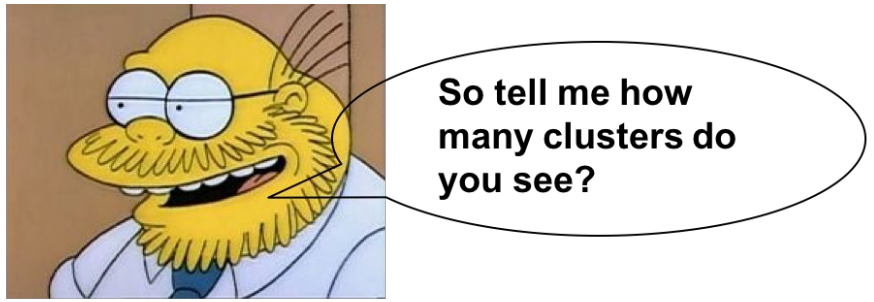
ANOVA continued, PCA and clustering



How many clusters?

Six Clusters

Two Clusters

Four Clusters

Overview

Review and continuation of ANOVAs

- Unbalanced data
- Repeated measures/block designs and random effects models

Principal components analysis (PCA)

If there is time: Clustering

ANOVA review

An Analysis of Variance (ANOVA) can be viewed as:

- A hypothesis test comparing multiple means
- A model for predicting means from categorical variables

In a **factorial ANOVA**, we model the response variable y as a function of **more than one** categorical predictor

For a two-way ANOVA we have:

$$y_{ijk} = \mu + \alpha_j + \beta_k + \gamma_{jk} + \varepsilon_{ijk}$$

Random error for the ijk^{th} data point

i^{th} response when:
- factor A has level j
- Factor B has level k

Overall mean

Main effect for factor A at level j

Main effect for factor B at level k

Specific interaction for j^{th} level of A and k^{th} level of B

Two-way ANOVA hypotheses

Main effect for A (bread type doesn't matter or institution type doesn't matter)

H_0: $\alpha_1 = \alpha_2 = \ldots = \alpha_J = 0$

H_A: $\alpha_j \neq 0$ for some j

Main effect for B (filling doesn't matter)

H_0: $\beta_1 = \beta_2 = \ldots = \beta_K = 0$

H_A: $\beta_k \neq 0$ for some k

Interaction effect:

H_0: All $\gamma_{jk} = 0$

H_A: $\gamma_{jk} \neq 0$ for some j, k

Where:

α_j: is the "effect" for factor A at level j

β_k: is the "effect" for factor B at level k

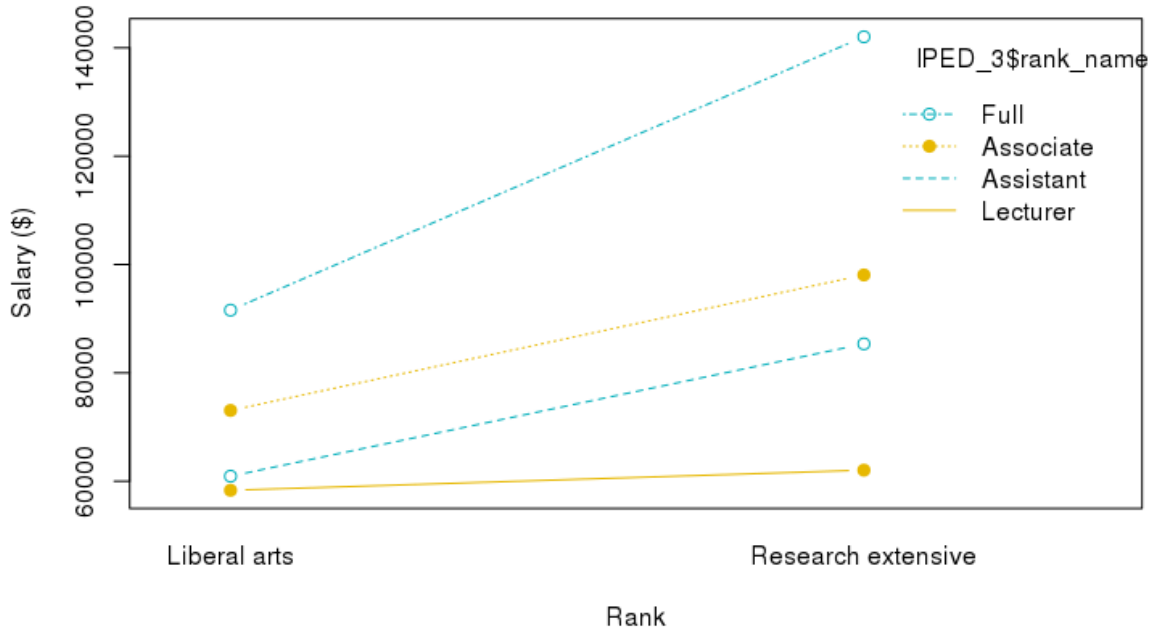
γ_{jk} : is the interaction between level j of factor A, and level k of factor B.

$$y_{ijk} = \mu + \alpha + \beta + \gamma_{jk} + \varepsilon_{ijk}$$

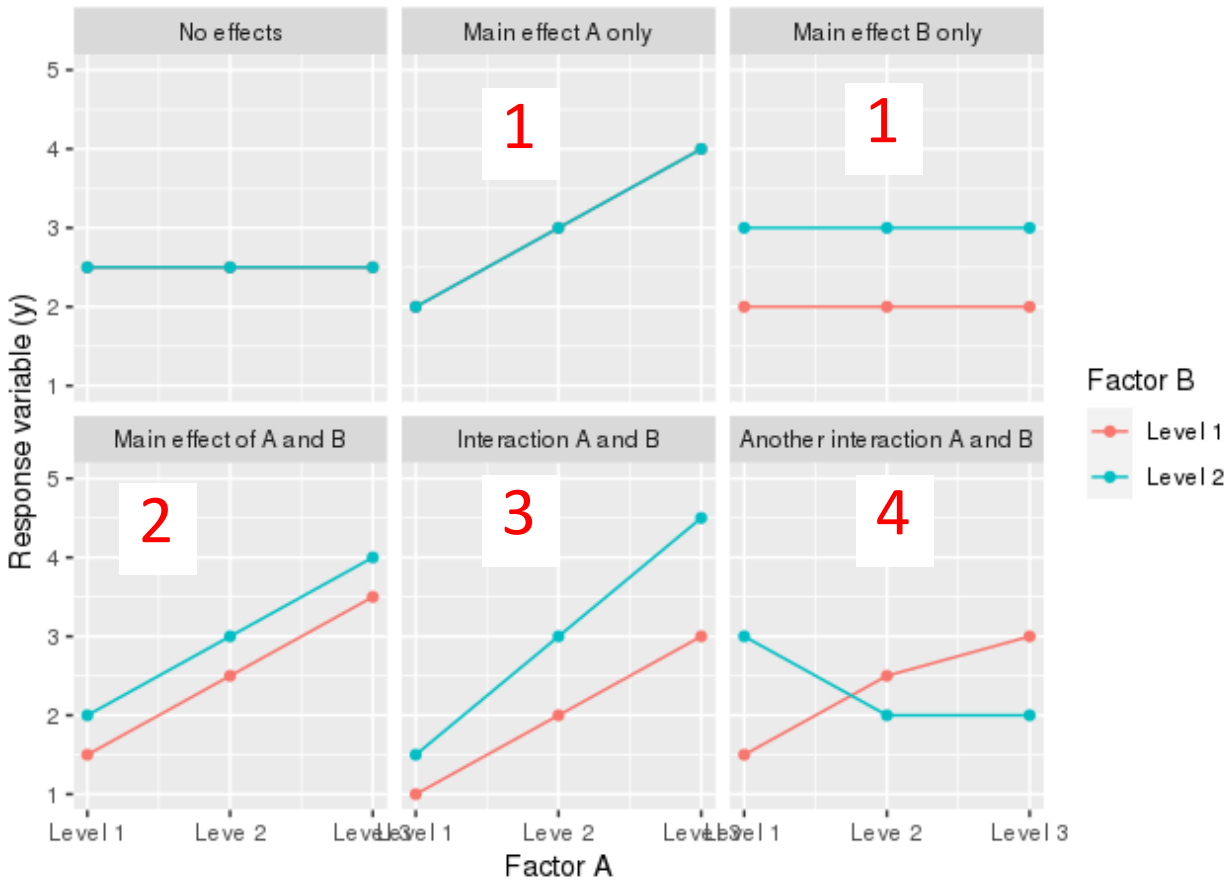
Interaction plots

Interaction plots can help us visualize main effects and interactions

- Plot the levels of one of the factors on the x-axis
- Plot the levels of the other factor as separate lines



Interpreting interaction through interaction plots



What are examples we have seen in class of the interactions in plots 1, 2, 3 and 4?

Complete and balanced designs

Complete factorial design: at least one measurement for each possible combination of factor levels

- E.g., in a two-way ANOVA for factors A and B, if there are K levels for factor A, and J levels for factor B, then there needs to be at least one measurement for each of the KJ levels

Balanced design: the sample size is the same for all combination of factor levels

- E.g., there are the same number of samples in each of the KJ level combinations.
- The computations and interpretations for non-balanced designs are a bit harder.

Unbalanced designs

For unbalanced designs, there are different ways to compute the sum of squares, and hence one can get different p-values

- The problem is analogous to multicollinearity. If two explanatory variables are correlated either can account for the variability in the response data.

Type I sum of squares, (also called sequential sum of squares) the order that terms are entered in the model matters.

- anova(lm(y ~ A*B)) gives different results than using anova(lm(y ~ B*A))
- SS(A) is taken into account before SS(B) is considered etc.

Type III sum of squares, the order that that terms are entered into the model does not matter.

- Car::Anova(lm(y ~ A*B) , type = "III") is the same as car::Anova(lm(y ~ B*A) , type = "III")
- For each factor, SS(A), SS(B), SS(AB) is taken into account after all other factors are added

Repeated measures ANOVA

In a **repeated measures ANOVA**, the same case/observational units are measured at each factor level.

Example: Do people prefer chocolate, butterscotch or caramel sauce?

Between subjects experiment: different people rate chocolate, butterscotch or caramel sauce.

- Run a between subjects ANOVA (as we have done before)

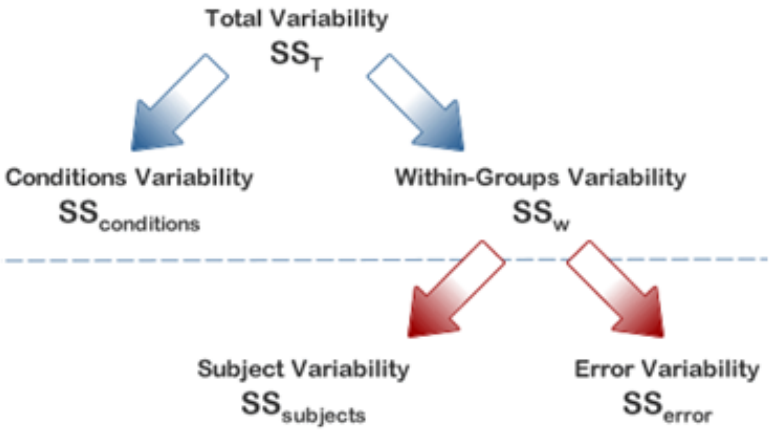
Within subjects experiment: each person in the experiment gives ratings for all three toppings.

- Run a repeated measures ANOVA

Repeated measures ANOVA

The advantages of a repeated measures ANOVA is that we can potentially reduce a lot of the variability between the cases

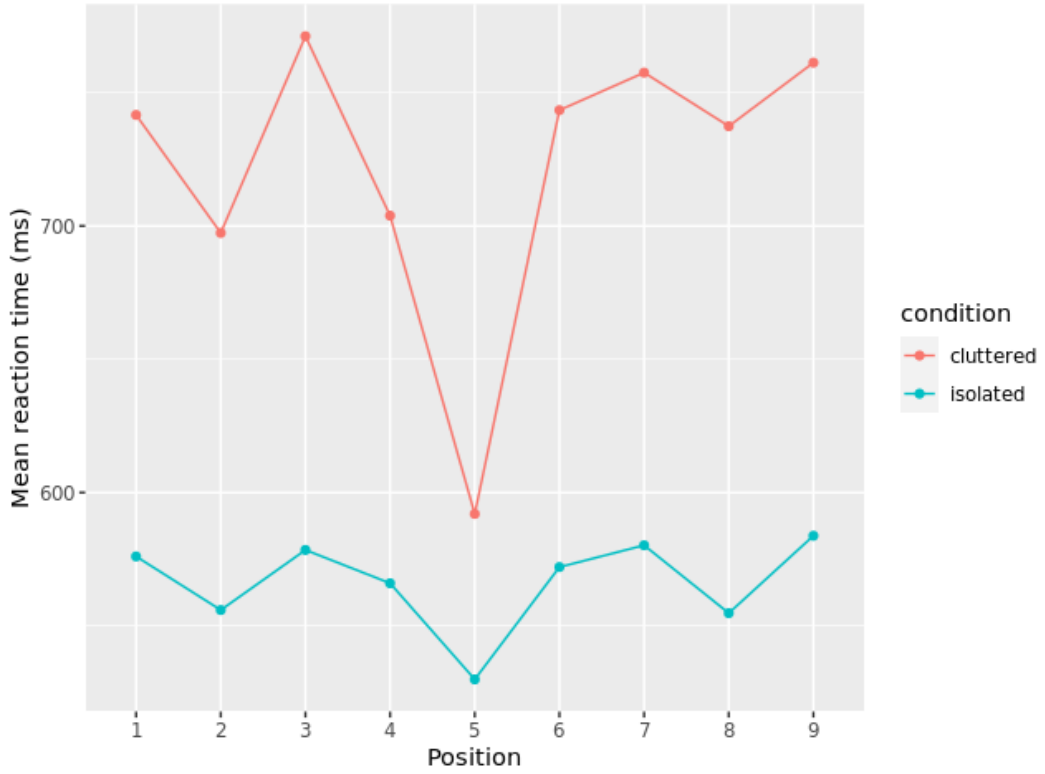
- This is a generalization of a paired t-test to more than two population means

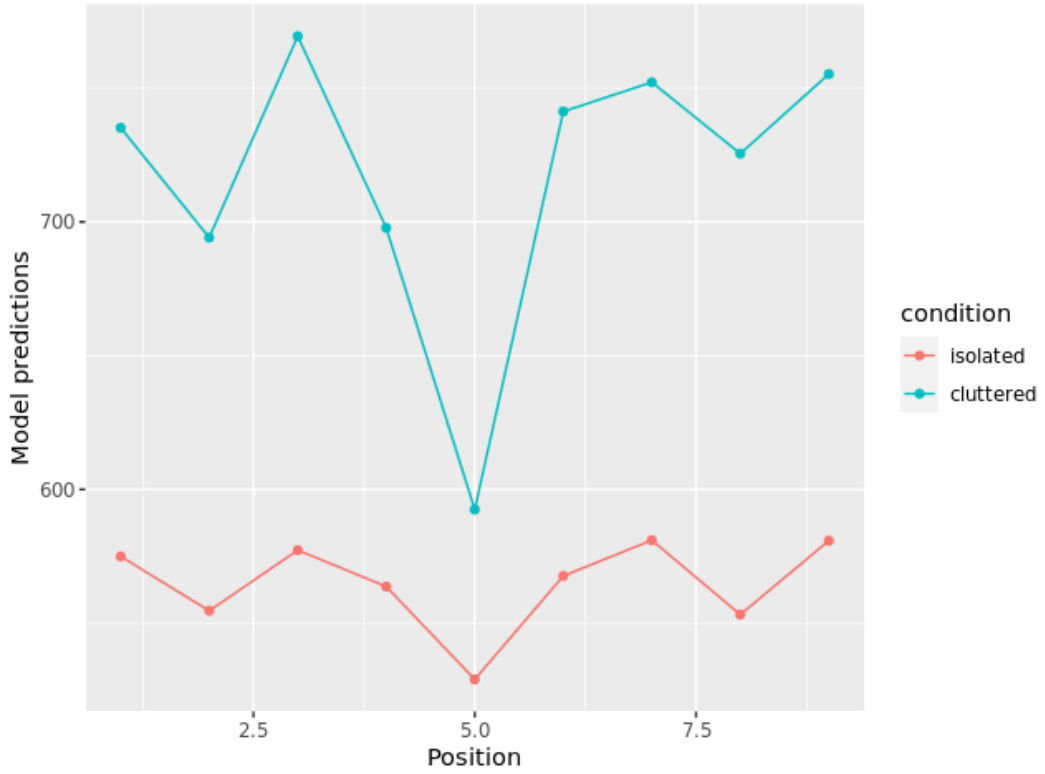


To run a repeated meseasures ANOVA, we use a factor called ID that has a unique value for each observational unit

```
aov(reaction_time ~ condition * position +  participant,
    data = popout_log_data)
```

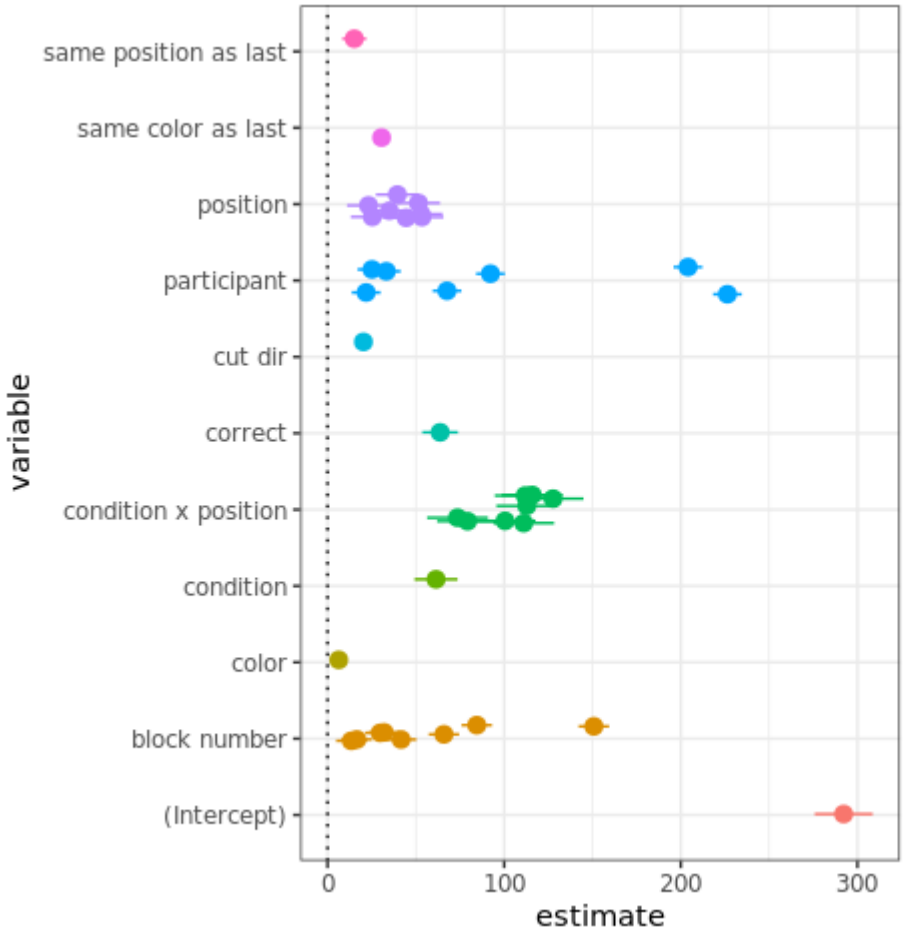
The ANOVA model – popout data

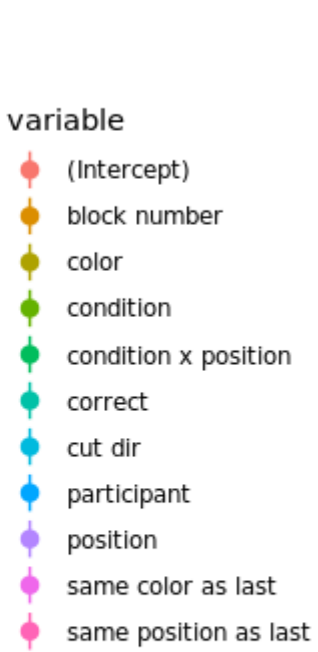


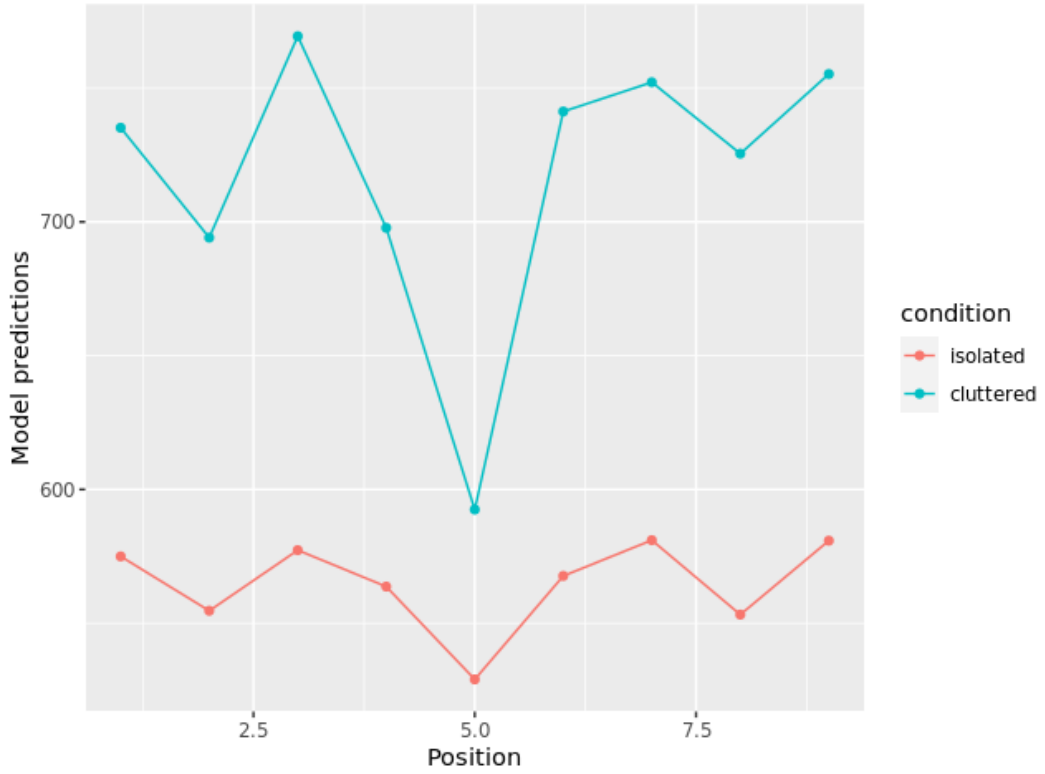


aov(reaction_time ~ condition + position + color + cut_dir + correct + block_number + participant + same_position_as_last + same_color_as_last + position * condition, data = popout_data)

The ANOVA model – popout data



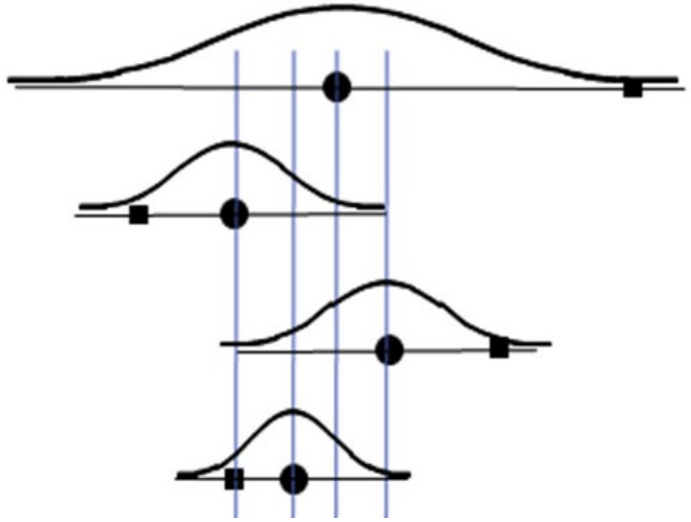




aov(reaction_time ~ condition + position + color + cut_dir + correct + block_number + participant + same_position_as_last + same_color_as_last + position * condition, data = popout_data)

Brief mention: random effects models

In a random effects ANOVA, factor levels are viewed as being randomly generated from an underlying distribution, rather than having a fixed number of levels.



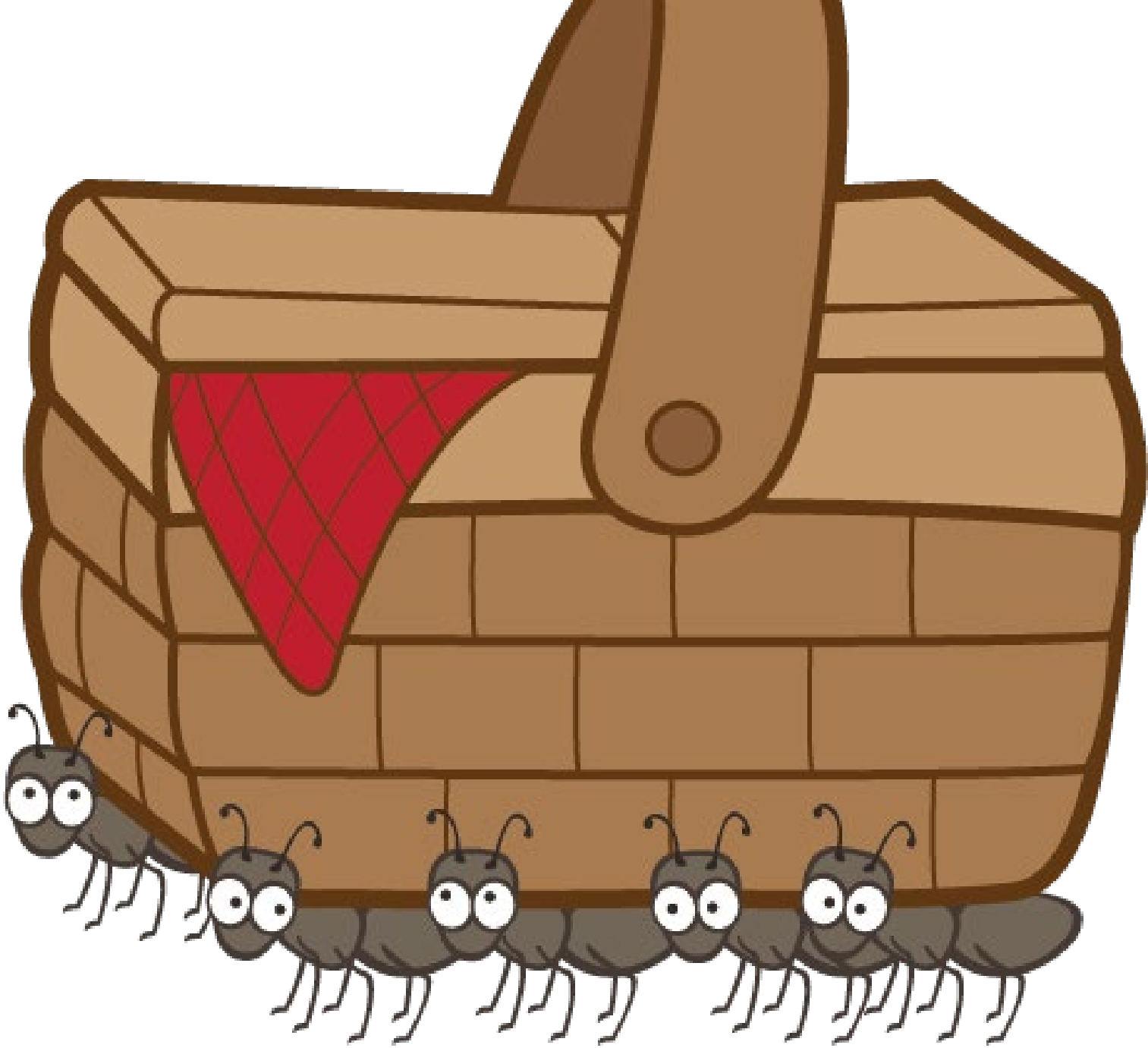
For example, we could view participants in an experiment as being a random sample from participants in a population.

- We then just estimate a mean and standard deviation for the underlying population, rather a separately ID for each participant.
  - This leads to few parameters and hence more degrees of freedom.

You can run mixed effects models in R using the lme4 package

- This is beyond what we will do in this class :/

Let’s these topics it R…



Principal Component Analysis

Supervised learning and unsupervised learning

In **supervised learning** we have a response variable y, along with explanatory variables $x_1, x_2, \ldots, x_k$

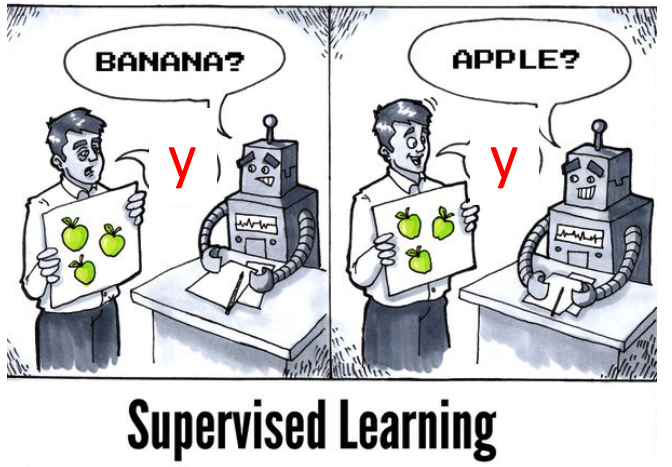
- For example, linear and logistic regression are supervised learning problems because we model a respond variable y as a function of several explanatory variables, $x_1, x_2, \ldots, x_k$

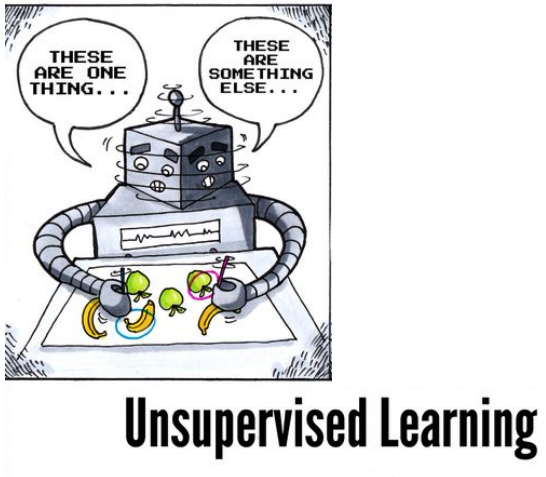
In **unsupervised learning**, we have explanatory variables $x_1, x_2, \ldots, x_k$ but **no** response variable y

Unsupervised learning can be useful in order to find structure in the data and to visualize patterns

A key challenge in unsupervised learning is that there is no real ground truth response variable y

- So we don't have measures like MSPE to see how well our model is fitting the data



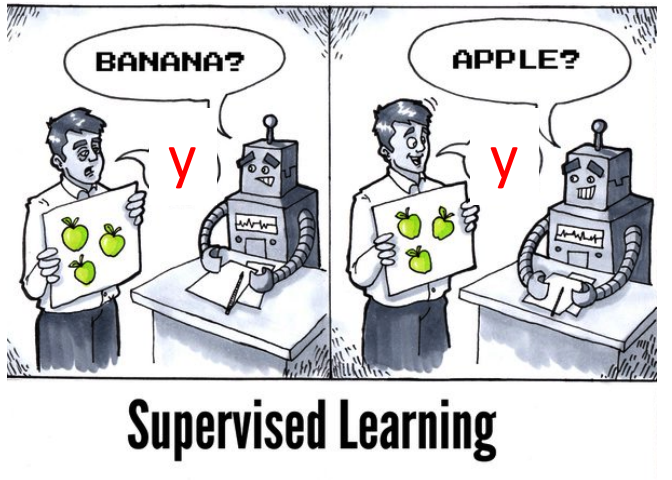


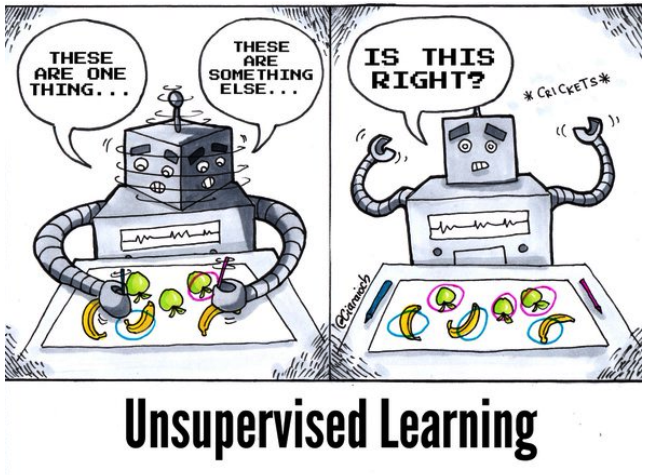
Unsupervised learning

We will discuss two types of unsupervised learning:

1. **Dimensionality reduction** where we try to find a smaller set of features that captures most of the variability in the data
   - Principal component analysis (PCA)

2. **Clustering** where we try to group similar data points together

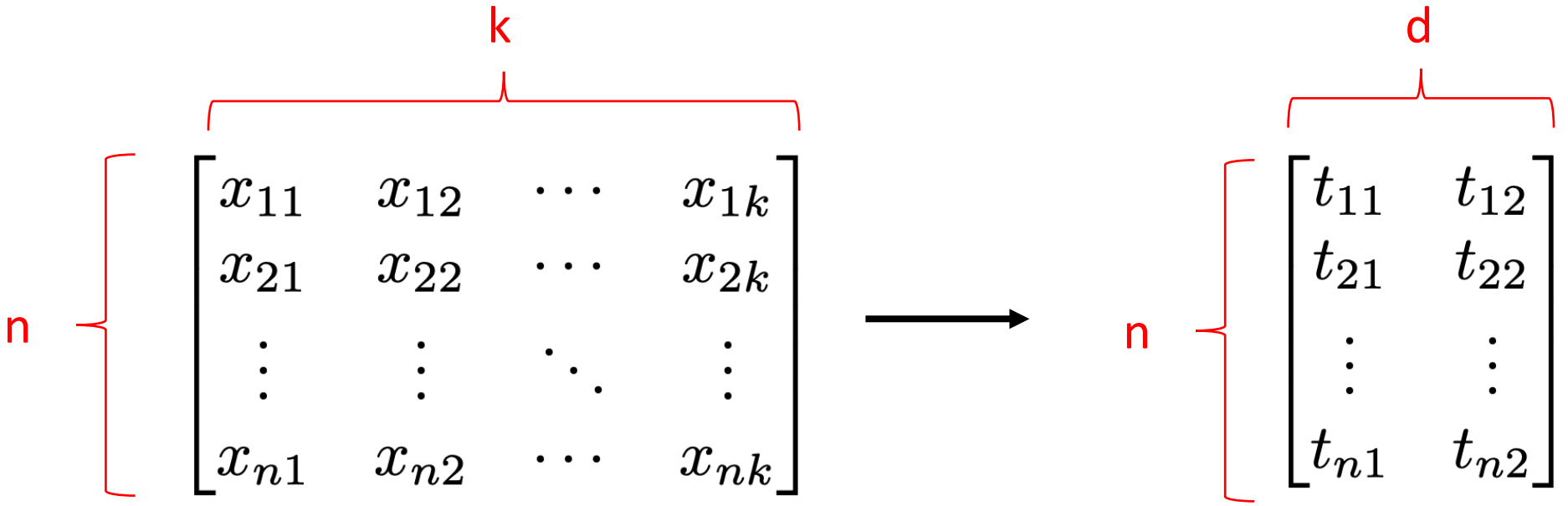




Principal Component Analysis

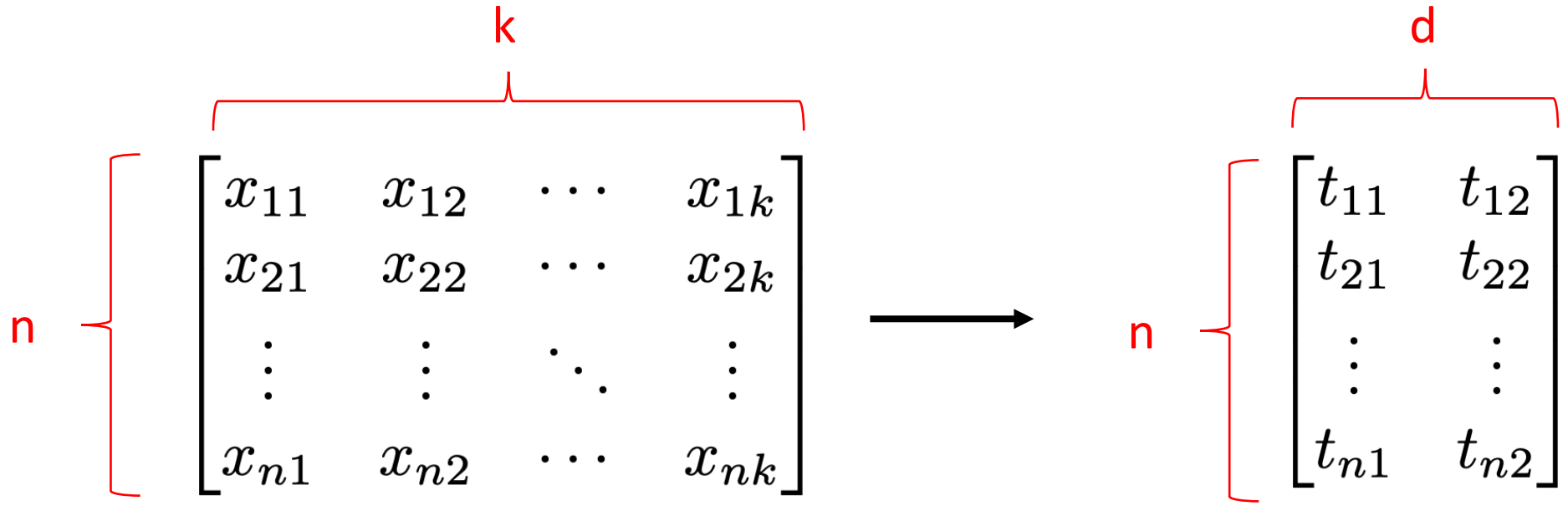
Dimensionality reduction methods find a new smaller set of explanatory variables that capture key properties in the data:

- $f(x_1, x_2, \ldots, x_k) \longrightarrow t_1, t_2, \ldots, t_d$ where $d << k$
- This can be useful for visualization if d is 2 or 3



Principal Component Analysis

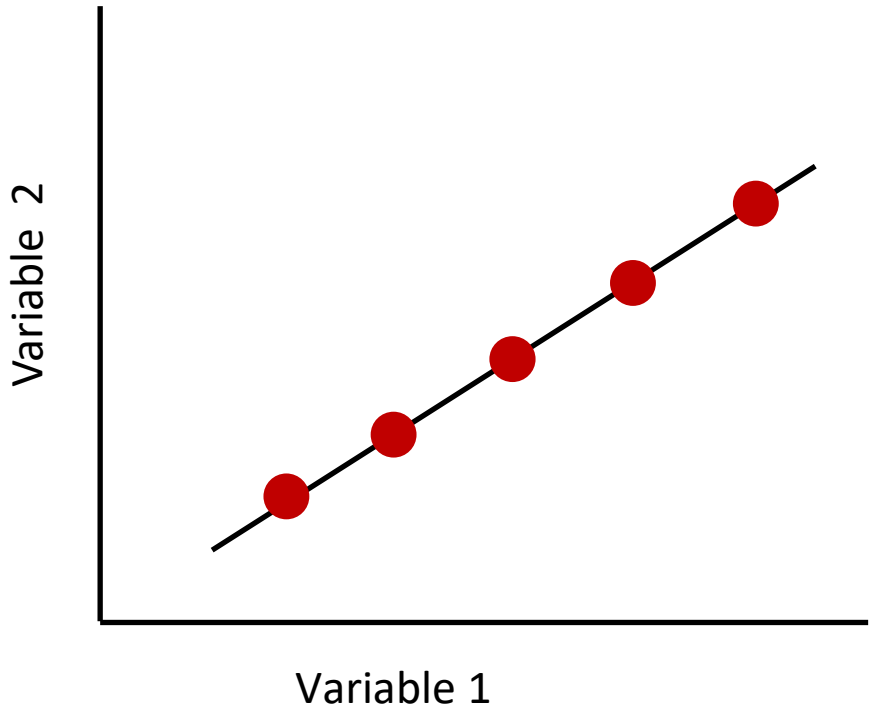
Principal Component Analysis is a dimensionality method that tries to capture most of the variability in the original data



Principal Component Analysis

Suppose that two features are highly correlated.

We can summarize their joint values (x_1, x_2) using a single features t_1



$$t_1 = \tfrac{1}{2} x_1 + \tfrac{1}{2} x_2$$

Principal Component Analysis

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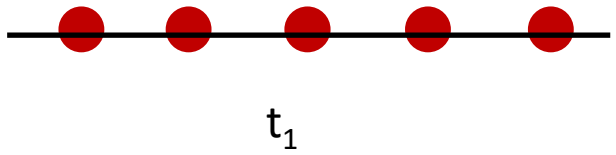
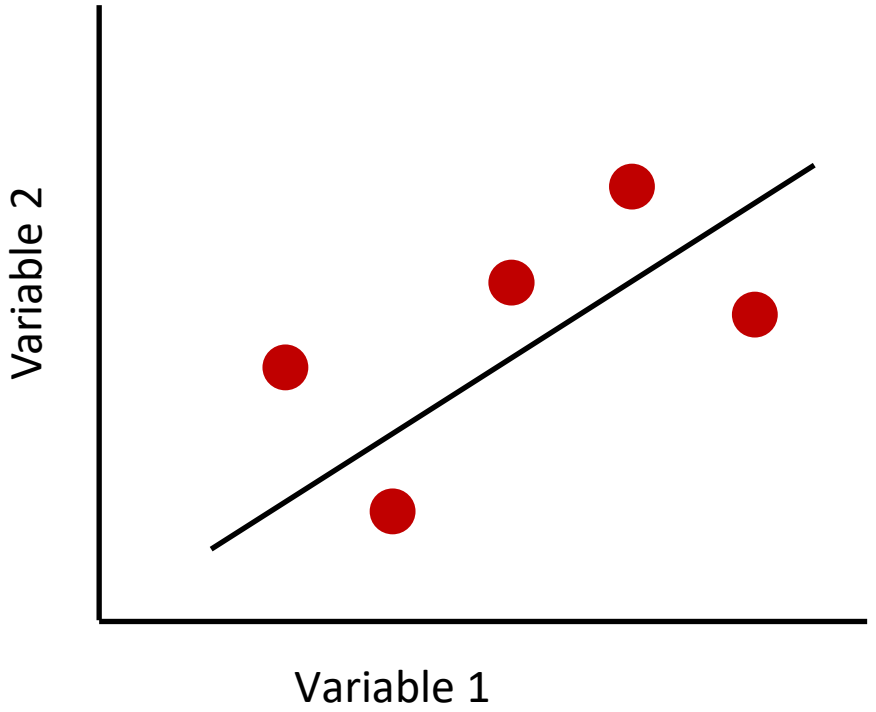


Principal Component Analysis

We can also do this even if the correlation is not perfect



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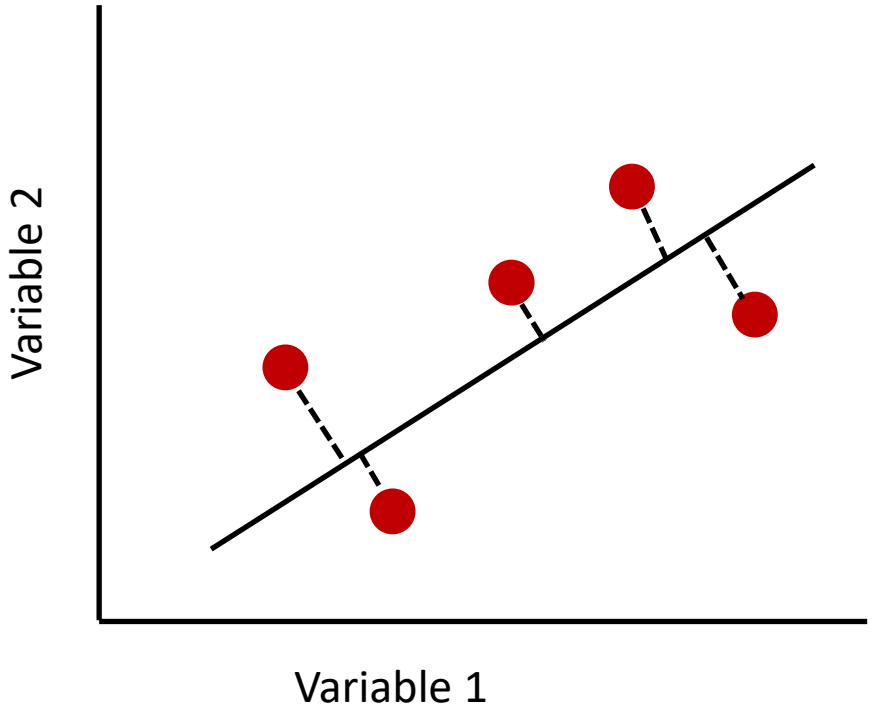

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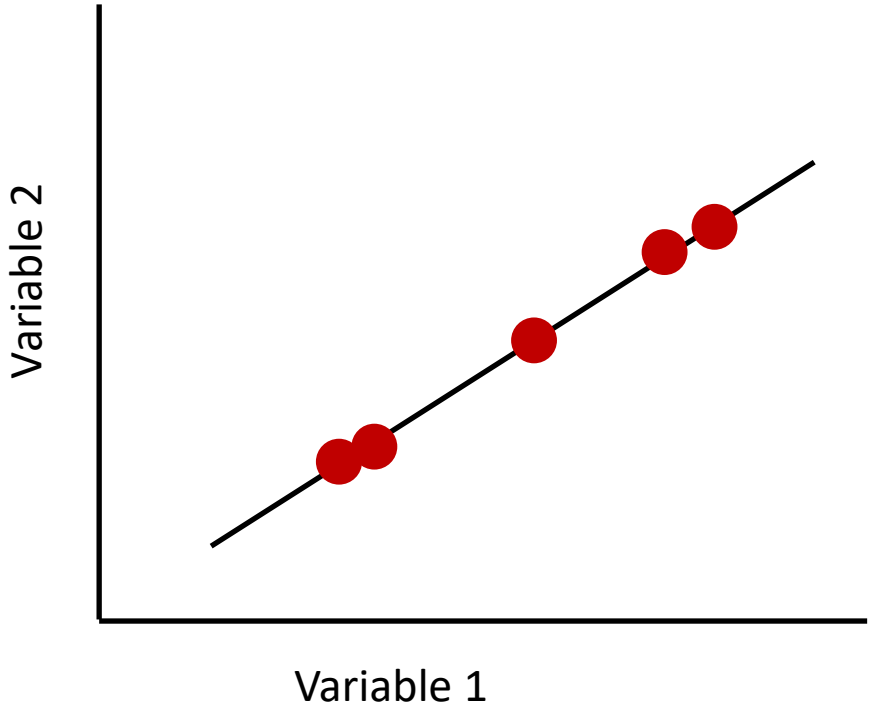


Principal Component Analysis

Principal component **scores** t_i's are linear combinations of the original variables x_{ij}'s:

$$t_{i1} = \alpha_{11}x_{i1} + \alpha_{21}x_{i2} + \ldots + \alpha_{k1}x_{ik}$$

α_{j1} are the **loadings** for the first principal component

- The "norm" of the loadings is 1

$$\sum_{j=1}^{k} \alpha_{j1}^2 = 1$$

$$\begin{bmatrix} t_{11} \\ t_{21} \\ \vdots \\ t_{n1} \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix} \begin{bmatrix} \alpha_{11} \\ \alpha_{21} \\ \vdots \\ \alpha_{k1} \end{bmatrix}$$

We can do this for each case in our data set we get values: $t_{11}, \ldots, t_{n1}$

Principal Component Analysis

To run PCA, we starts by centering each variable x_i so that it has a mean of 0

We also usually divide all variables by their standard deviation

- i.e., z-score the transform the features before performing PCA
- We divide by the s_i's so that variables with large variances don't dominate

$$\begin{bmatrix} t_{11} \\ t_{21} \\ \vdots \\ t_{n1} \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix} \begin{bmatrix} \alpha_{11} \\ \alpha_{21} \\ \vdots \\ \alpha_{k1} \end{bmatrix}$$

$$\begin{bmatrix} \bar{x}_1 & \bar{x}_2 & \dots & \bar{x}_k \end{bmatrix}$$

$$\begin{bmatrix} s_1 & s_2 & \dots & s_k \end{bmatrix}$$

Principal Component Analysis

The loadings for the first principal component are found by finding the projection vector $A_1 = (\alpha_{11}, \alpha_{21}, \alpha_{k1})$ such that the variance of the t_i is maximized

$$\begin{bmatrix} t_{11} \\ t_{21} \\ \vdots \\ t_{n1} \end{bmatrix} = \begin{bmatrix} z_{11} & z_{12} & \cdots & z_{1k} \\ z_{21} & z_{22} & \cdots & z_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & \cdots & z_{nk} \end{bmatrix} \begin{bmatrix} \alpha_{11} \\ \alpha_{21} \\ \vdots \\ \alpha_{k1} \end{bmatrix}$$

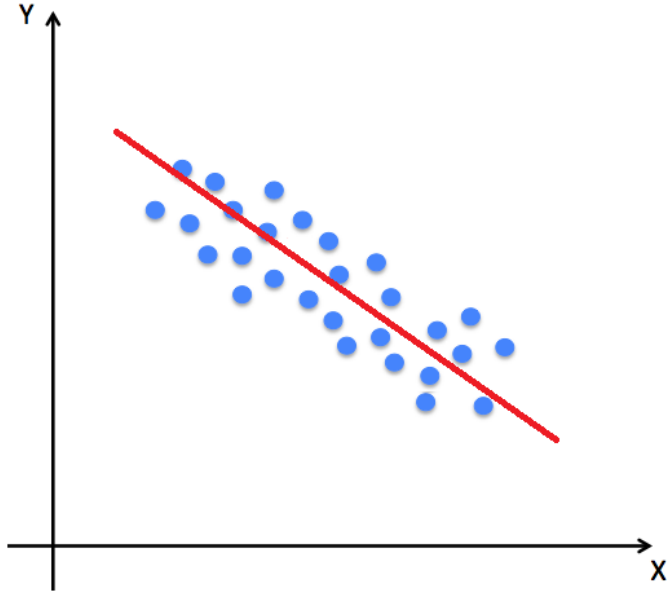
Find the α's that maximize:

$$\frac{1}{n-1}\sum_{i=1}^{n} t_i^2 = \frac{1}{n-1}\sum_{i=1}^{n}(\alpha_{11}z_{i1} + \alpha_{21}z_{i2} + \ldots + \alpha_{k1}z_{ik})^2$$

Subject to the constraint:

$$\sum_{j=1}^{k} \alpha_{j1}^2 = 1$$

Principal Component Analysis



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Find the α's that maximize:

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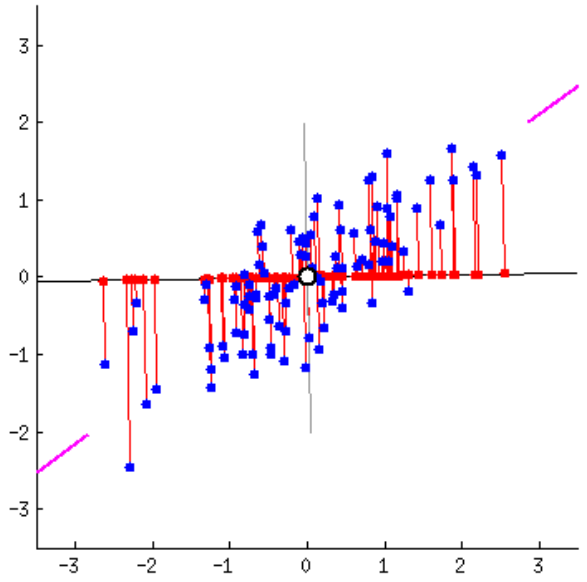

Subject to the constraint:

$$\sum_{j=1}^{k} \alpha_{j1}^2 = 1$$

The Second Principal Component

The second principal component scores t_{i2} is the linear combination of the $z_1, z_2, \ldots, z_k$ that has maximal variance and is **uncorrelated** with the first principal component scores t_{i1}

- $t_{i2} = \alpha_{12}z_1 + \alpha_{22}z_2 + \ldots + \alpha_{k2}z_k$
- $cor(T_1, T_2) = 0$

This is equivalent of having A_1 be orthogonal to A_2

- $A_1^T A_2 = 0$

$$\sum_{j=1}^{k} \alpha_{j1} \cdot \alpha_{j2} = 0$$

First principal component

$$\begin{bmatrix} t_{11} \\ t_{21} \\ \vdots \\ t_{n1} \end{bmatrix} = \begin{bmatrix} z_{11} & z_{12} & \cdots & z_{1k} \\ z_{21} & z_{22} & \cdots & z_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & \cdots & z_{nk} \end{bmatrix} \begin{bmatrix} \alpha_{11} \\ \alpha_{21} \\ \vdots \\ \alpha_{k1} \end{bmatrix}$$

Second principal component

$$\begin{bmatrix} t_{12} \\ t_{22} \\ \vdots \\ t_{n2} \end{bmatrix} = \begin{bmatrix} z_{11} & z_{12} & \cdots & z_{1k} \\ z_{21} & z_{22} & \cdots & z_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & \cdots & z_{nk} \end{bmatrix} \begin{bmatrix} \alpha_{12} \\ \alpha_{22} \\ \vdots \\ \alpha_{k2} \end{bmatrix}$$

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$$\sum_{j=1}^{k} \alpha_{j1} \cdot \alpha_{j2} = 0$$

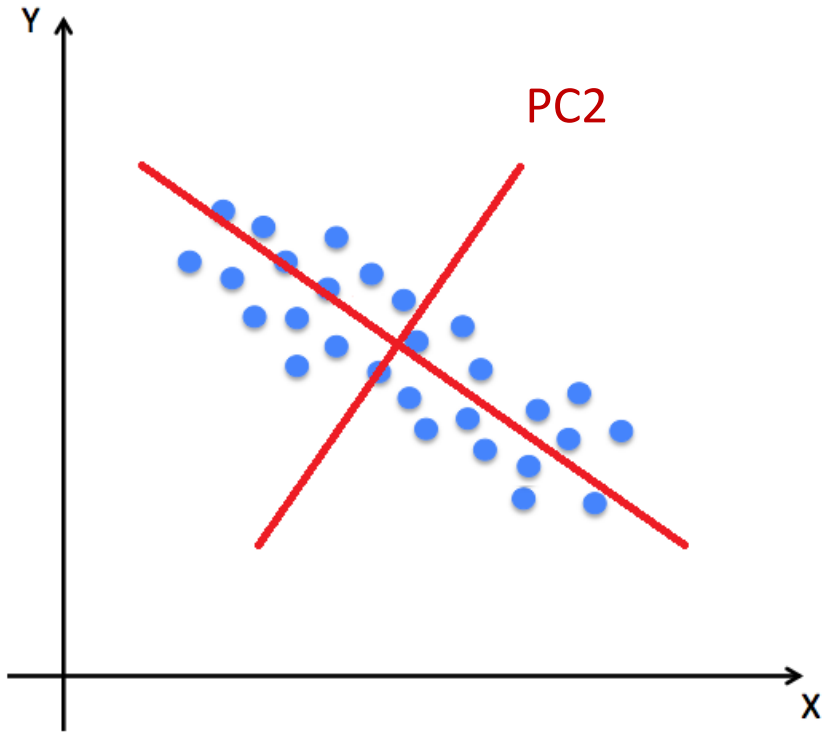
First and second principal components

$$\begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \\ \vdots & \vdots \\ t_{n1} & t_{n2} \end{bmatrix} = \begin{bmatrix} z_{11} & z_{12} & \cdots & z_{1k} \\ z_{21} & z_{22} & \cdots & z_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & \cdots & z_{nk} \end{bmatrix} \begin{bmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \\ \vdots & \vdots \\ \alpha_{k1} & \alpha_{k2} \end{bmatrix}$$

Geometric interpretation of the second PC

Find the direction that maximizes the variance of t_i's

- Data projected on to the principal component is most spread out that is perpendicular (orthogonal) to the other PCs



Higher Principal Components

We continue this process until we find all the principal component scores, T_1, T_2, … T_d

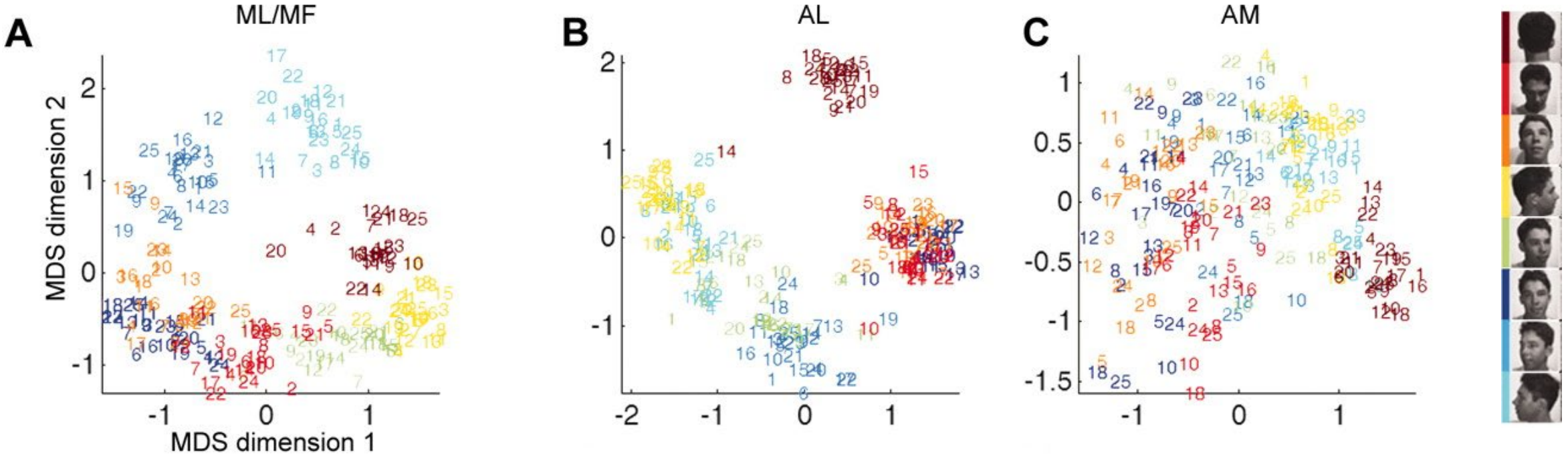
- The principal component scores are unique up to a sign flip $T_i = -T_i$
  - To find the principal components what is really done is an eigenvalue decomposition of the covariance matrix.

All principal components

$$\begin{bmatrix} t_{11} & t_{12} & \dots & t_{1d} \\ t_{21} & t_{22} & \dots & t_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ t_{n1} & t_{n2} & \dots & t_{nd} \end{bmatrix} = \begin{bmatrix} z_{11} & z_{12} & \dots & z_{1k} \\ z_{21} & z_{22} & \dots & z_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ z_{n1} & z_{n2} & \dots & z_{nk} \end{bmatrix} \begin{bmatrix} \alpha_{11} & \alpha_{12} & \dots & \alpha_{1d} \\ \alpha_{21} & \alpha_{22} & \dots & \alpha_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{k1} & \alpha_{k2} & \dots & \alpha_{kd} \end{bmatrix}$$

Neuroscience example

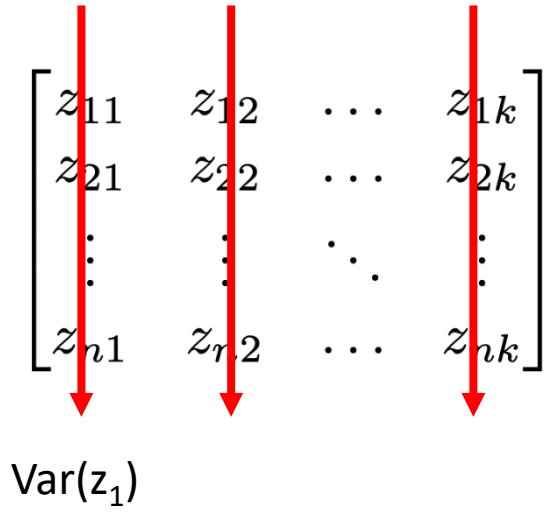
Freiwald and Tsao (Science 2010) used dimensionality reduction to reduce the activity of a large population of neurons to two dimensions so that they could visualize how different brain regions represent faces.



Proportion of Variance Explained

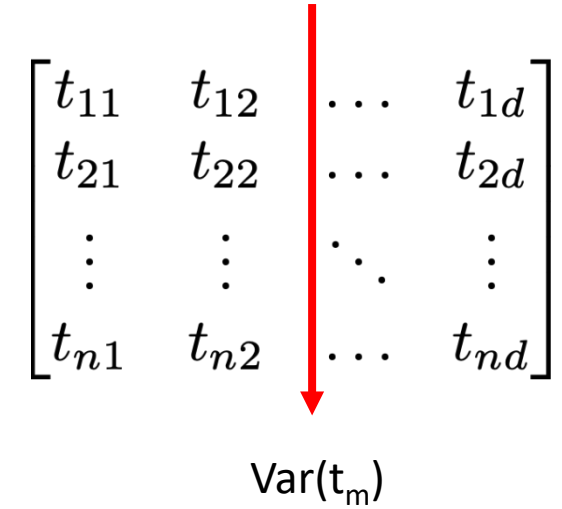
In order to know how many principal components to use, it is usual to assess the **proportion of variance explained** (PVE) by each PC

Total variance: $$\sum_{j=1}^{k} Var(z_j) = \sum_{j=1}^{k} \frac{1}{n-1} \sum_{i=1}^{n} (z_{ij})^2$$



Variance explained by mth principal component:

$$Var(t_m) = \frac{1}{n-1} \sum_{i=1}^{n} t_{im}^2 = \frac{1}{n-1} \sum_{i=1}^{n} (\sum_{j=1}^{k} \alpha_{jm} z_{ij})^2$$

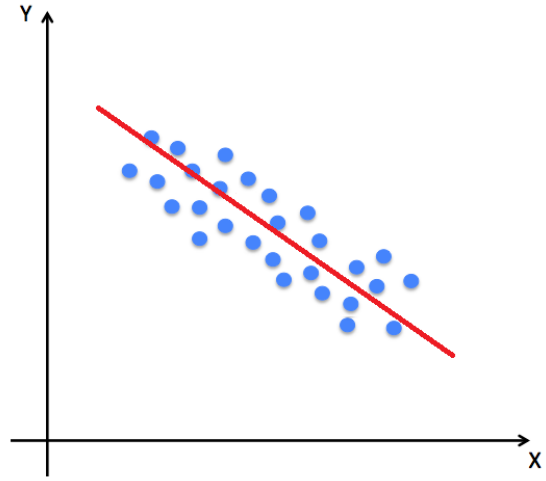


Proportion of Variance Explained

Proportion *of variance that is explained* by each PC:

$$\text{PVE}_{mv} = \frac{\text{Variance explained by m}^{th}\text{ principal component}}{\text{Total variance}}$$

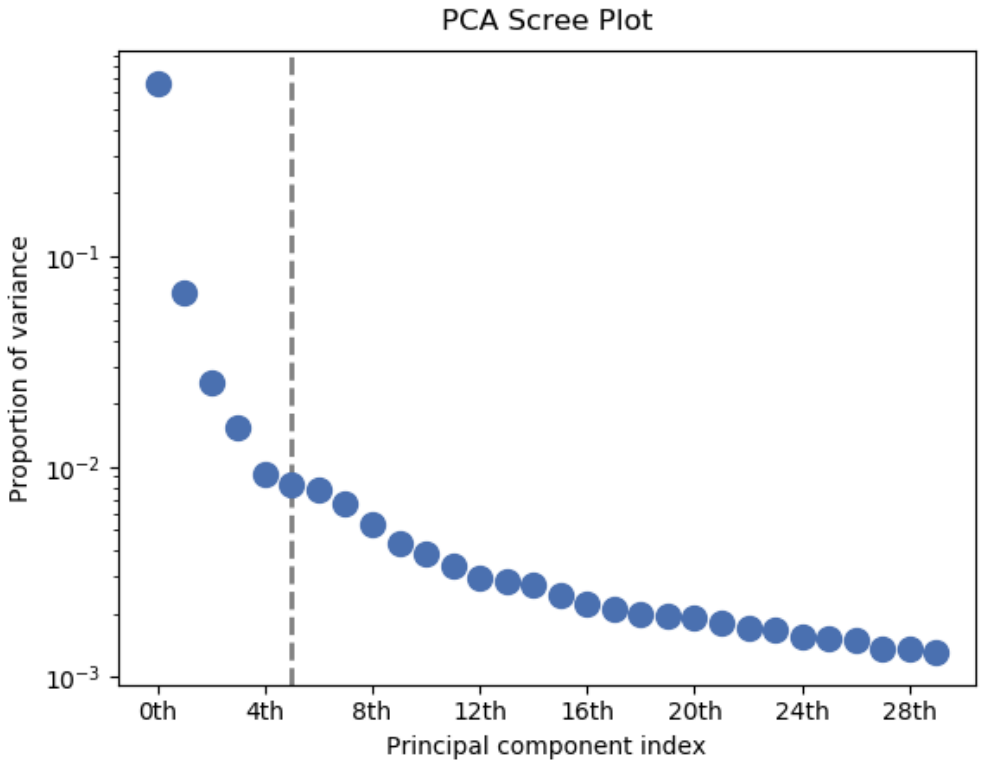
$$PVE_m = \frac{Var(t_m)}{Var(total)} = \frac{\sum_{i=1}^{n}(\sum_{j=1}^{k}\alpha_{jm}z_{ij})^2}{\sum_{j=1}^{k}\sum_{i=1}^{n}z_{ij}^2}$$



Deciding how many PCs to use

A **scree plot** shows the PVE as a function of PC number

- The number of PCs chosen is often selected by looking for the “elbow” in this plot
  - i.e., point where PVE stop dramatically dropping and levels off



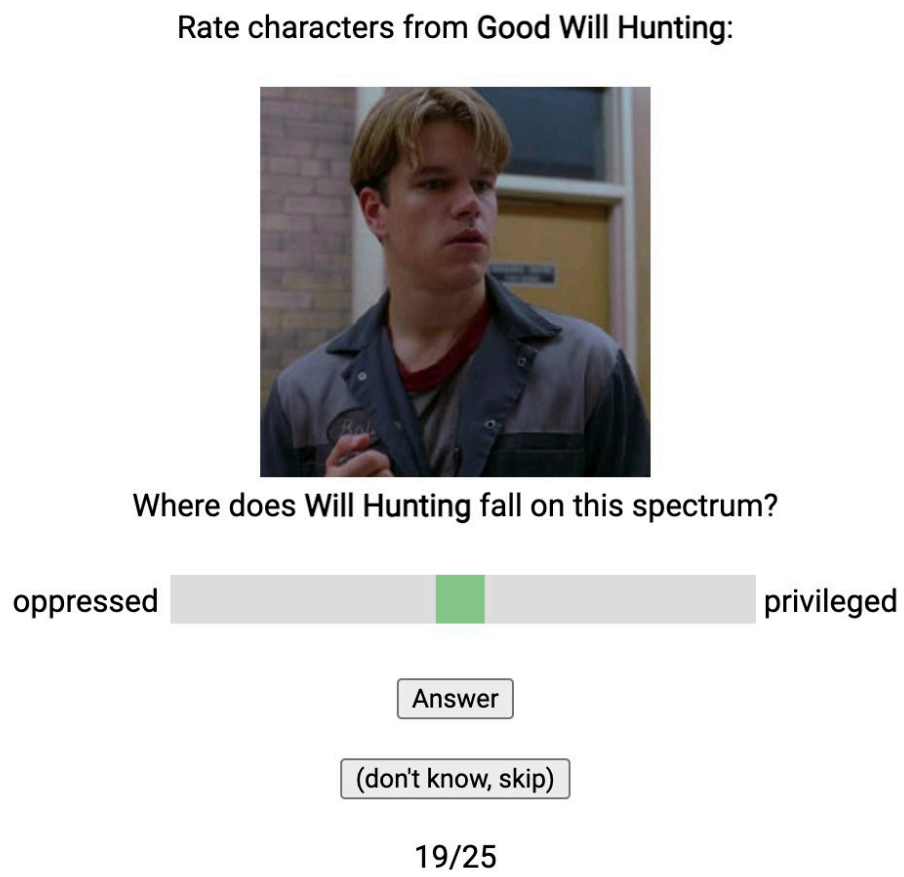
PCA example: personality traits of fictional characters

The Open-Source Psychometrics Project conducted a survey where they got ratings of 235+ personality traits from 800 fictional characters.

Let's use PCA to assess:

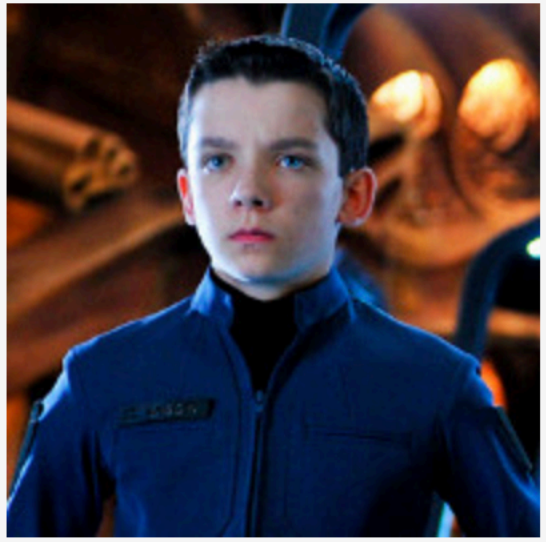
- How to personality traits commonly covary
- Which fictional characters are most similar

If you want to find out which fictional character you are most similar you can take their "Which Character" personality quiz



Let’s try the PCA in R…

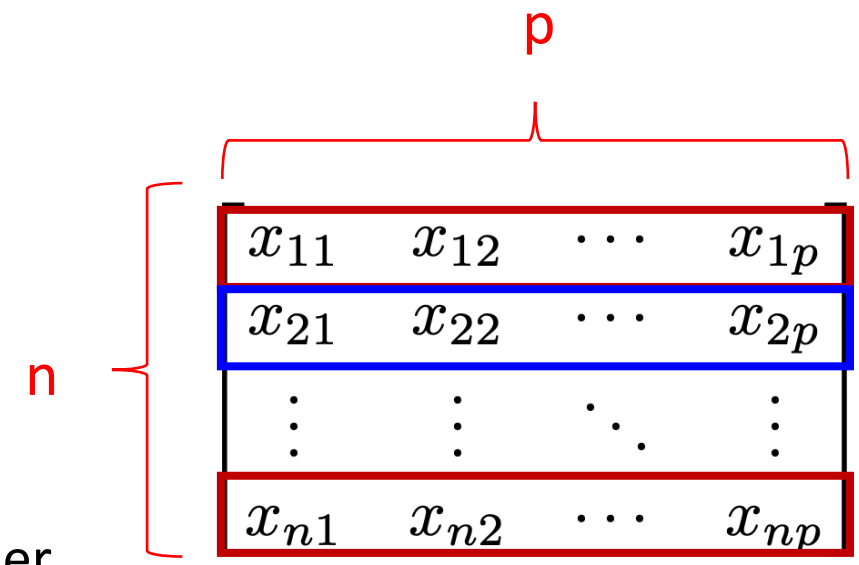
The best match between the self assessment you provided and the profile of a fictional character as rated by other people who have taken this survey is the character **Ender Wiggin** (Ender's Game).



84% match

Your traits versus their traits are graphed below (click on points for labels).

Clustering



Clustering divides n data points x_i's into subgroups

- Data points in the same group are similar/homogeneous
- Data points in different groups are different from each other

Examples:

- Examining gene expression levels to group cancer types together
- Examining consumer purchasing behavior to perform market segmentation

Clustering can be:

- **Flat**: no structure beyond dividing points into groups
- **Hierarchical**: Population is divided into smaller and smaller groups (tree like structure)

K-means clustering

K-means clustering partitions the data into ***K*** distinct, non-overlapping clusters

- i.e., each data point x_i belongs to exactly one cluster C_k

The number of clusters, ***K***, needs to be specified prior to running the algorithm

The goal is to minimize the within-cluster variation for some measure $W(C_k)$

$$\underset{C_1,\ldots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} W(C_k) \right\}$$

K-means clustering

A common within cluster similarity measure $W(C_k)$ is the sum of the **Euclidean distance** between all pairs of points in a cluster:

$$\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

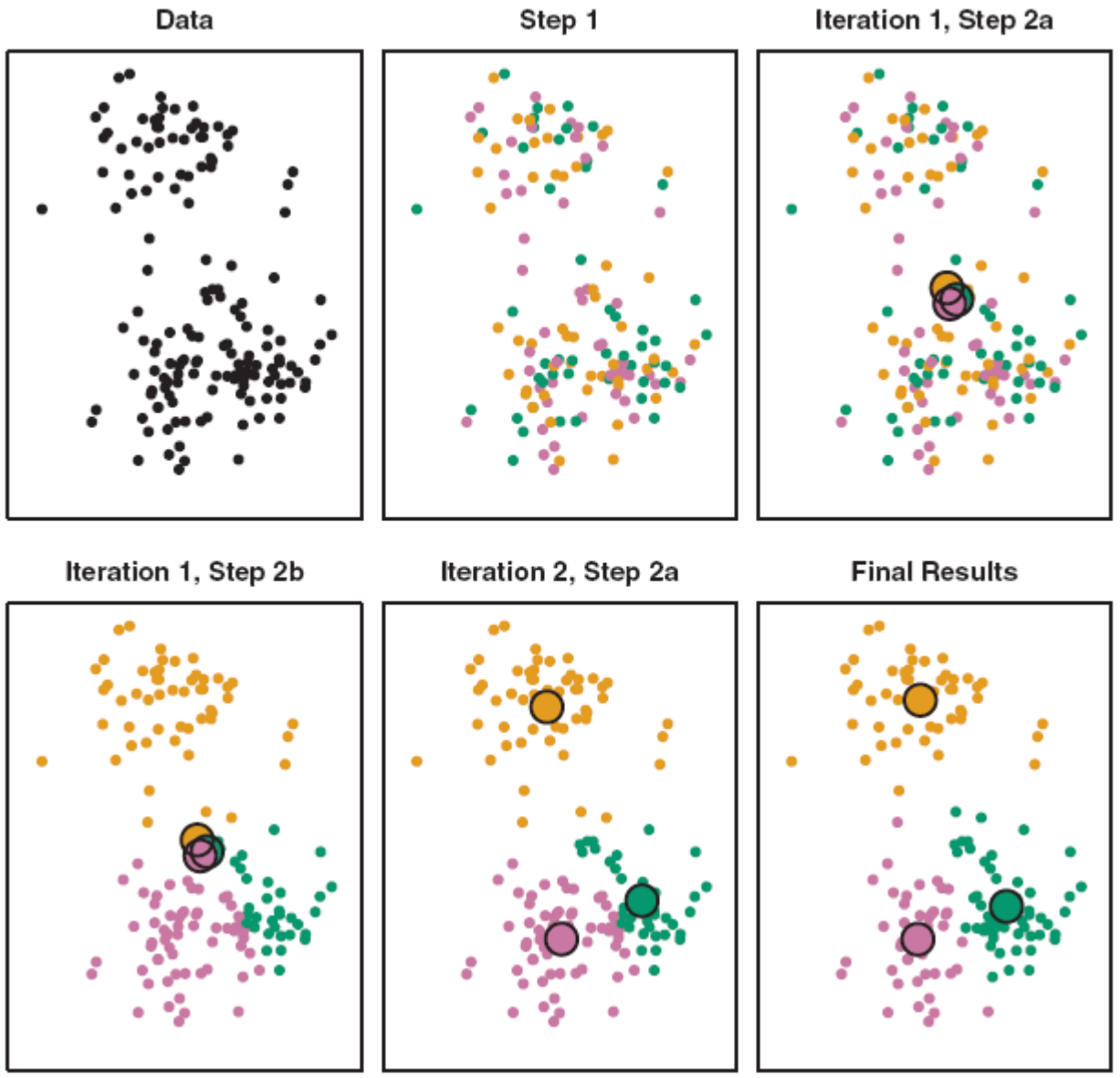
$$\underset{C_1,\ldots,C_K}{\text{minimize}} \left\{ \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 \right\}$$

This is equivalent to minimizing: $\frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = 2 \sum_{i \in C_k} \sum_{j=1}^{p} (x_{ij} - \bar{x}_{kj})^2$

Finding the exact optimal solution is computationally intractable (there are k^n possible partitions), but a simple algorithm exists to find a local optimum which is often works well in practice.

K-means clustering

1. Randomly assign points to clusters C_k
2. Calculate cluster centers as means of points in each cluster
3. Assign points to the closest cluster center
4. Recalculate cluster center as the mean of points in each cluster
5. Repeat steps 3 and 4 until convergence



K-means clustering

Because only a local minimum is found, different random initializations will lead to different solutions

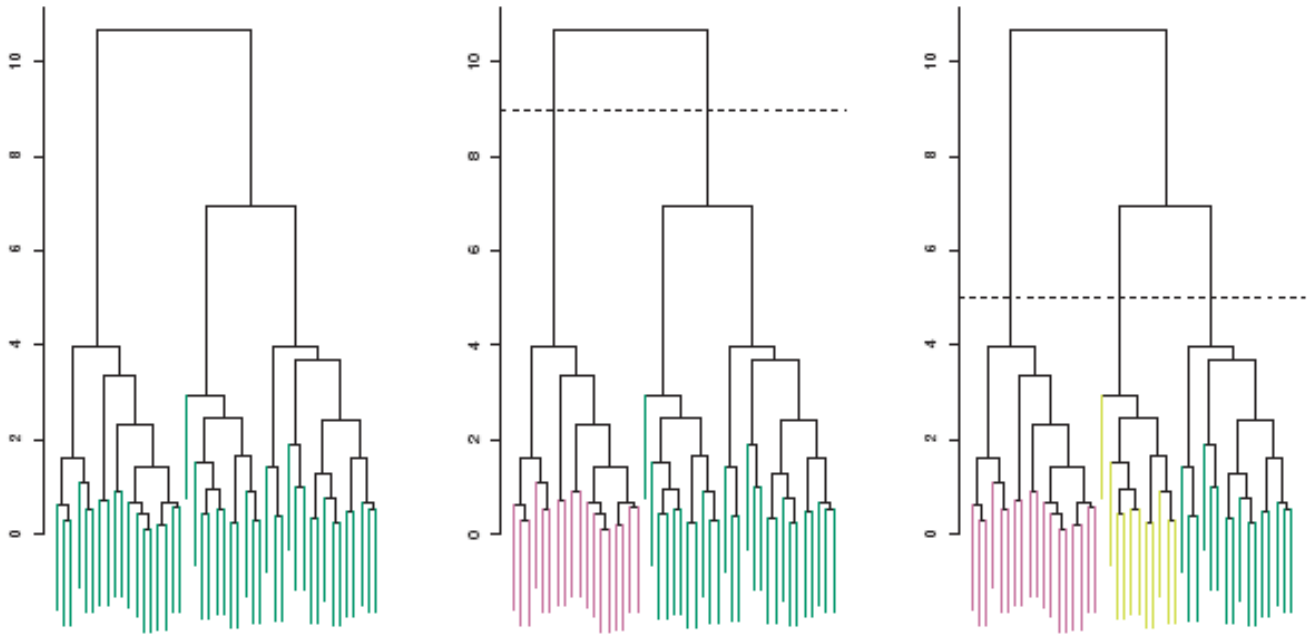
- One should run the algorithm multiple times to get better solutions

Hierarchical clustering

In **hierarchical clustering** we create a dendrogram which is a tree-based representation of successively larger clusters.

We can cut the dendrogram at any point to create as many clusters as desired

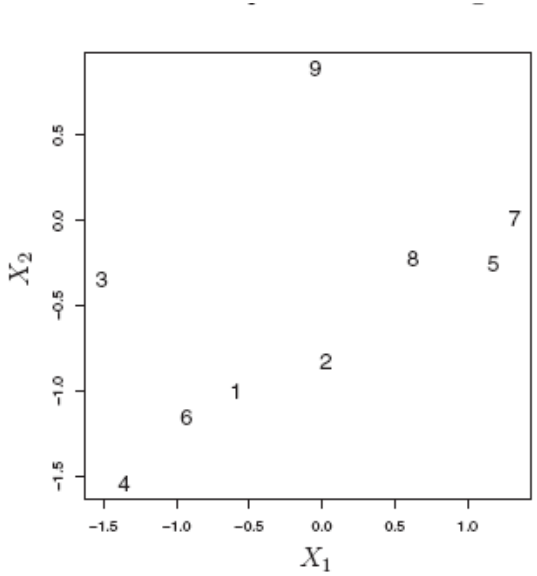
- i.e., don't need to specify the number of clusters, K, beforehand



Hierarchical clustering

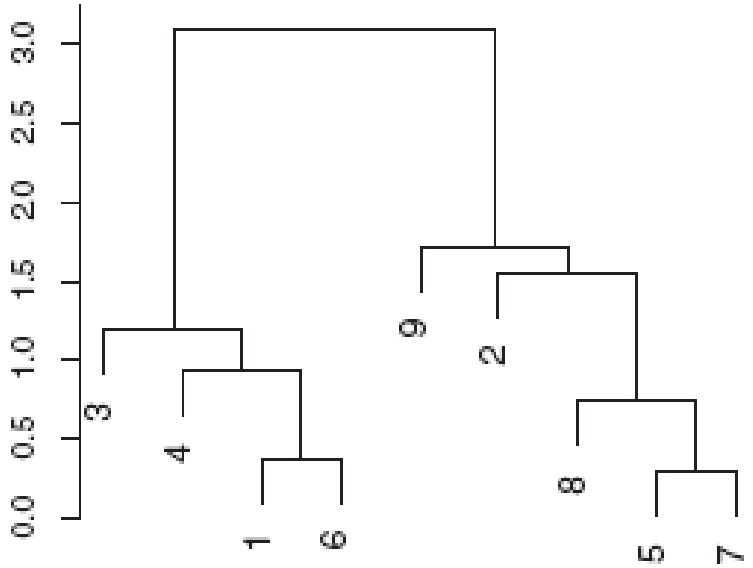
We can create a hierarchical clustering of the data using simple bottom-up agglomerative algorithm:

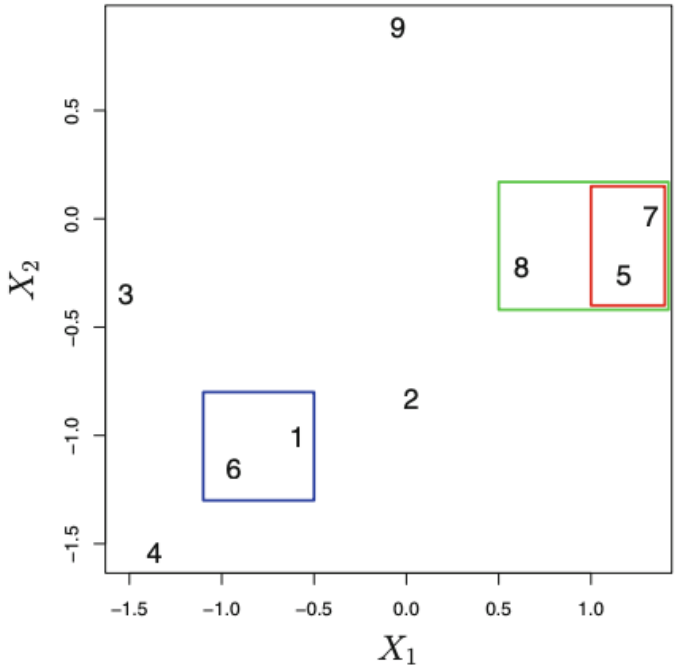
1. Choosing a (dis)similarity measure
   - E.g., The Euclidean distance
2. Initializing the clustering by treating each point as its own cluster
3. Successively merging the pair of clusters that are most similar
   - i.e., calculate the similarity between all pairs of clusters and merging the pair that is most similar
4. Stopping when all points have been merged into a single cluster



Hierarchical clustering

The vertical height that two clusters/points merge show how similar the two ***clusters*** are





Note: horizontal distance between ***individual points*** is not important:

- point 9 is considered as similar to point 2 as it is to point 7

Hierarchical clustering choices

We can define the similarity between two data points using the Euclidean distance or another measure, but how do we define similarity between groups of data points?

- A few choices for ‘linkage’ functions are:

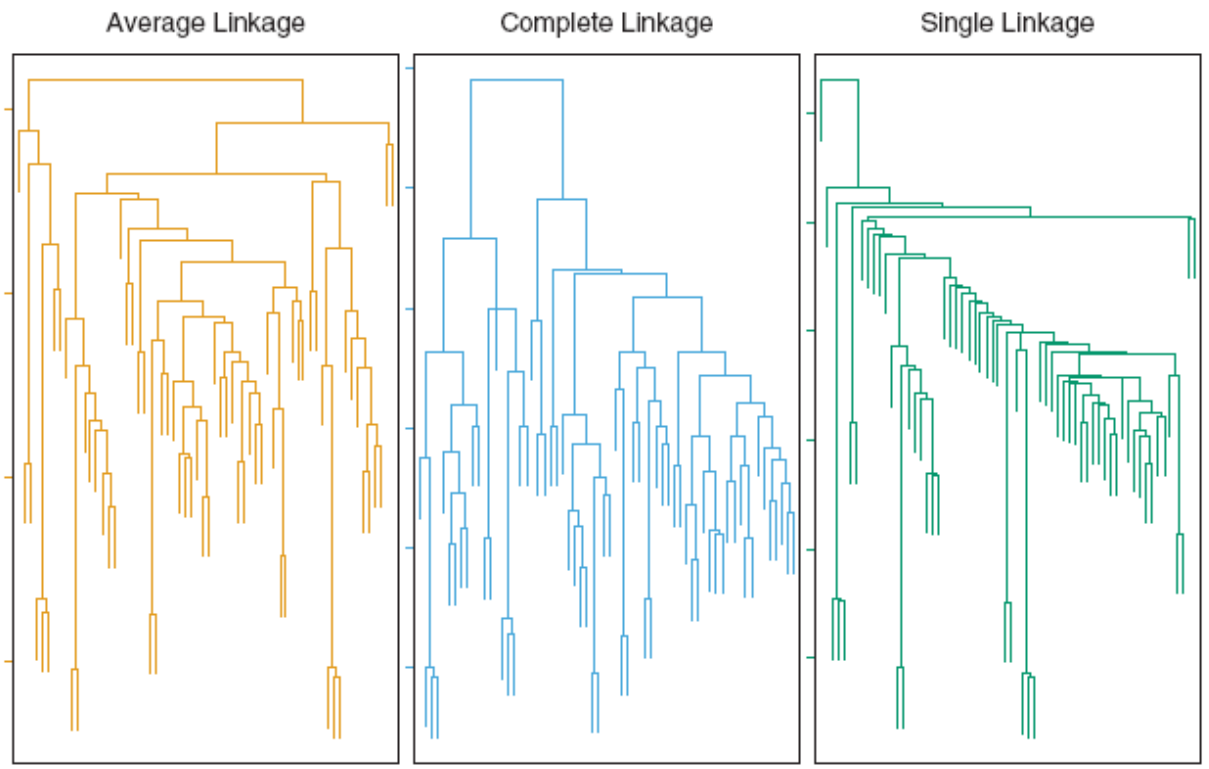
Complete	Compute the dissimilarity between all pairs of points in the two clusters. The cluster dissimilarity is defined as the ***maximum dissimilarity*** between all points.
Single	Compute the dissimilarity between all pairs of points in the two clusters. The cluster dissimilarity is defined as the ***minimum dissimilarity*** between all points.
Average	Compute the dissimilarity between all pairs of points in the two clusters. The cluster dissimilarity is defined as the ***average dissimilarity*** between all points.
Centroid	Compute the dissimilarity between centroids (i.e., the means) of the two clusters.

Hierarchical clustering choices

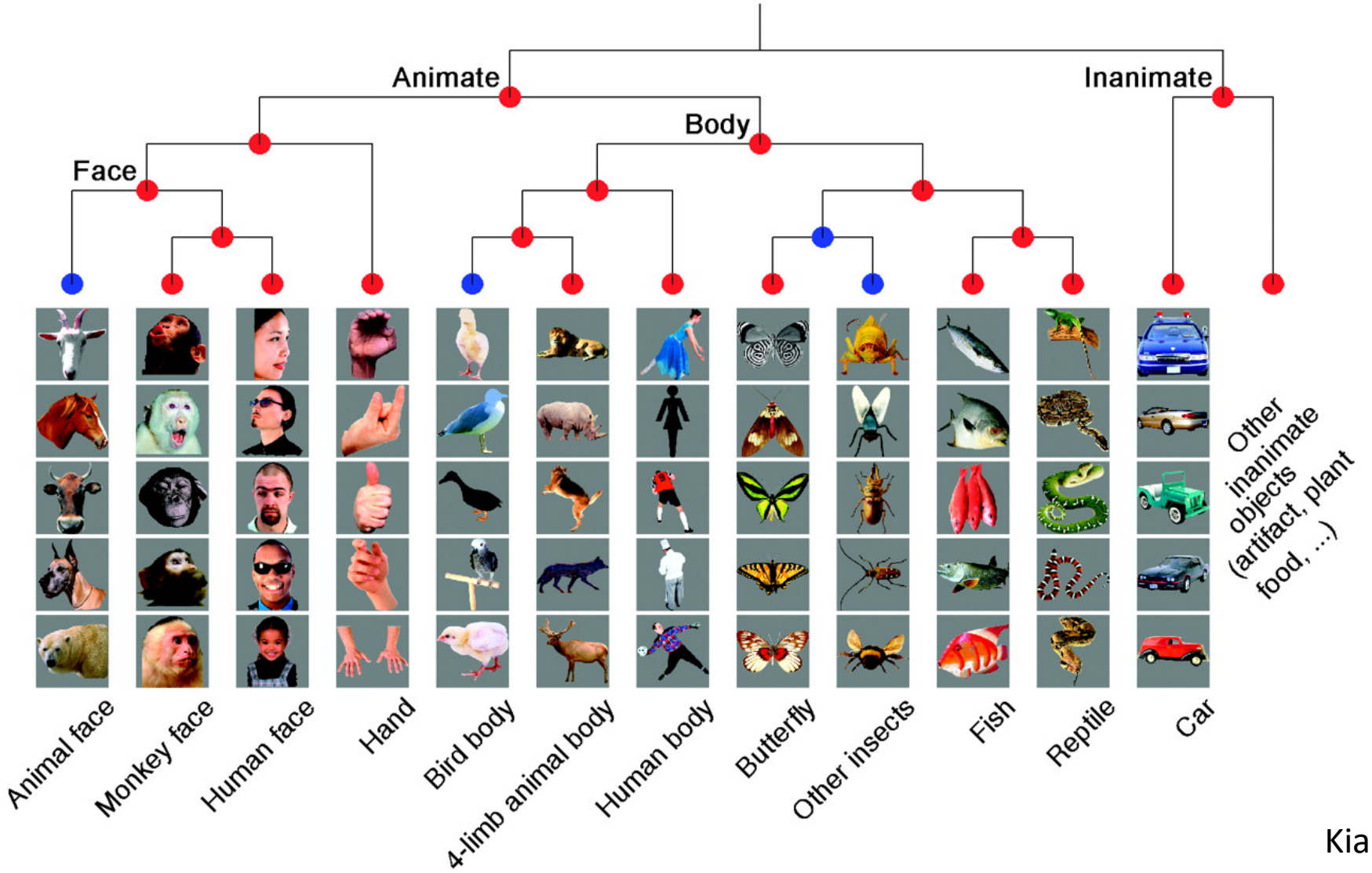
Generally average and complete linkage chosen over single linkage since they tend to yield more balanced trees

Centroid linkage can lead to inversions in which two clusters can be merged below the height of the individual clusters

- This makes it impossible to visualization the clustering as a tree



Hierarchical clustering example

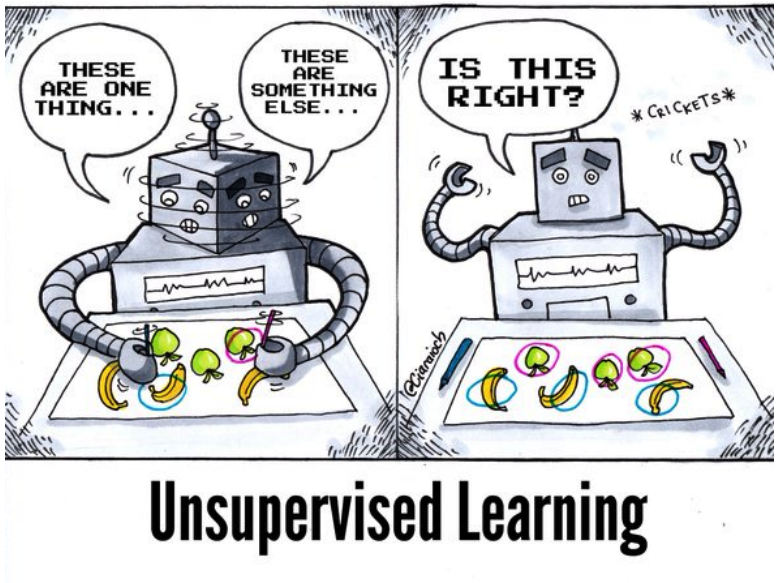


Kiani et al, 2007

Issues with clustering

Choices made can effect the results:

- Feature normalization and/or dissimilarity measure
- K-means: choice of K
- For hierarchical cluster: linkage and cut height



Potential approaches to deal with these issues:

- Try a few methods and see if one gives interesting/useful results
- Validate that you get similar results on a second set of data

Let’s try clustering in R…