Visualising High-dimensional Data with R

Session 1

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https://dicook.github.io/mulgar_tutorial/

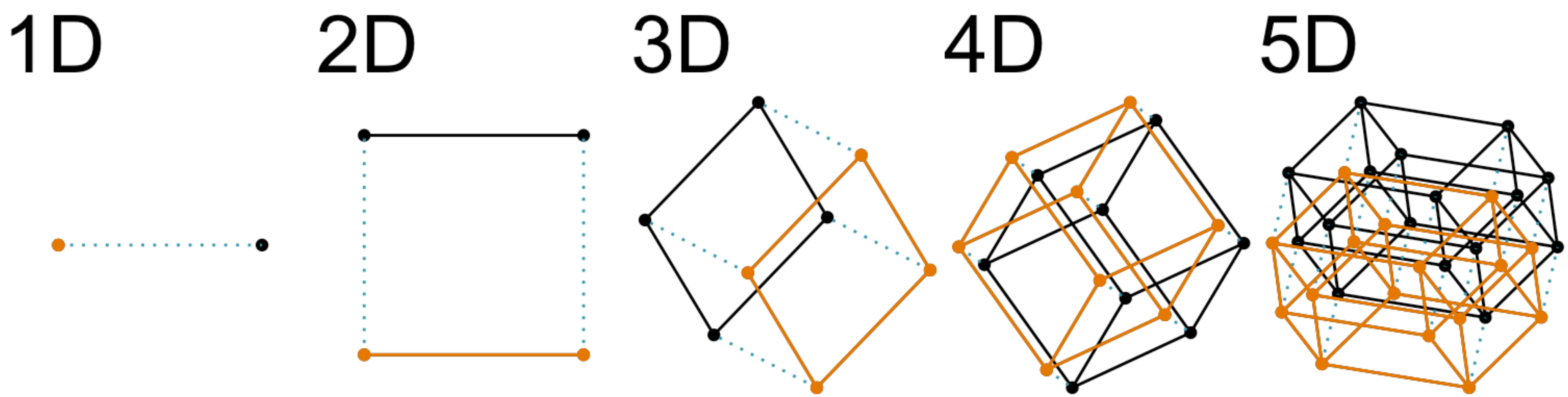
Session 1

Outline

time	topic
1:30-1:40	Introduction: What is high-dimensional data, why visualise and overview of methods
1:50-2:10	Basics of linear projections, and recognising high-d structure
2:10-2:30	Effectively reducing your data dimension, in association with non-linear dimension reduction
2:30-3:00	BREAK

Introduction

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

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

Notation: Projection

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

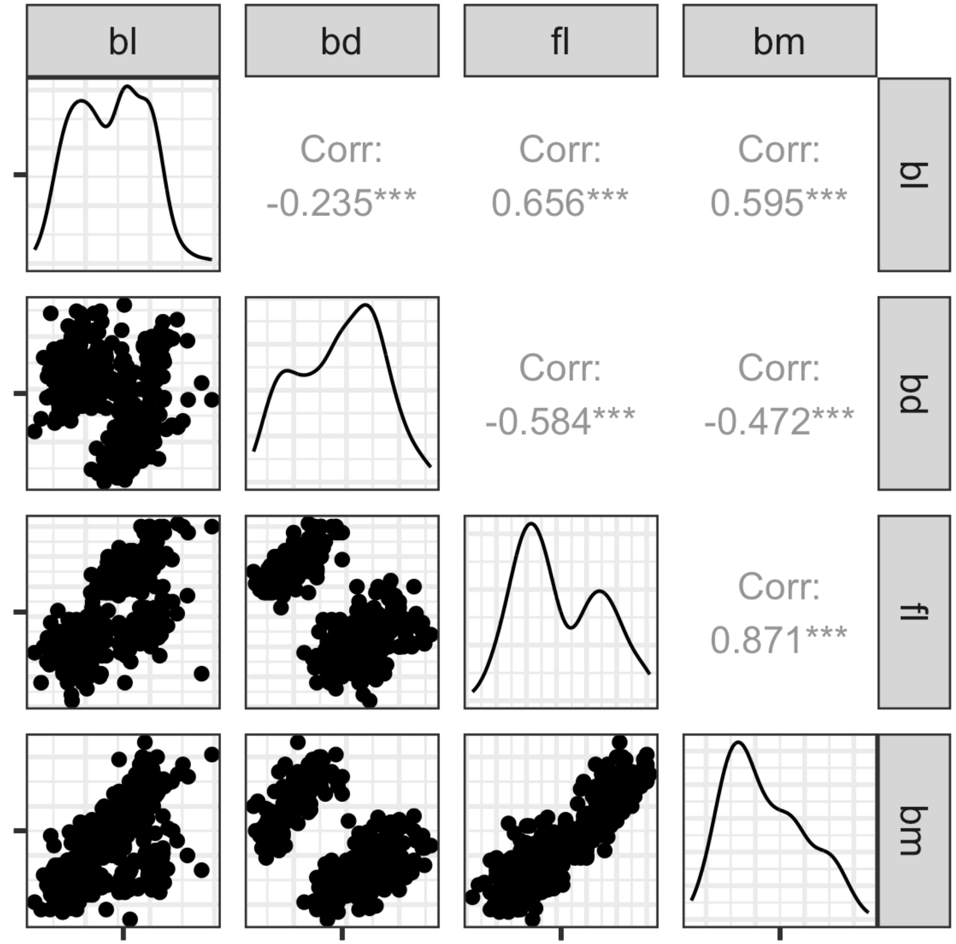
Notation: Projected data

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

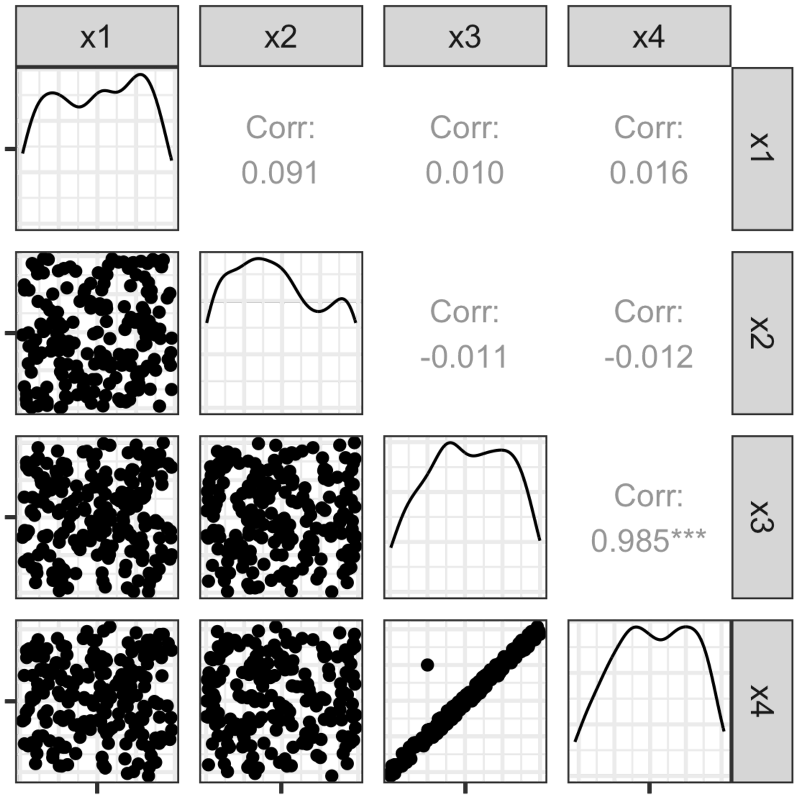
Why? (1/2)

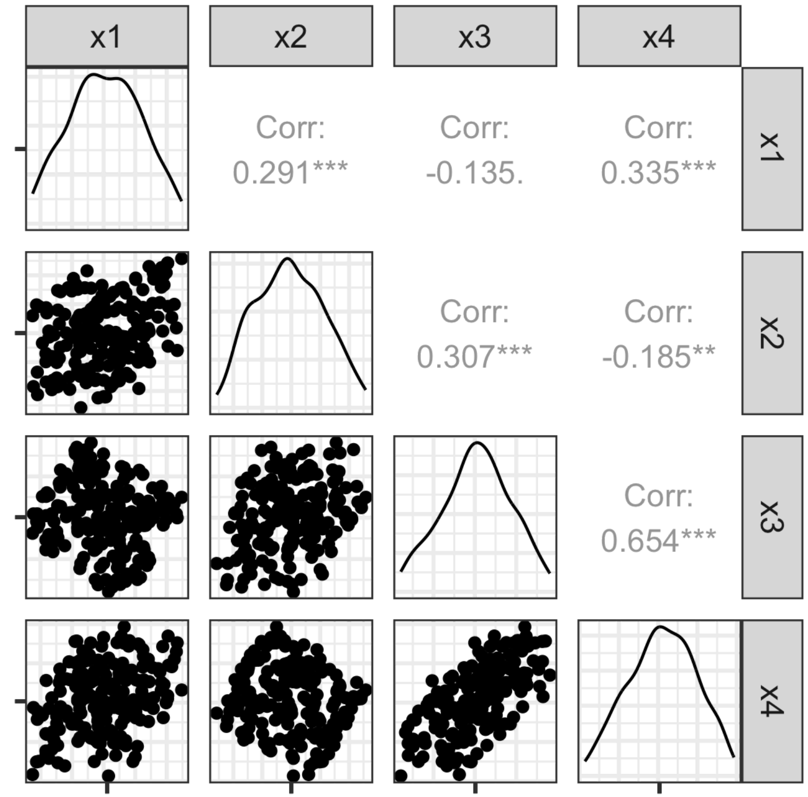
Scatterplot matrix

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



Why? (2/2)

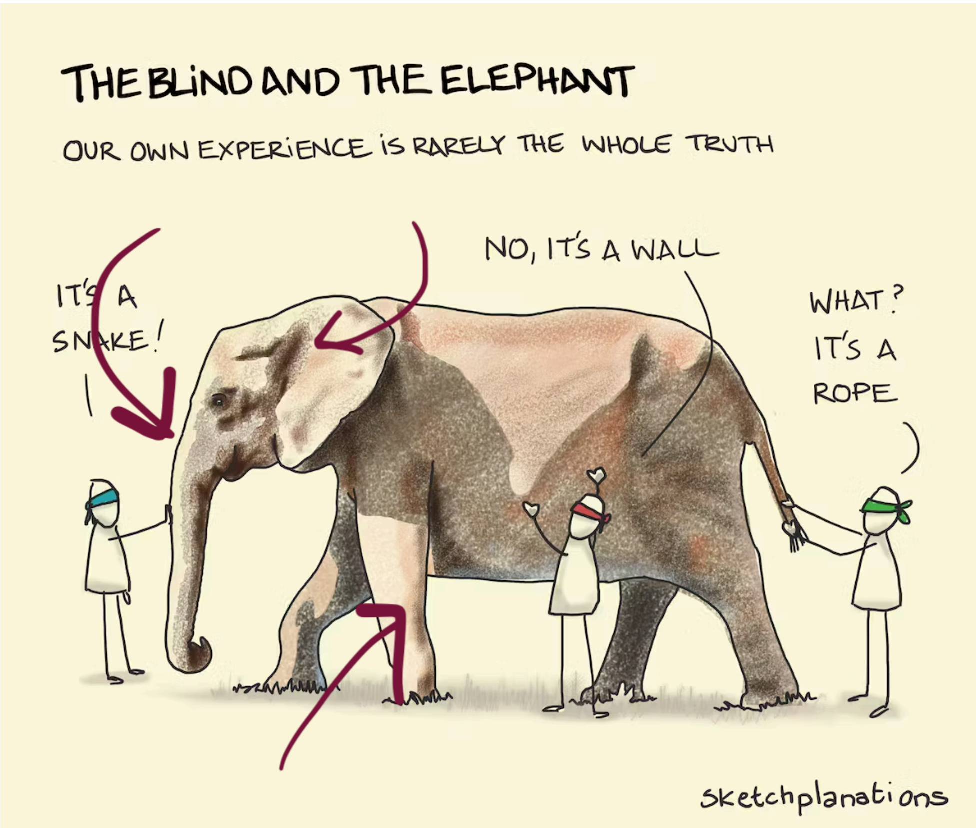




There is an outlier in the data on the right, like the one in the left, but it is hidden in a combination of variables. It's not visible in any pair of variables.

And help to see the data as a whole

To avoid misinterpretation …



… see the bigger picture!

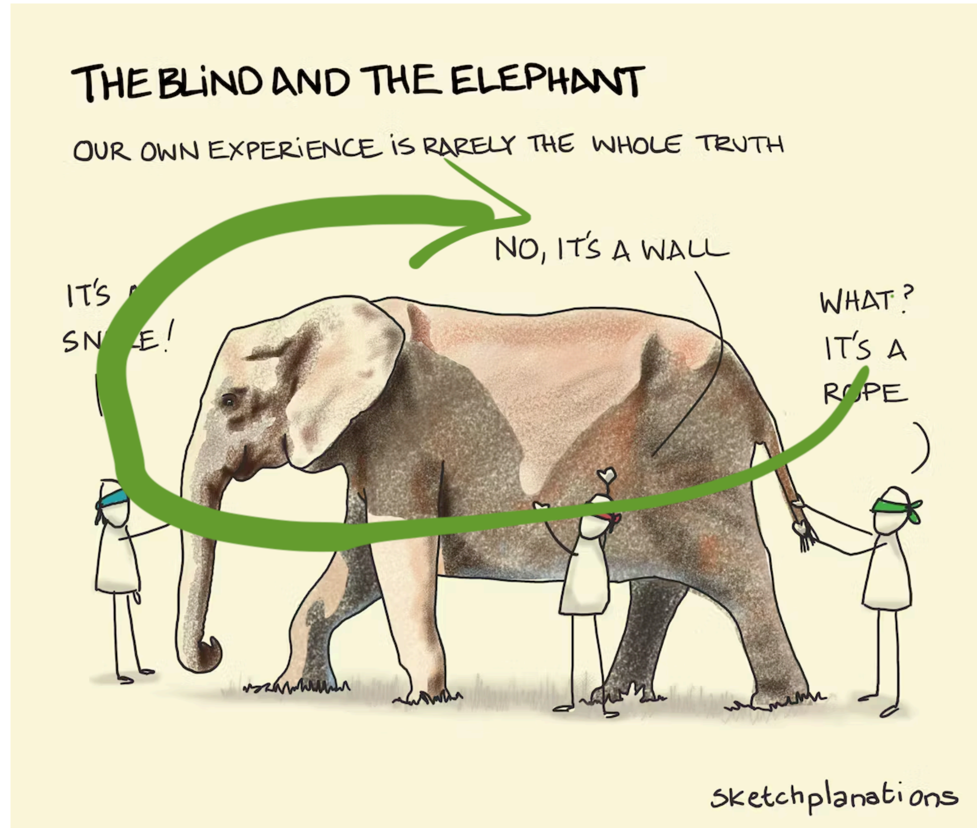
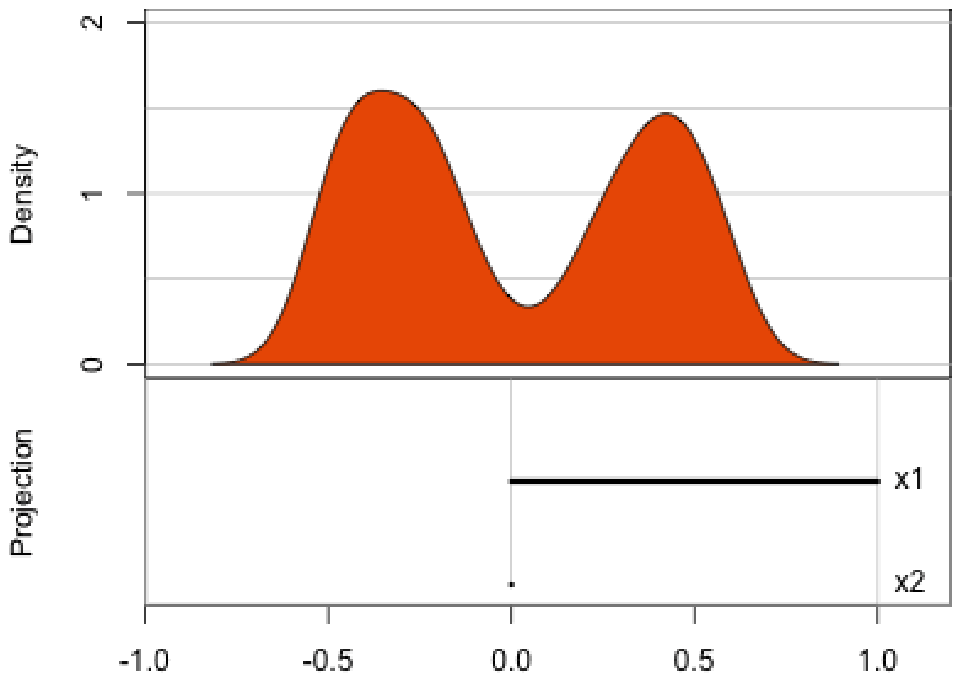


Image: Sketchplanations.

Tours of linear projections

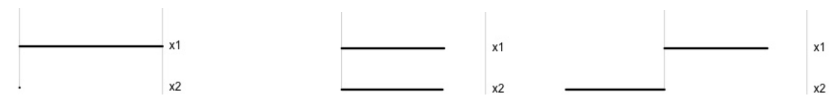


Data is 2D: $p = 2$

Projection is 1D: $d = 1$

$$A_{2\times 1} = \begin{bmatrix} a_{11} \\ a_{21} \end{bmatrix}_{2\times 1}$$

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



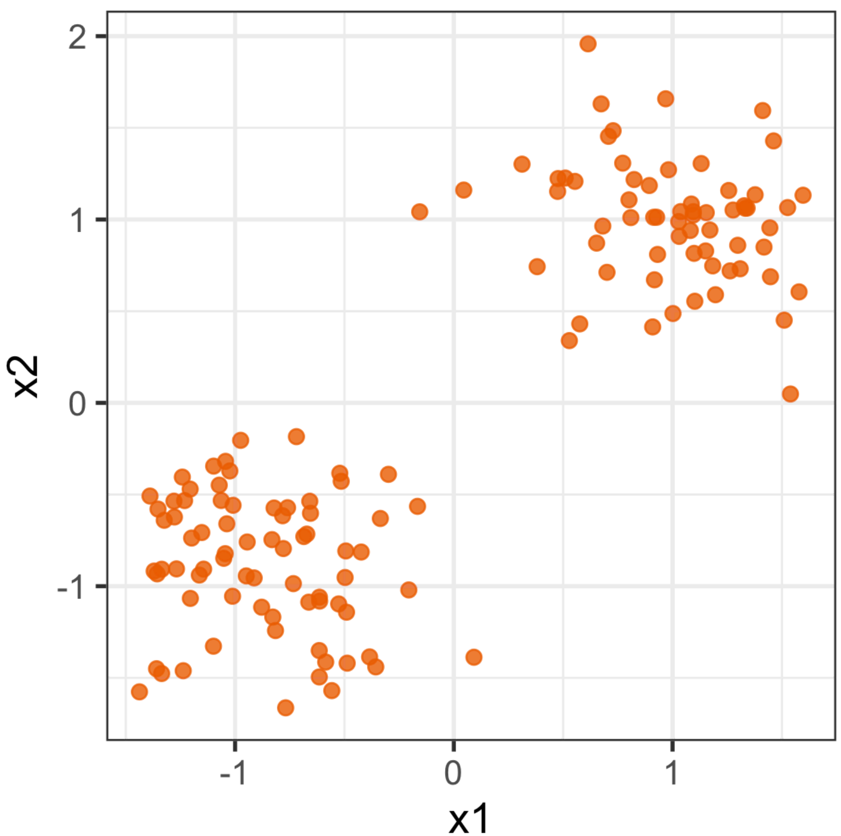
$A = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $A = \begin{bmatrix} 0.7 \\ 0.7 \end{bmatrix}$ $A = \begin{bmatrix} 0.7 \\ -0.7 \end{bmatrix}$

watching the 1D shadows we can see:

- unimodality
- bimodality, there are two clusters.

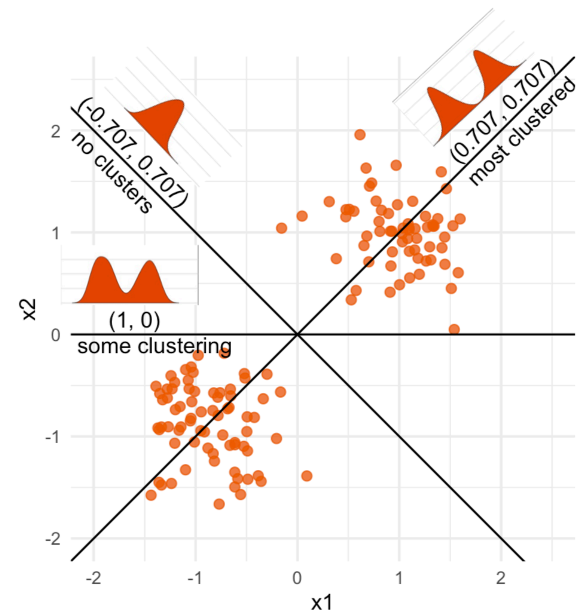
What does the 2D data look like? Can you sketch it?

Tours of linear projections



←

The 2D data



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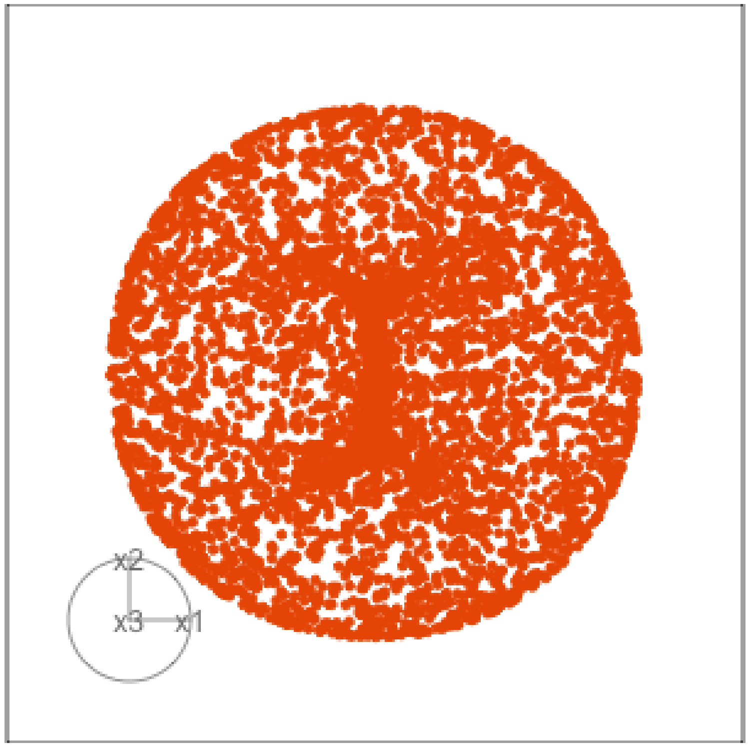
Tours of linear projections



Data is 3D: $p = 3$

Projection is 2D: $d = 2$

$$A_{3\times 2} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}_{3\times 2}$$

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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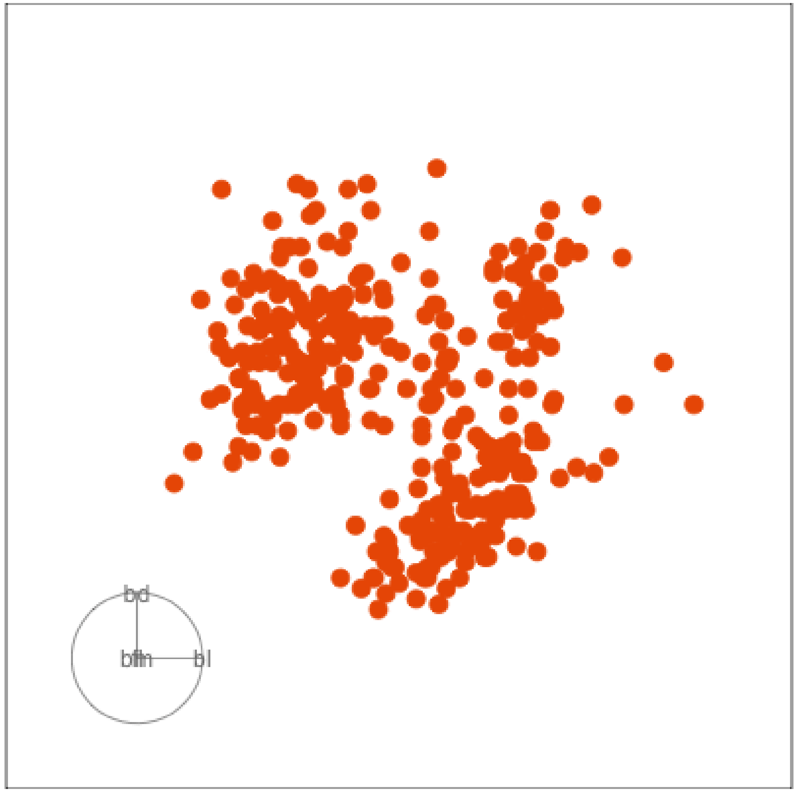
Tours of linear projections



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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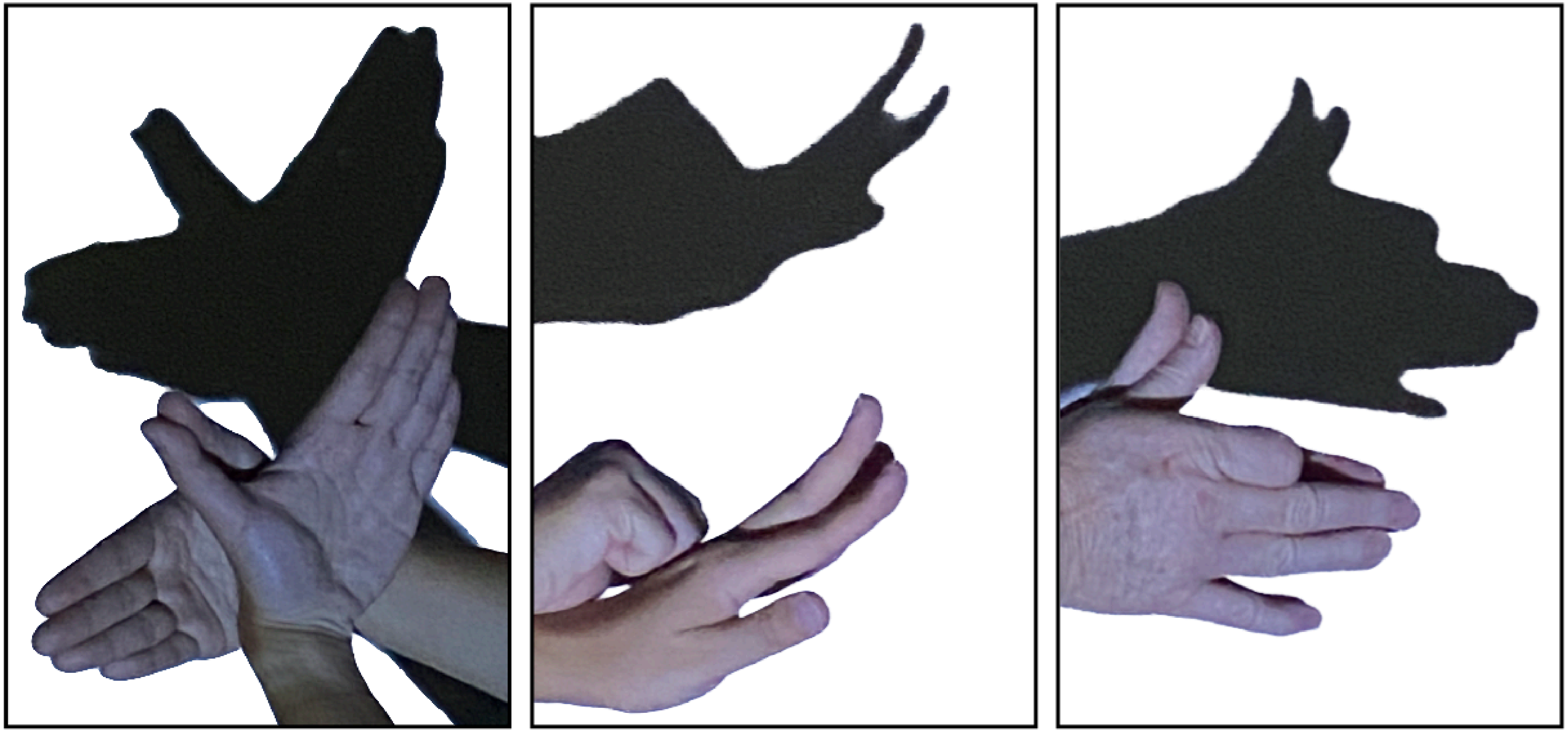
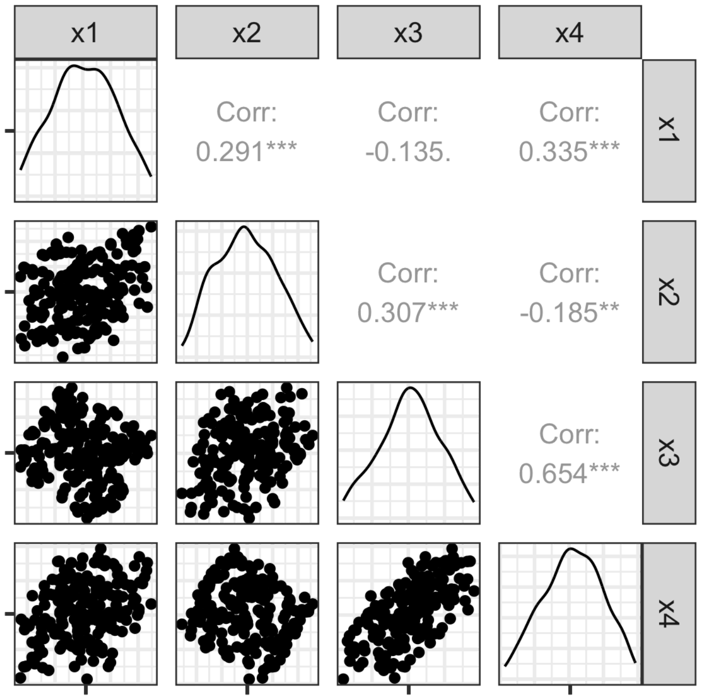
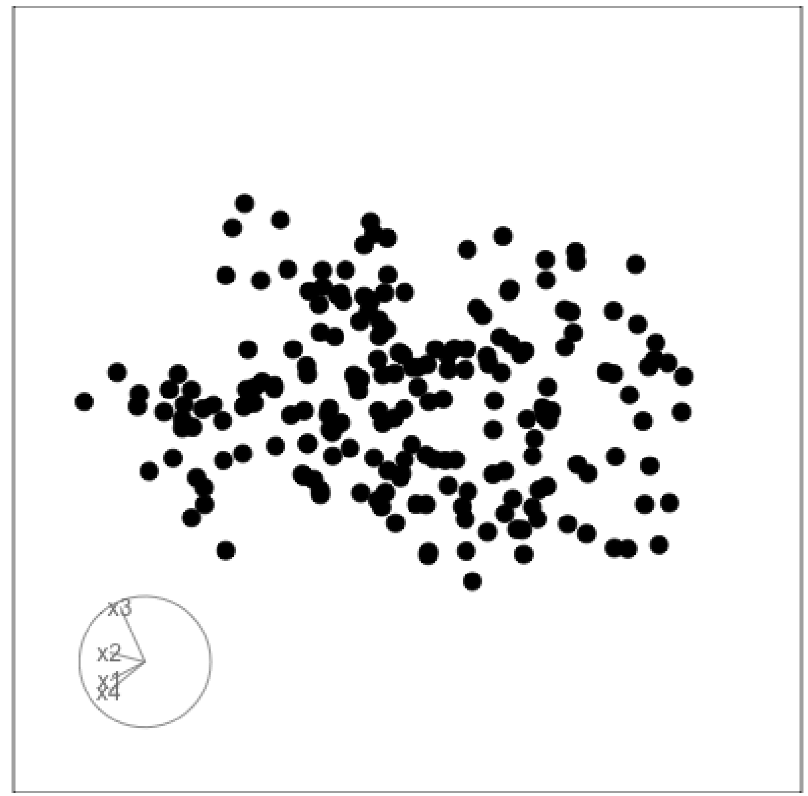
Intuitively, tours are like …



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)
```

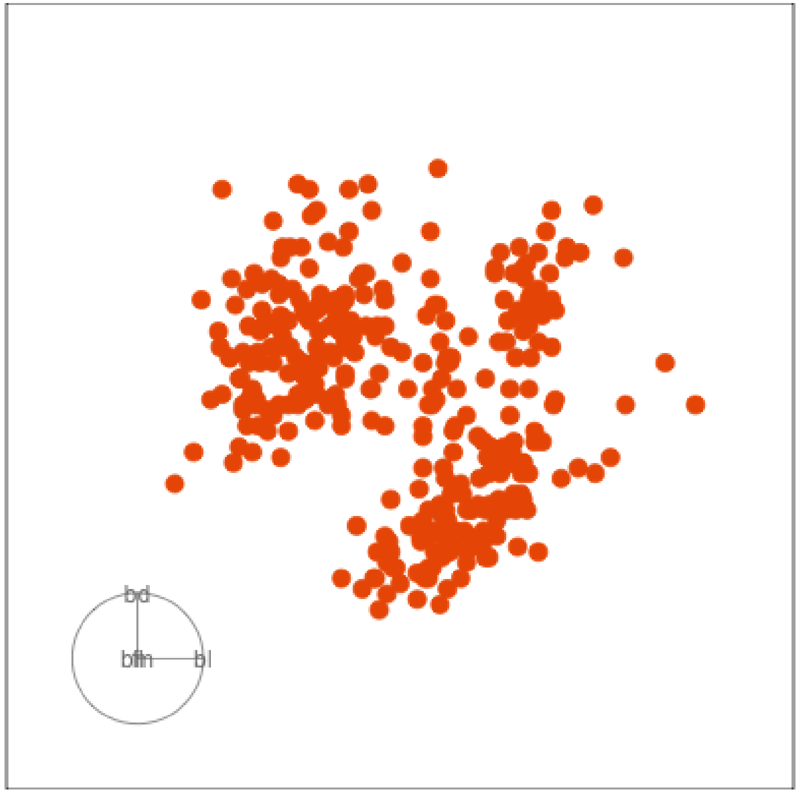
You can specifically guide the tour choice of projections using

```
animate_xy(flea[, 1:6],
           tour_path = guided_tour(holes()),
           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, 2),
                       mvar = 6),
           rescale = TRUE,
           col = flea$species)
```

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="#EC5C00",
             half_range=3.8,
             axes="bottomleft", cex=2.5),
           gif_file = "gifs/penguins1.gif",
           apf = 1/60,
           frames = 1500,
           width = 500,
           height = 400)
```

Your turn

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

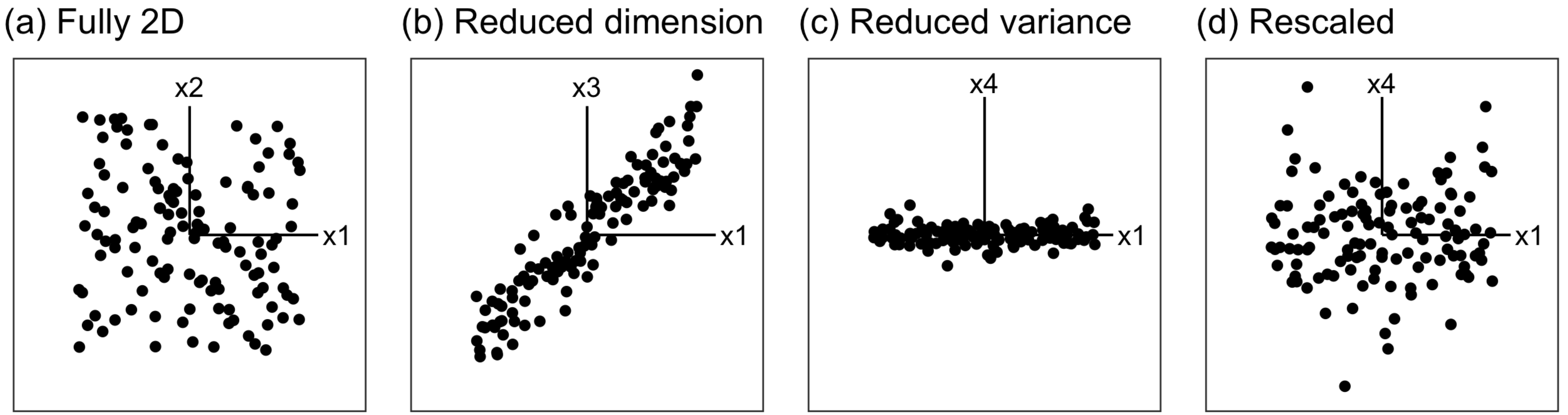
```
library(tourr)
library(mulgar)
animate_xy(c1)
```

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

05:00

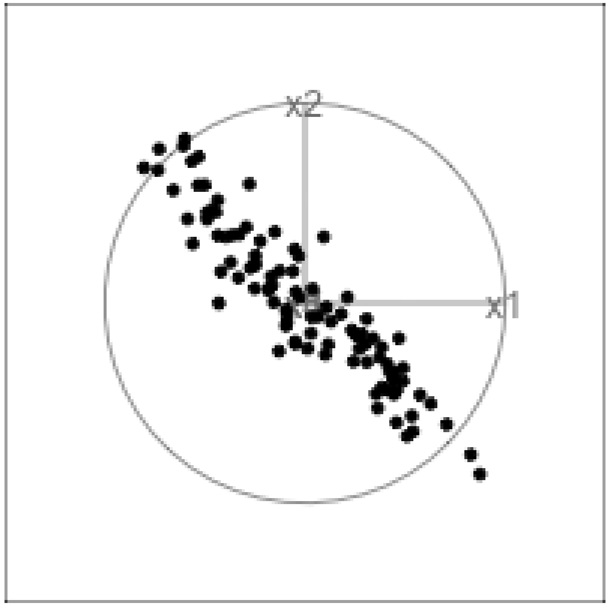
Dimension reduction

What is dimensionality?

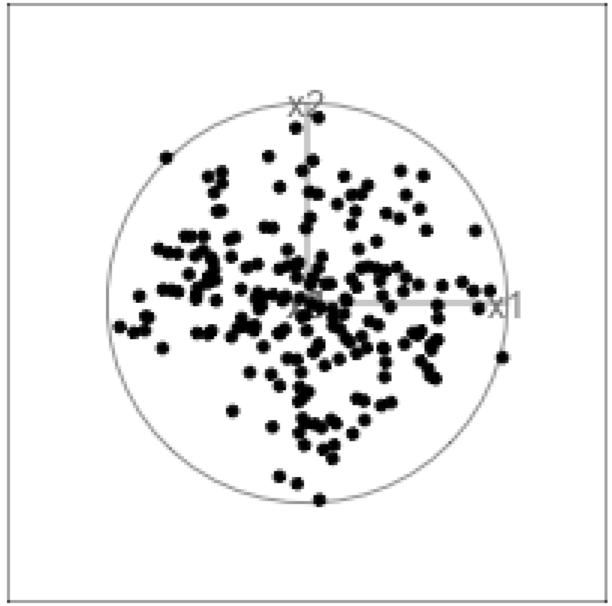


When an axis extends out of a direction where the points are collapsed, it means that this variable is partially responsible for the reduced dimension.

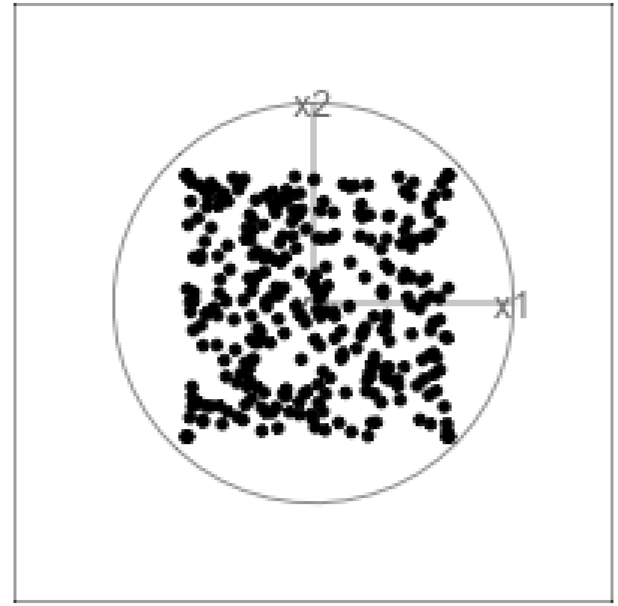
In high-dimensions



2D plane in 5D



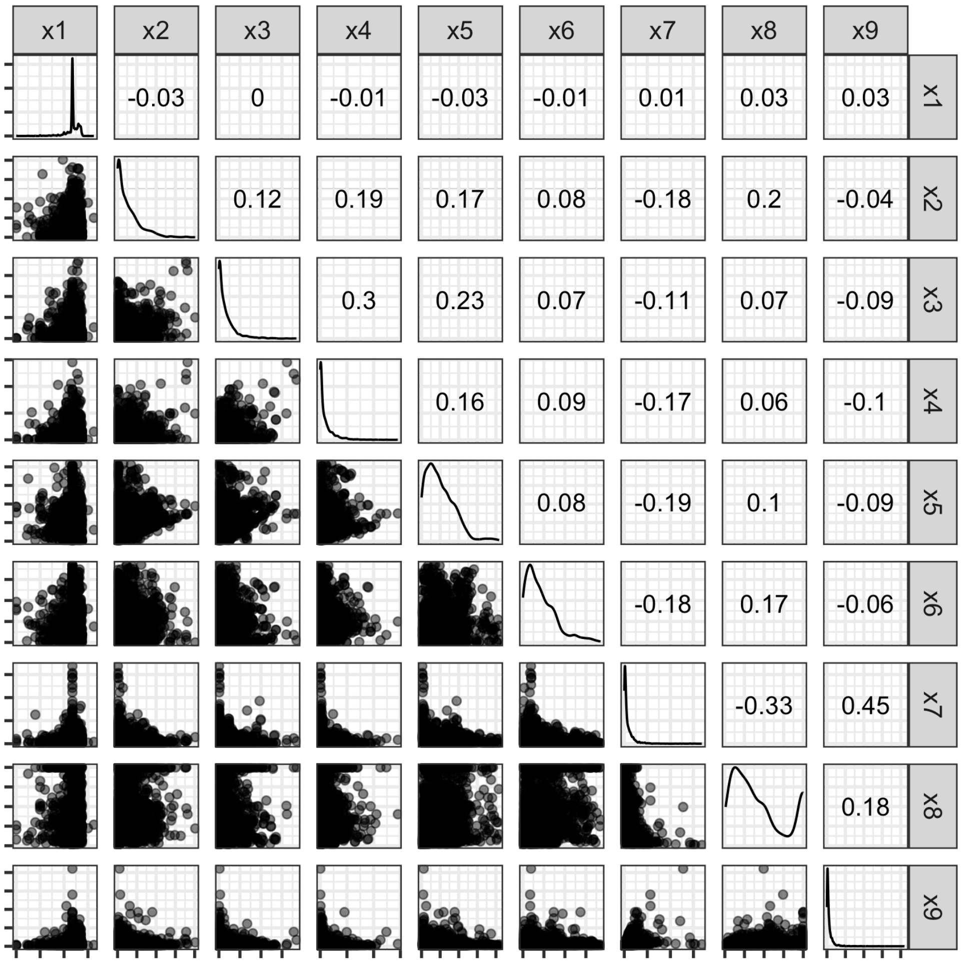
3D plane in 5D

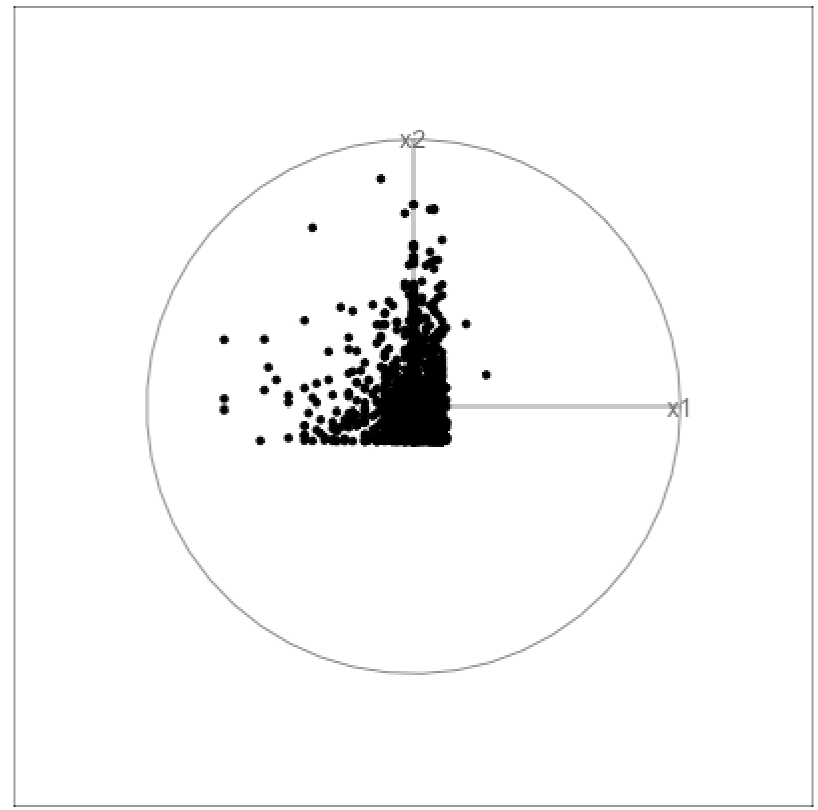


5D plane in 5D

Principal component analysis (PCA) will detect these dimensionalities.

Some data is basically univariate





Mostly skewed variables, some outliers, without much association.

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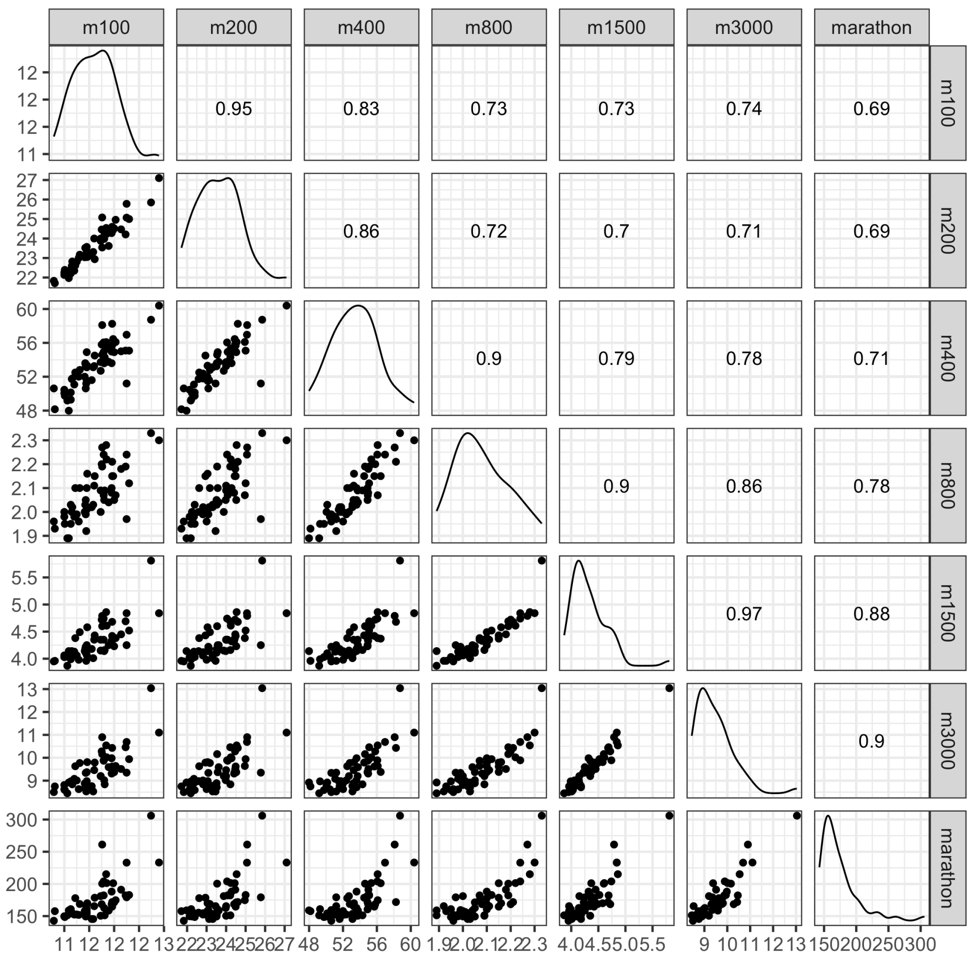
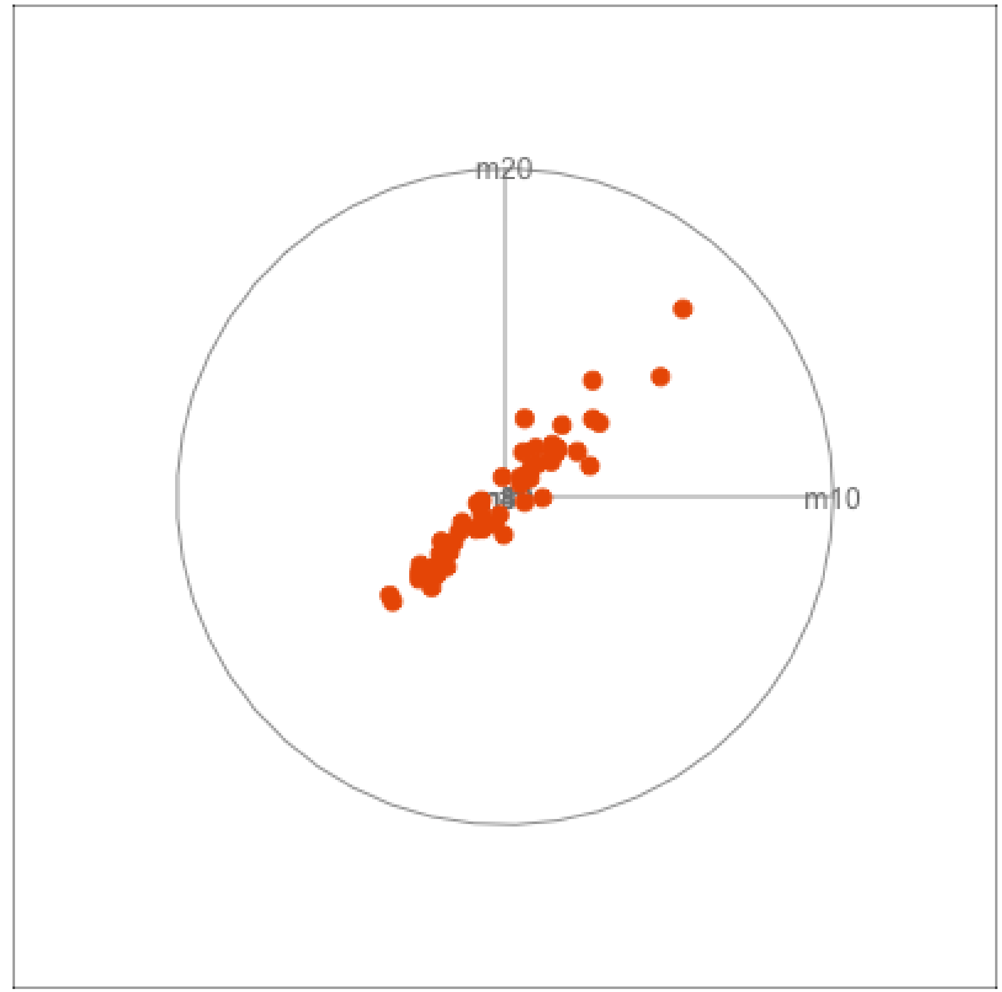
Example: womens' track records (1/3)





Source: Johnson and Wichern, Applied multivariate analysis

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Example: PCA summary (2/3)

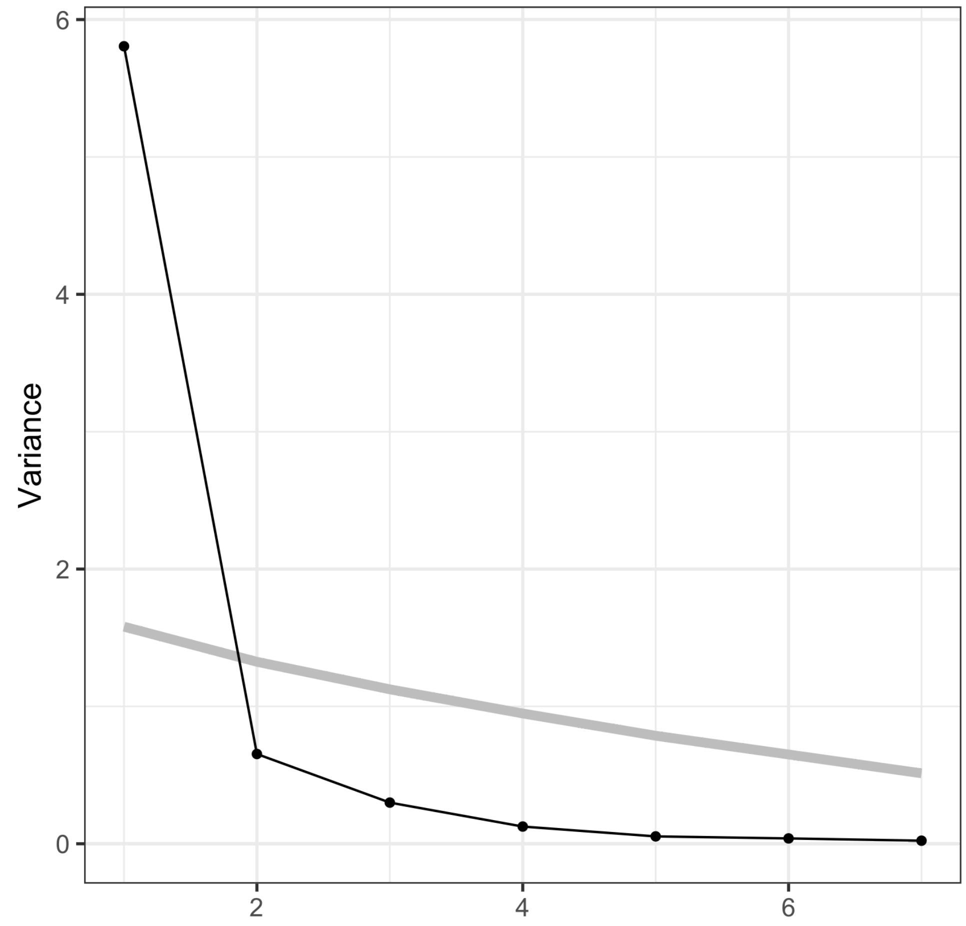
Variances/eigenvalues

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

Component coefficients

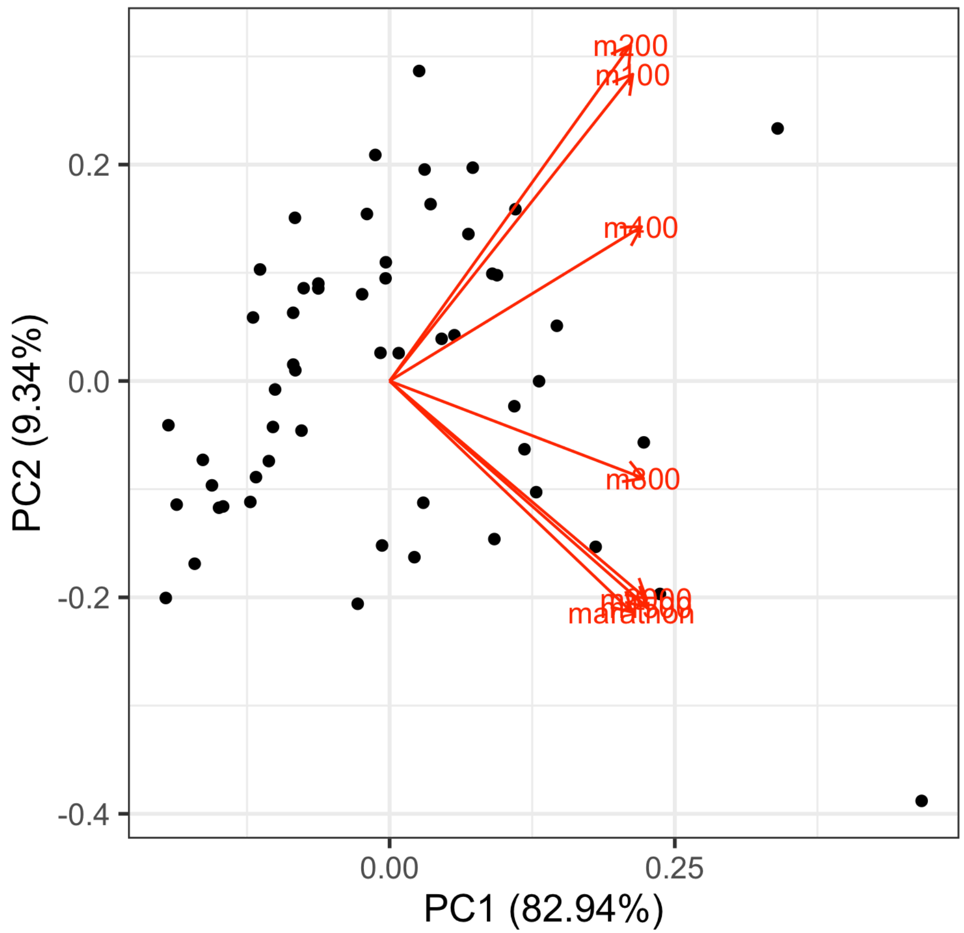
```
          PC1   PC2    PC3    PC4
m100     0.37  0.49 -0.286  0.319
m200     0.37  0.54 -0.230 -0.083
m400     0.38  0.25  0.515 -0.347
m800     0.38 -0.16  0.585 -0.042
m1500    0.39 -0.36  0.013  0.430
m3000    0.39 -0.35 -0.153  0.363
marathon 0.37 -0.37 -0.484 -0.672
```

How many PCs?

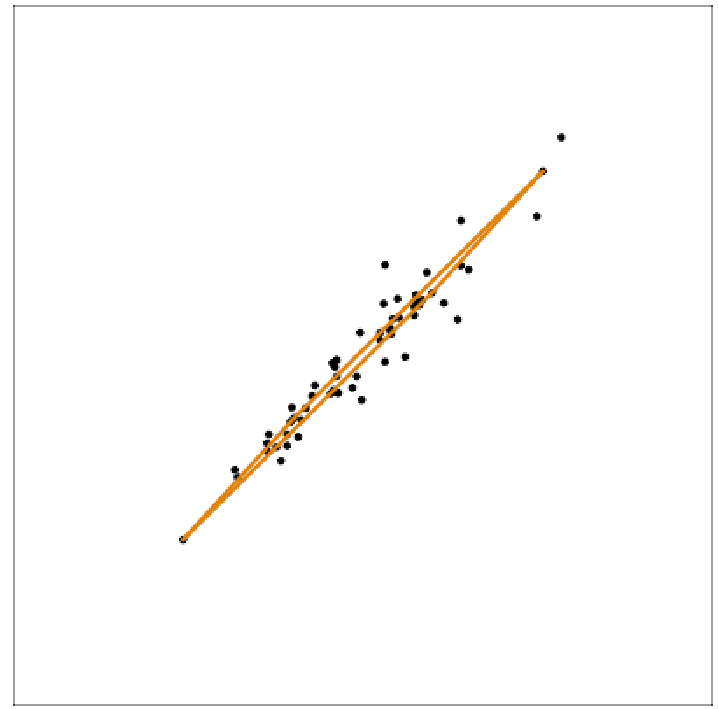


Example: Visualise (3/3)

Biplot: data in the model space



2D model in data space



```
track_model <- mulgar::pca_model(track_std_pca, d=2, s=2)
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")
```

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:

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

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.

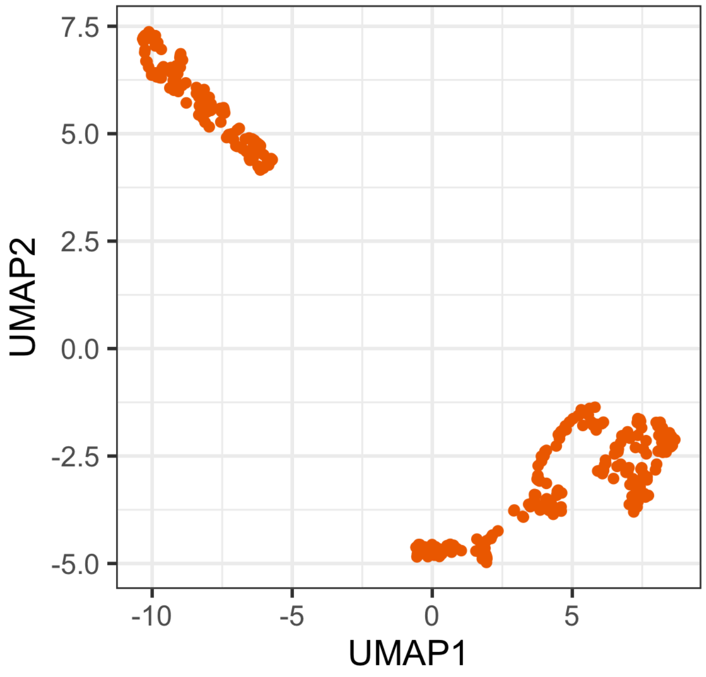
Many variations being developed:

- 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.

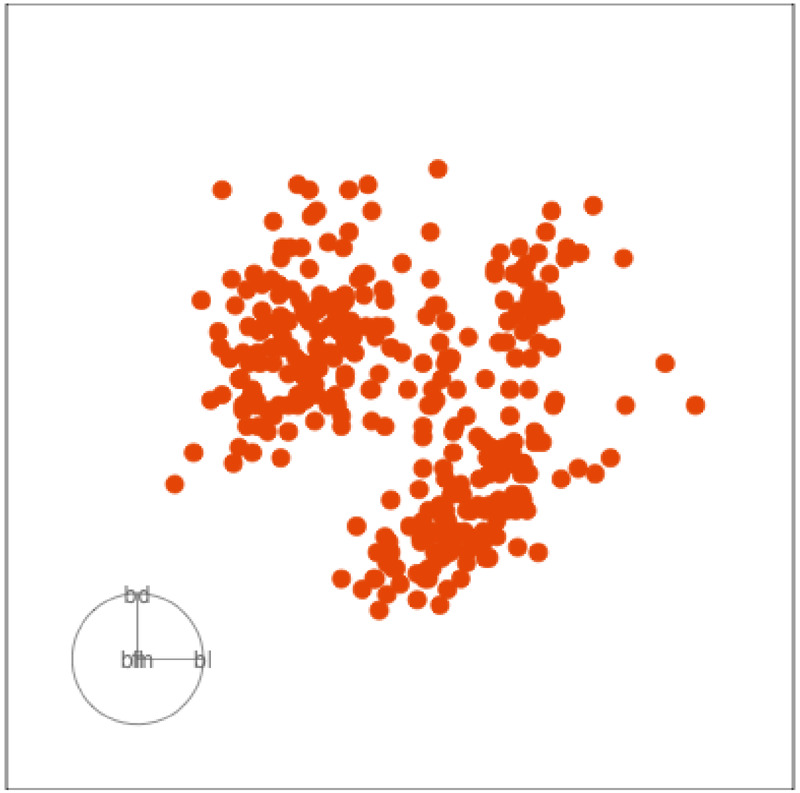
NLDR can be useful but it can also make some misleading representations.

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 = "spca")
```

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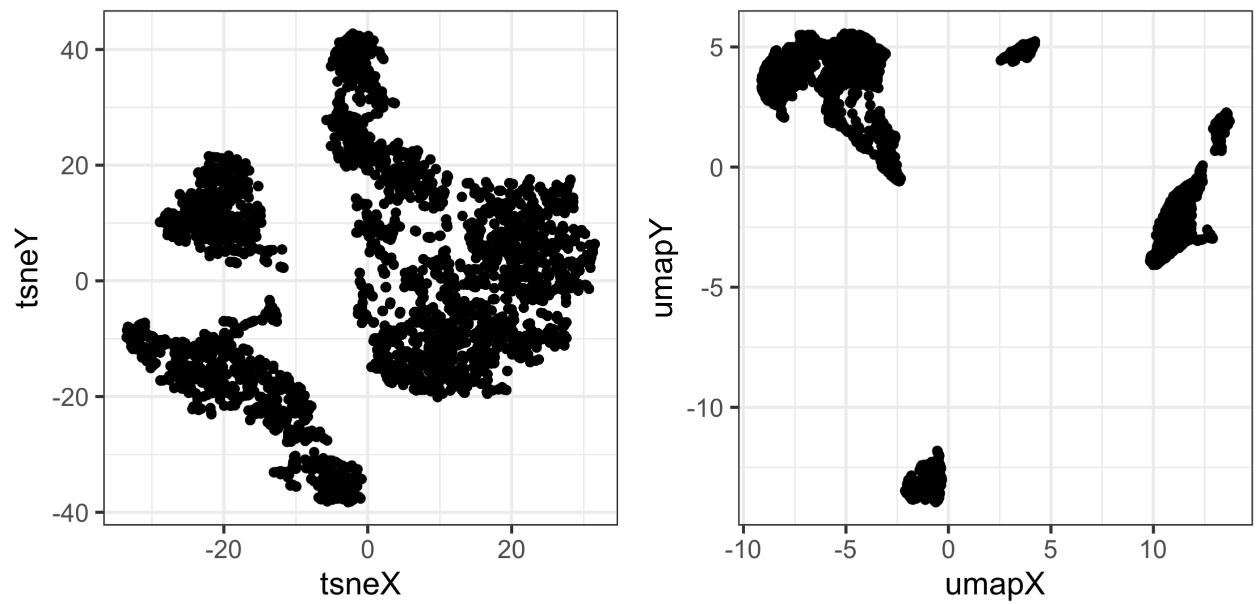
Your turn

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])
```

05:00

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