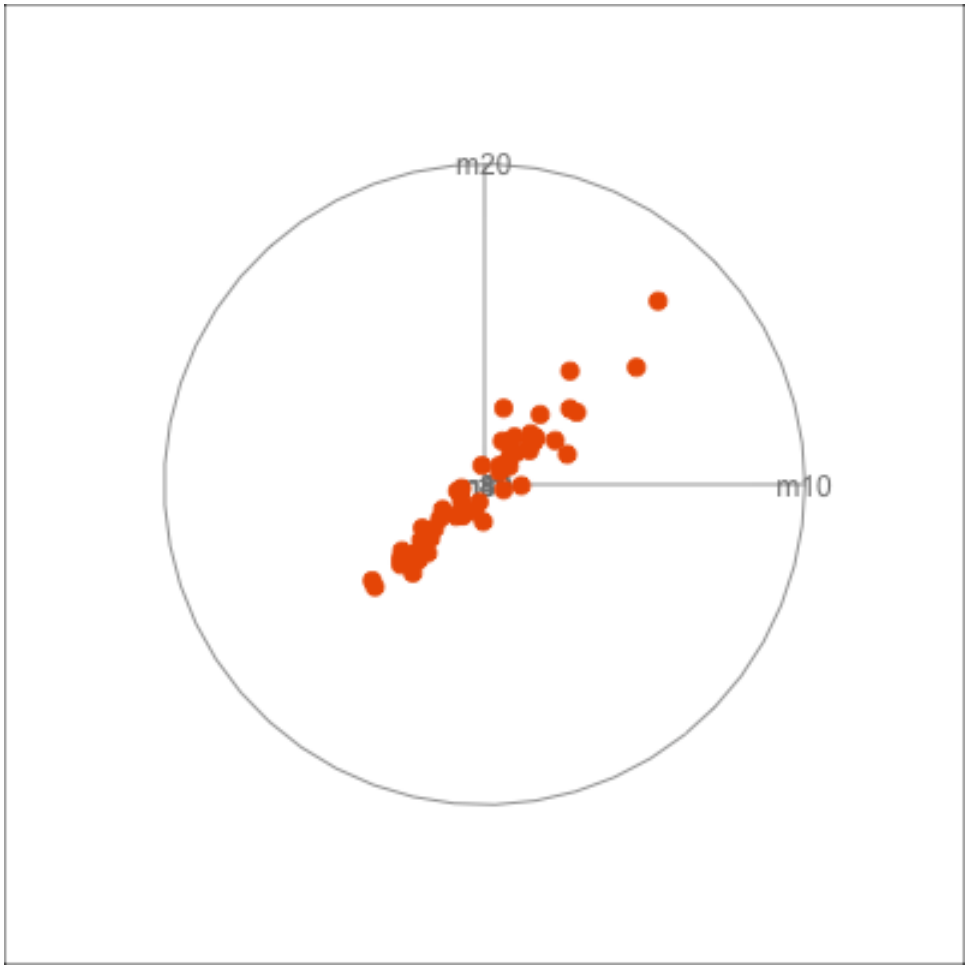
Example: womens' track records (1/3)





Source: Johnson and Wichern, Applied multivariate analysis

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Example: PCA summary (2/3)

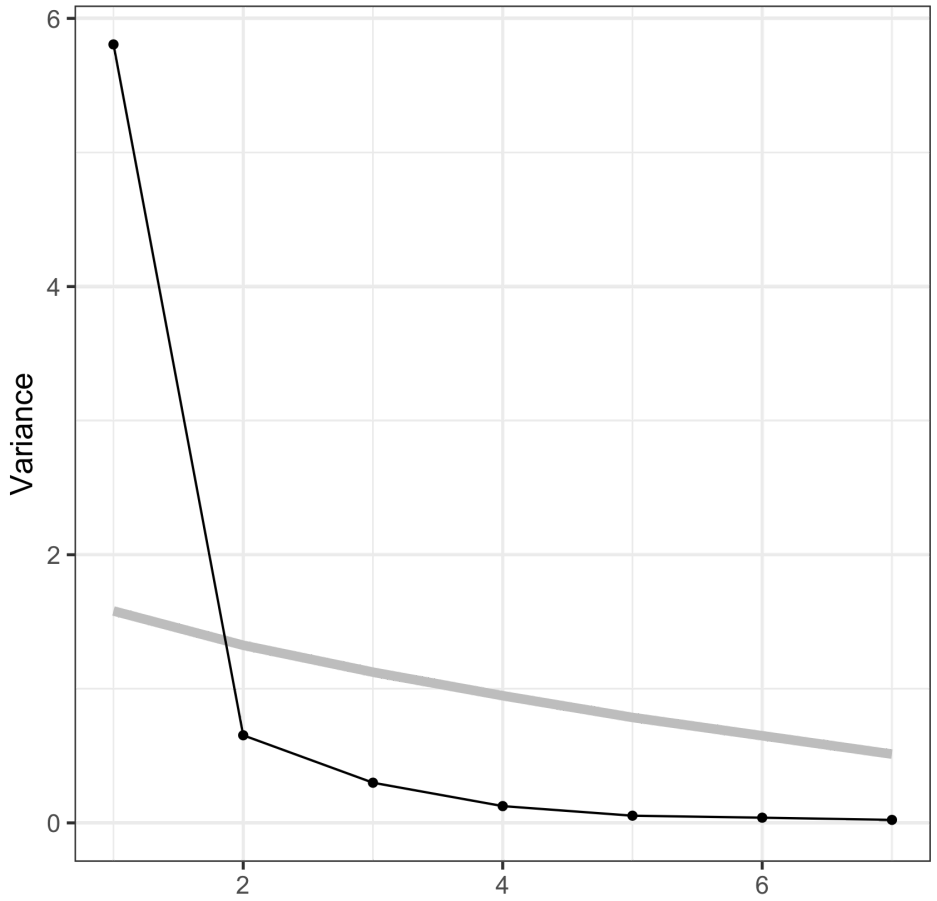
Variances/eigenvalues

```
[1] 5.806 0.654 0.300 0.125 0.054
0.039 0.022
```

Component coefficients

	PC1	PC2	PC3	PC4
m100	0.37	0.49	-0.286	0.319
m200	0.37	0.54	-0.230	-0.083
m400	0.38	0.25	0.515	-0.347
m800	0.38	-0.16	0.585	-0.042
m1500	0.39	-0.36	0.013	0.430
m3000	0.39	-0.35	-0.153	0.363
marathon	0.37	-0.37	-0.484	-0.672

How many PCs?



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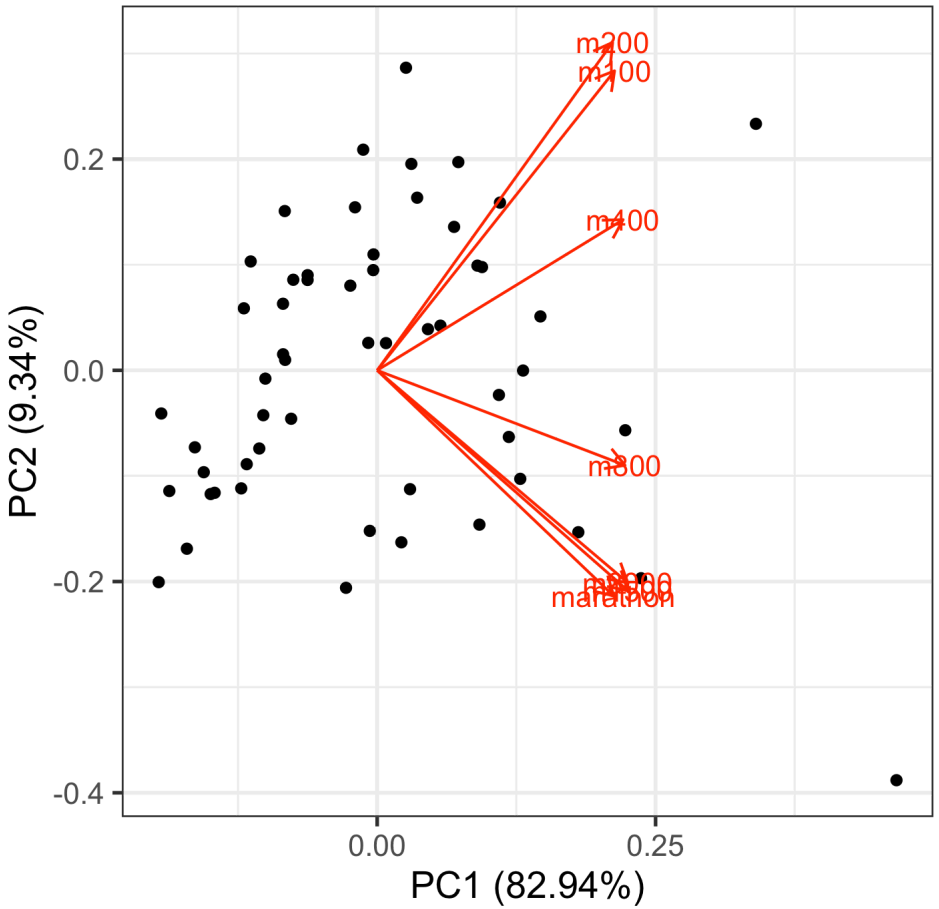
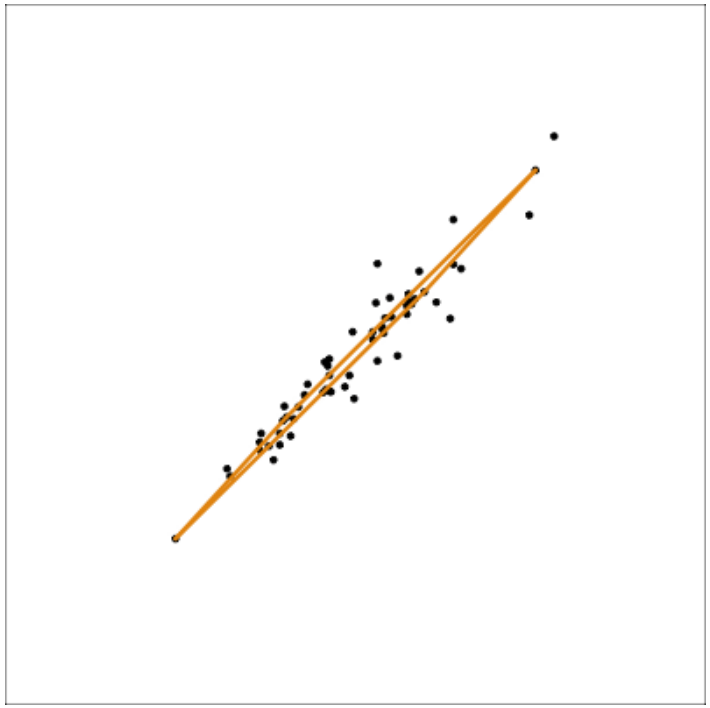
Example: Visualise (3/3)

Biplot: data in the model space



2D model in data space



```
track_model <- mulgar::pca_model(track_std_pca, d=2, s=
track_all <- rbind(track_model$points, track_std[,1:7])
animate_xy(track_all, edges=track_model$edges,
           edges.col="#E7950F",
           edges.width=3,
           axes="off")
```

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Non-linear dimension reduction (1/2)

Find some low-dimensional layout of points which approximates the distance between points in high-dimensions, with the purpose being to have a useful representation that reveals high-dimensional patterns, like clusters.

Multidimensional scaling (MDS) is the original approach:

$$\text{Stress}_D(x_1, \ldots, x_n) = \left(\sum_{i,j=1; i \neq j}^{n} (d_{ij} - d_k(i,j))^2 \right)^{1/2}$$

where D is an $n \times n$ matrix of distances (d_{ij}) between all pairs of points, and $d_k(i,j)$ is the distance between the points in the low-dimensional space.

PCA is a special case of MDS. The result from PCA is a linear projection, but generally MDS can provide some non-linear transformation.

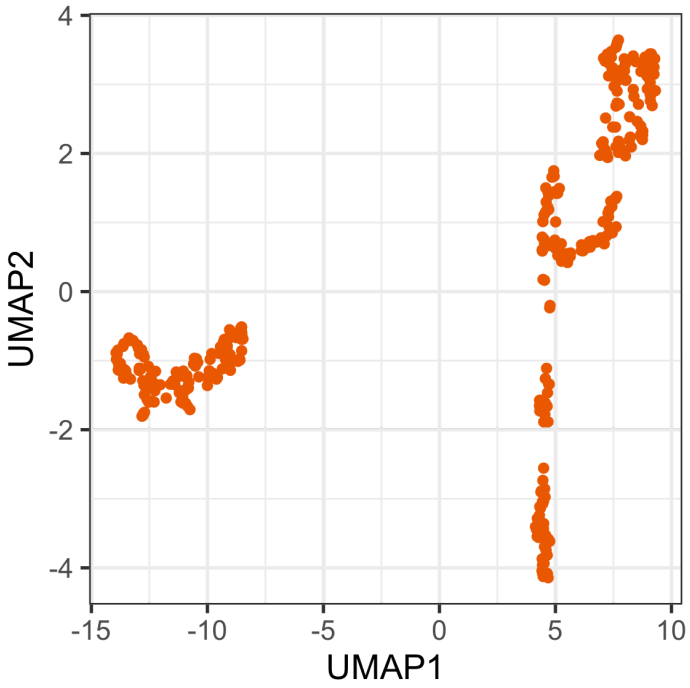
Many variations being developed:

- t-stochastic neighbourhood embedding (t-SNE): compares interpoint distances with a standard probability distribution (eg t-distribution) to exaggerate local neighbourhood differences.
- uniform manifold approximation and projection (UMAP): compares the interpoint distances with what might be expected if the data was uniformly distributed in the high-dimensions.

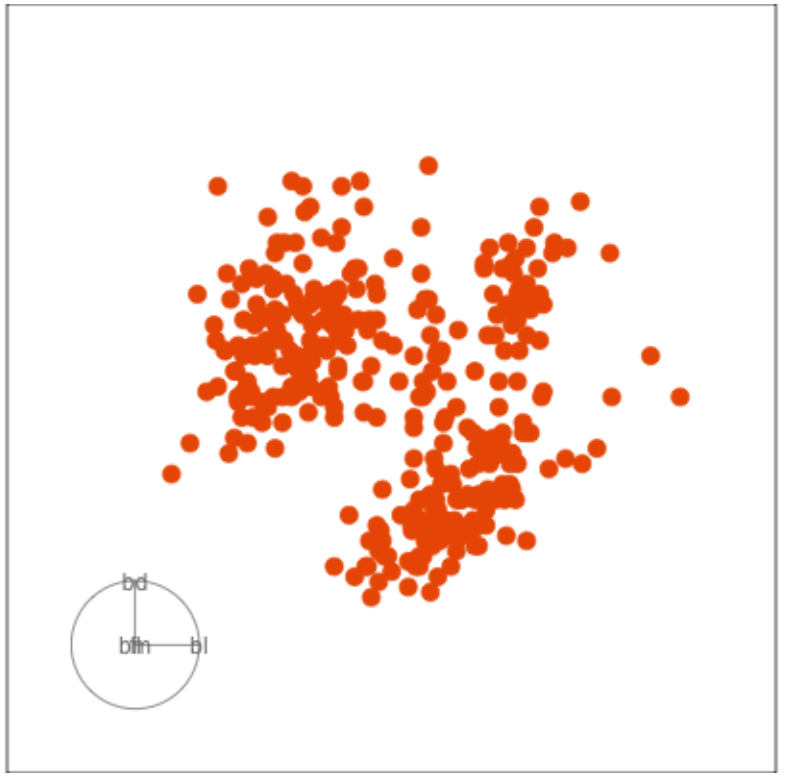
NLDR can be useful but it can also make some misleading representations.

Non-linear dimension reduction (2/2)

UMAP 2D representation



Tour animation of the same data




```
library(uwot)
set.seed(253)
p_tidy_umap <- umap(p_tidy_std[,2:5], init = "
```

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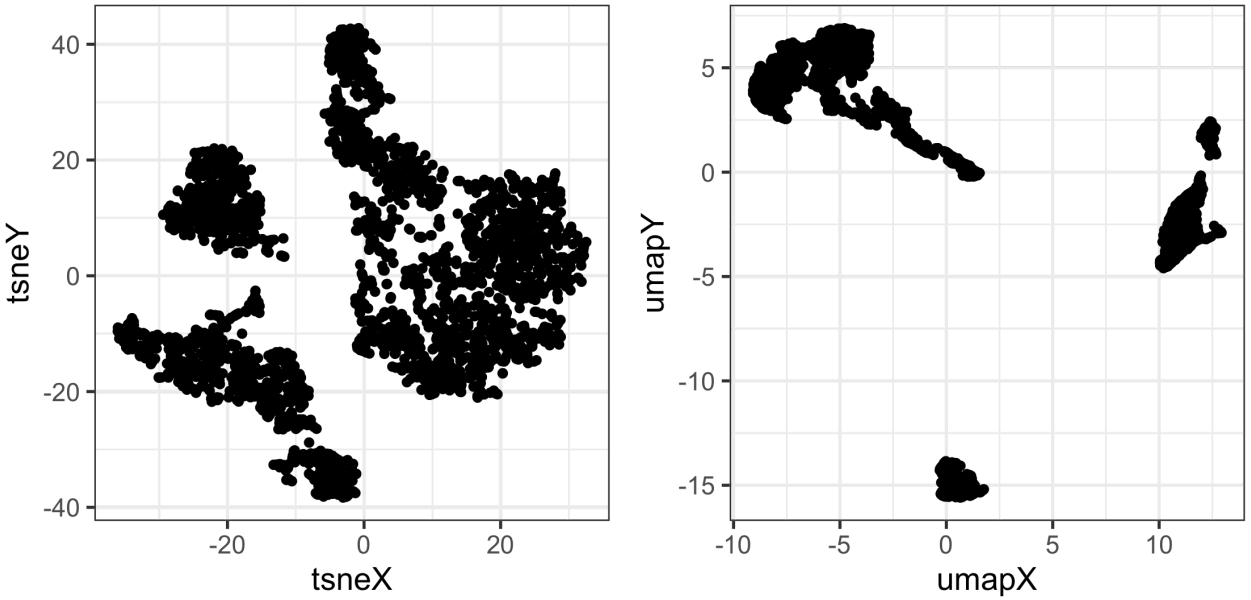
Your turn

Which is the best representation, t-SNE or UMAP, of this 9D data?



You can use this code to read the data and view in a tour:

```
pbmc <- readRDS("data/pbmc_pca_50.rds")
animate_xy(pbmc[,1:9])
```

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Key conceptual points

- Avoid misinterpretation, by using your high-dimensional visualisation skills to look at the **data as a whole**.
- Examine model fit by by examining the model overlaid on the data, **model-in-the-data-space**. (Wickham et al (2015) Removing the Blindfold)

End of session 1

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