

PSY9511: Seminar 6

Unsupervised learning

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03.11.25



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Outline

1. Overview of unsupervised learning
2. Clustering
 - K-means
 - Hierarchical
3. Dimensionality reduction
 - Principal component analysis (PCA)
 - Independent component analysis (ICA)
 - Partial least squares (PLS)



Unsupervised learning



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Unsupervised learning: Motivation

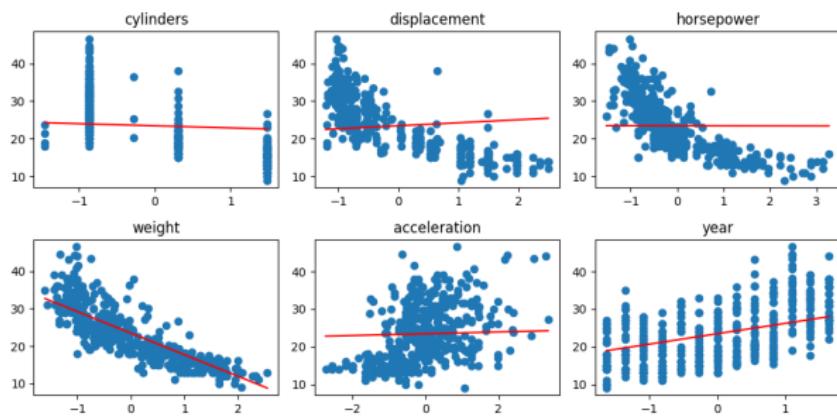
Supervised learning: Find $\hat{y} = \hat{f}(X)$



Unsupervised learning: Motivation

Supervised learning: Find $\hat{y} = \hat{f}(X)$

- Descriptive: Understand the relationship between X and y



Unsupervised learning: Motivation

Supervised learning: Find $\hat{y} = \hat{f}(X)$

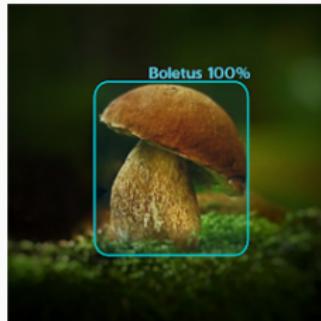
- Descriptive: Understand the relationship between X and y
- Predictive: Predict y given new X .



Unsupervised learning: Motivation

Supervised learning: Find $\hat{y} = \hat{f}(X)$

- Descriptive: Understand the relationship between X and y
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 - Because the predictions are useful



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- Predictive: Predict y given new X .
 - Because the predictions are useful
 - Because we want to know if it is possible



→ [Depression?]

A large gray arrow points from the brain image towards a dashed rectangular box containing the text "Depression?".

Unsupervised learning: Motivation

Supervised learning: Find $\hat{y} = \hat{f}(X)$

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Unsupervised learning: Are there interesting patterns in X ?



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Unsupervised learning: Are there interesting patterns in X ?

- Can we find subgroups or interesting axes of variability?



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Unsupervised learning: Are there interesting patterns in X ?

- Can we find subgroups or interesting axes of variability?
- Exploratory analyses
- Visualization



Clustering



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Clustering: Background

Are there some (naturally occurring) subgroups in our dataset?



Clustering: Background

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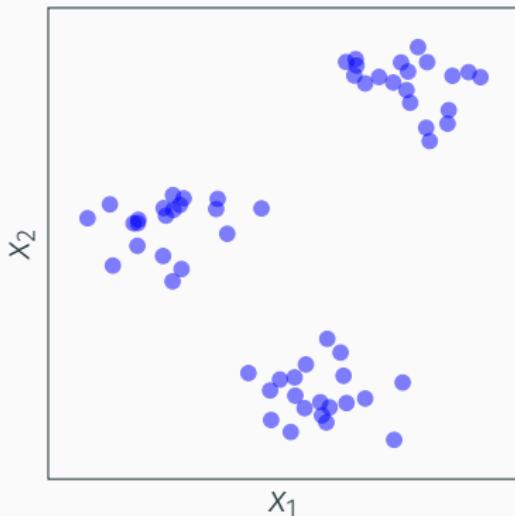
x_1	x_2
0.20	-0.26
0.15	-0.33
0.03	0.07
-0.07	-0.01
-0.06	0.00
0.28	-0.24
0.21	-0.35
0.20	-0.32
0.30	0.25
0.00	-0.12



Clustering: Background

Are there some (naturally occurring) subgroups in our dataset?

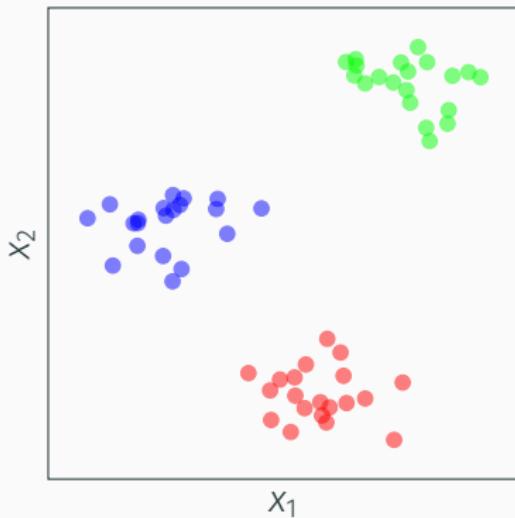
x_1	x_2
0.20	-0.26
0.15	-0.33
0.03	0.07
-0.07	-0.01
-0.06	0.00
0.28	-0.24
0.21	-0.35
0.20	-0.32
0.30	0.25
0.00	-0.12



Clustering: Background

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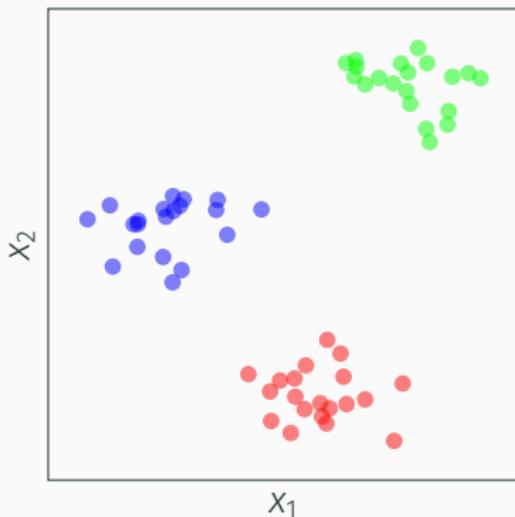
x_1	x_2
0.20	-0.26
0.15	-0.33
0.03	0.07
-0.07	-0.01
-0.06	0.00
0.28	-0.24
0.21	-0.35
0.20	-0.32
0.30	0.25
0.00	-0.12



Clustering: Background

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x_1	x_2
0.20	-0.26
0.15	-0.33
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0.28	-0.24
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0.20	-0.32
0.30	0.25
0.00	-0.12



K-means clustering: Definition

K-means clustering: Find k clusters in the data to minimize the *within-cluster variance*:

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



K-means clustering: Definition

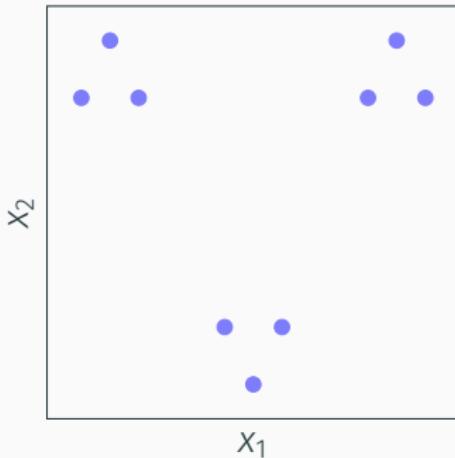
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K-means clustering: Definition

x_1	x_2
1	1
1.5	1
1.25	1.25
-1	1
-1.5	1
-1.25	1.25
0.25	0
-0.25	0
0	-0.25

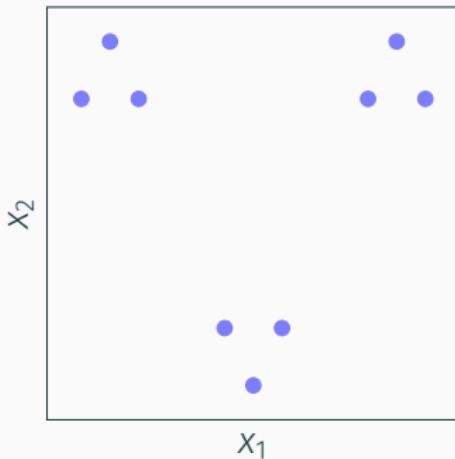


$$\underset{C_1, \dots, C_k}{\text{minimize}} \left(\sum_{k=1}^K \frac{1}{|C_k|} \sum_{i, i' \in C_k} \sqrt{\sum_{j=1}^p (x_{ij} - x_{i'j})^2} \right)$$



K-means clustering: Definition

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-1	1
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-1.25	1.25
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-0.25	0
0	-0.25



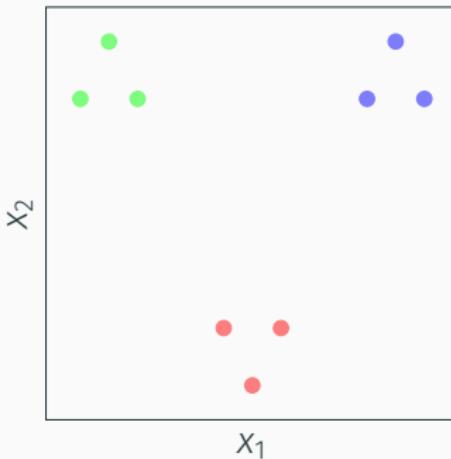
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1	1
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0	-0.25

C_1
 C_1
 C_1
 C_2
 C_2
 C_2
 C_3
 C_3
 C_3



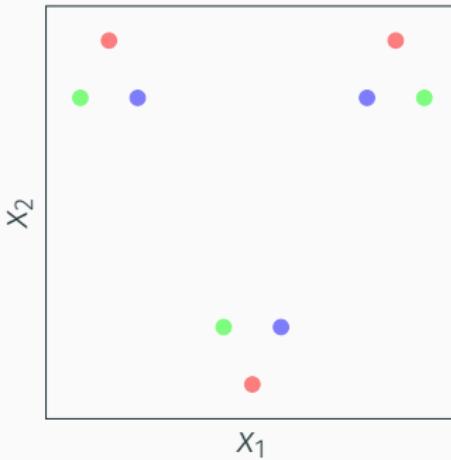
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C_1
 C_2
 C_3



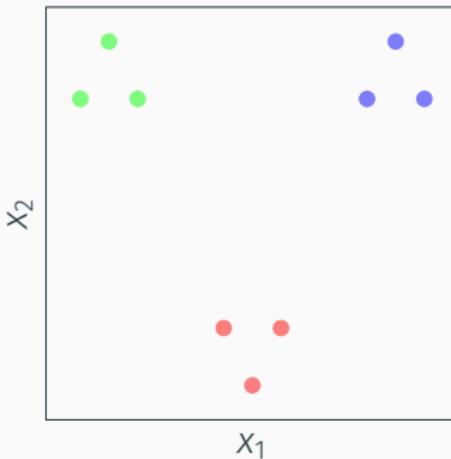
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C_1
 C_1
 C_1
 C_2
 C_2
 C_2
 C_3
 C_3
 C_3



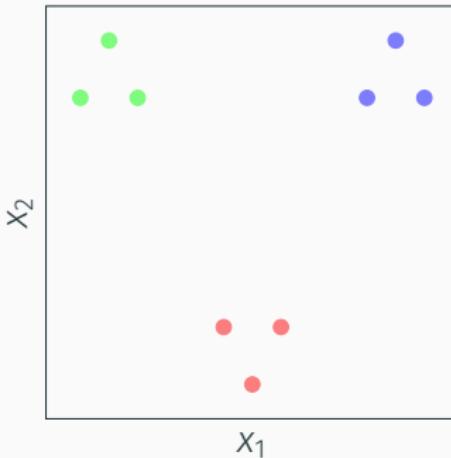
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C_1
 C_1
 C_1
 C_2
 C_2
 C_2
 C_3
 C_3
 C_3



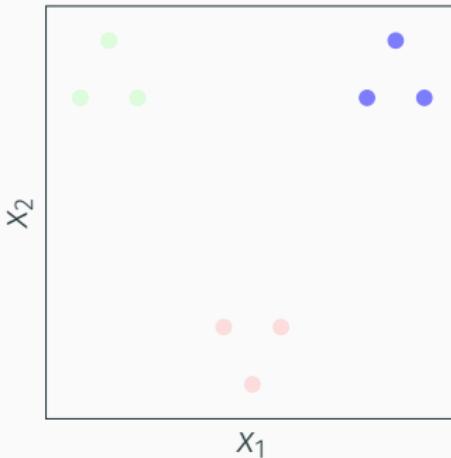
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C_1
 C_1
 C_1
 C_2
 C_2
 C_2
 C_3
 C_3
 C_3



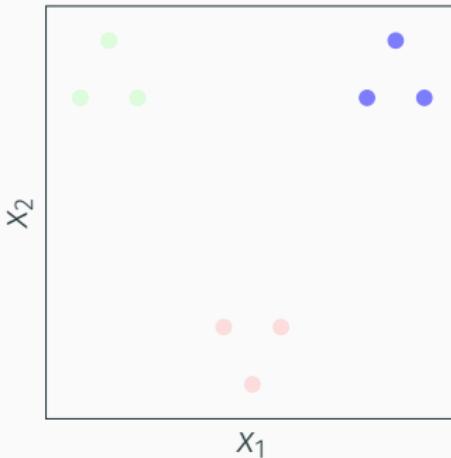
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C_1
 C_1
 C_1
 C_2
 C_2
 C_2
 C_3
 C_3
 C_3



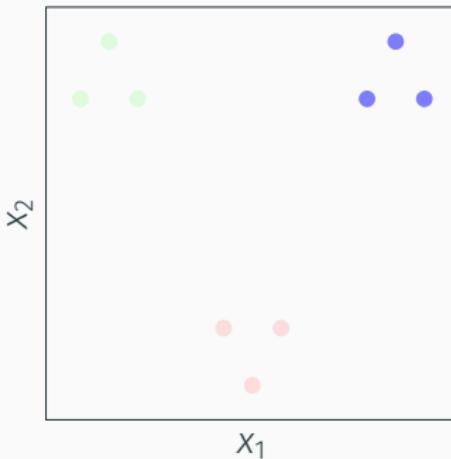
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C_1
 C_1
 C_1
 C_2
 C_2
 C_2
 C_3
 C_3
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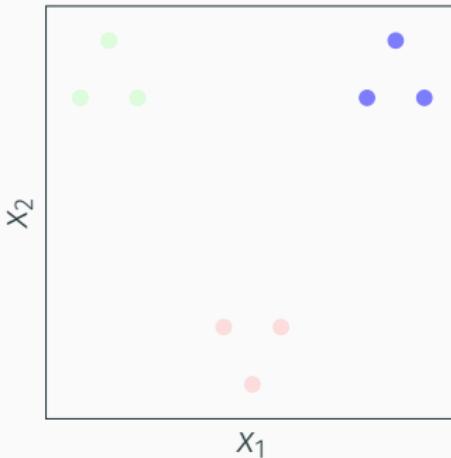


K-means clustering: Definition

↑
 i, i'
↓

	x_1	x_2
i	1	1
i'	1.5	1
	1.25	1.25
	-1	1
	-1.5	1
	-1.25	1.25
	0.25	0
	-0.25	0
	0	-0.25

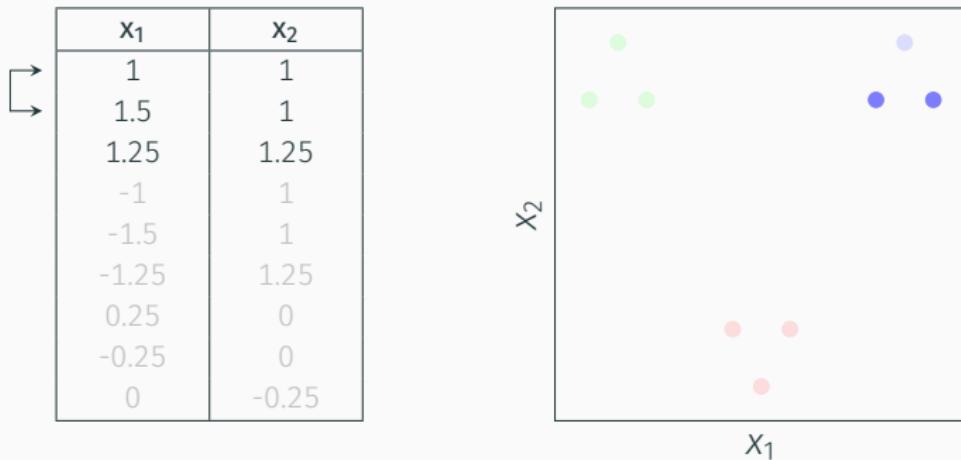
C_1
 C_1
 C_1
 C_2
 C_2
 C_2
 C_3
 C_3
 C_3



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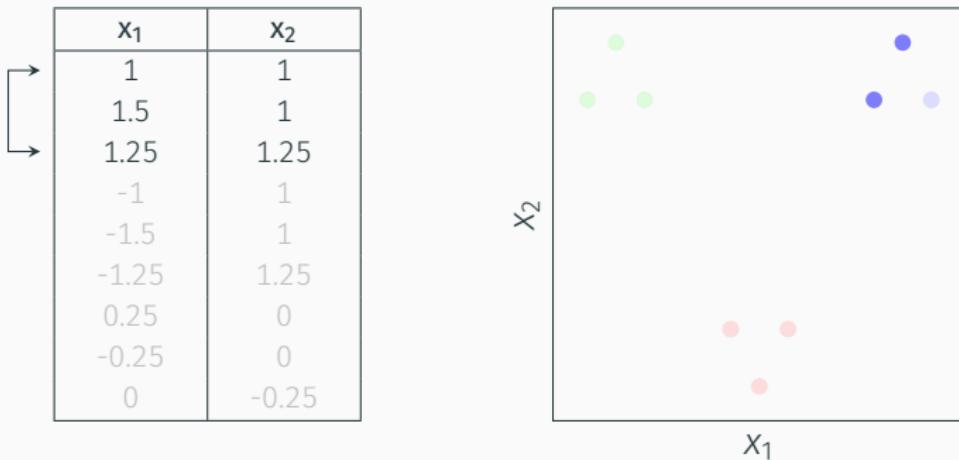
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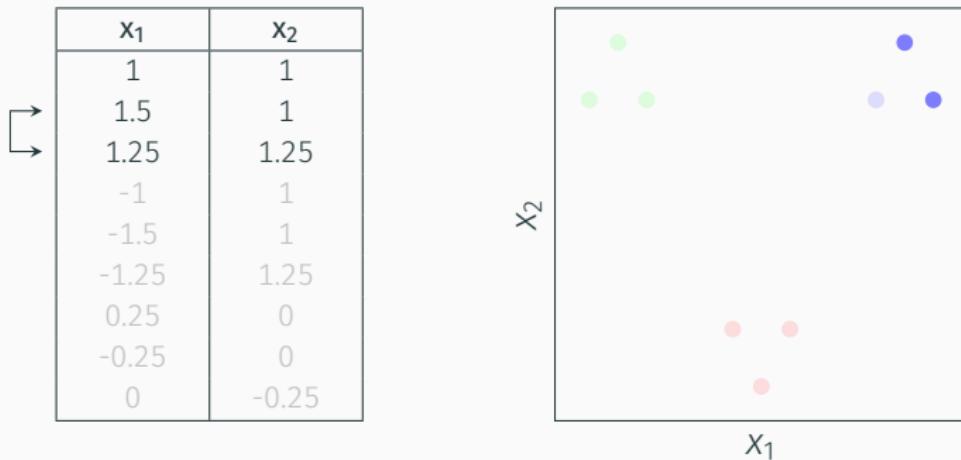
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K-means clustering: Definition

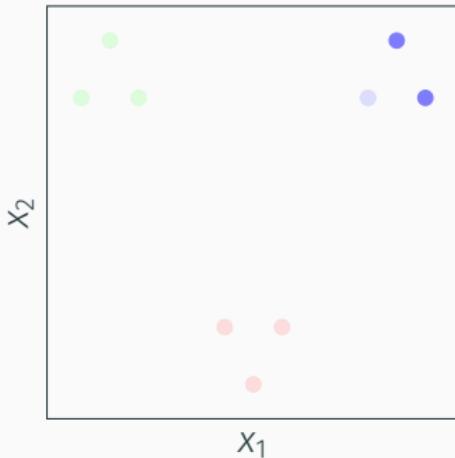


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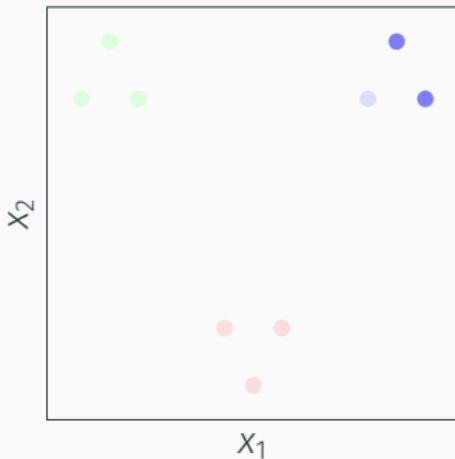


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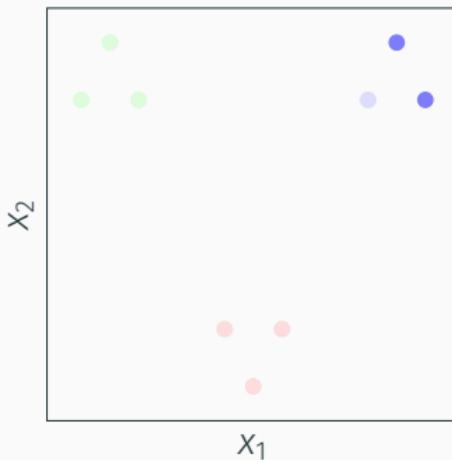
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K-means clustering: Definition

↔ j →

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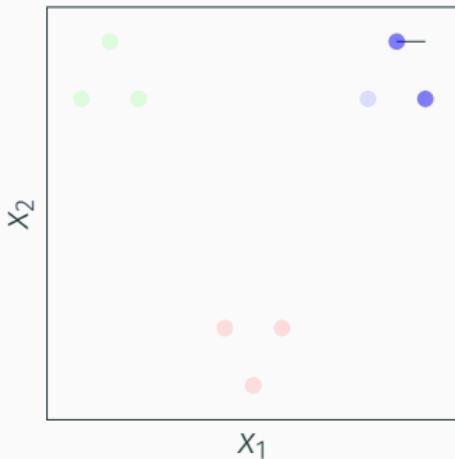


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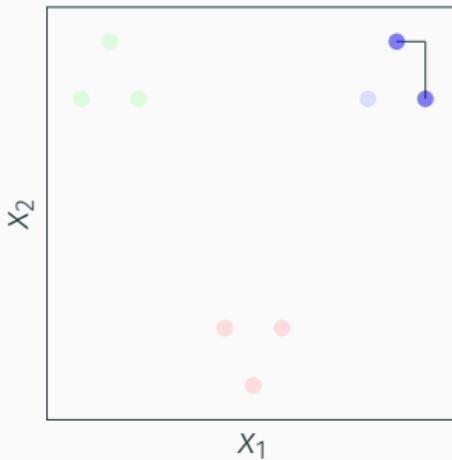


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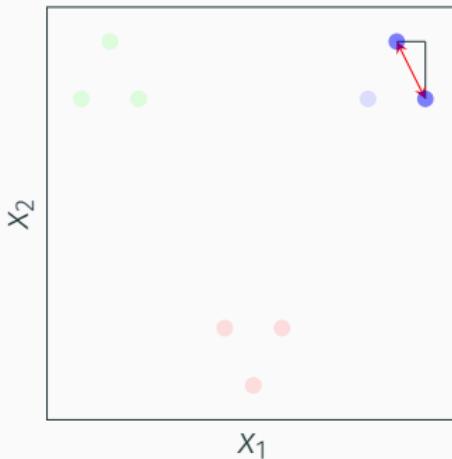


$$\underset{C_1, \dots, C_k}{\text{minimize}} \left(\sum_{k=1}^K \frac{1}{|C_k|} \sum_{i, i' \in C_k} \sqrt{\sum_{j=1}^p (x_{ij} - x_{i'j})^2} \right)$$



K-means clustering: Definition

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1.5	1
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K-means clustering: Definition

We want to find an assignment of clusters that for each cluster, for each pair of points within the cluster, minimizes the distance between them

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



K-means clustering: Definition

x_1	x_2
1	1
1.5	1
1.25	1.25
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-1.5	1
-1.25	1.25
0.25	0
-0.25	0
0	-0.25

C_1

C_1

C_1

C_2

C_2

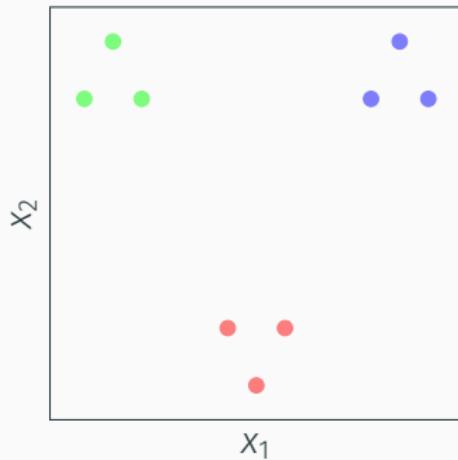
C_2

C_3

C_3

C_3

C_3



K-means clustering: Definition

x_1	x_2
1	1
1.5	1
1.25	1.25
-1	1
-1.5	1
-1.25	1.25
0.25	0
-0.25	0
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C_1

C_2

C_3

C_1

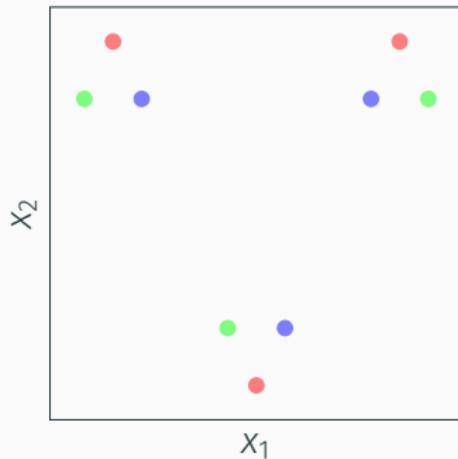
C_2

C_3

C_1

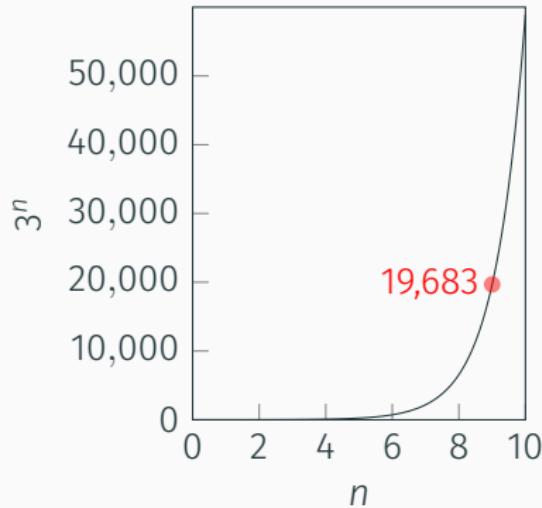
C_2

C_3



K-means clustering: Definition

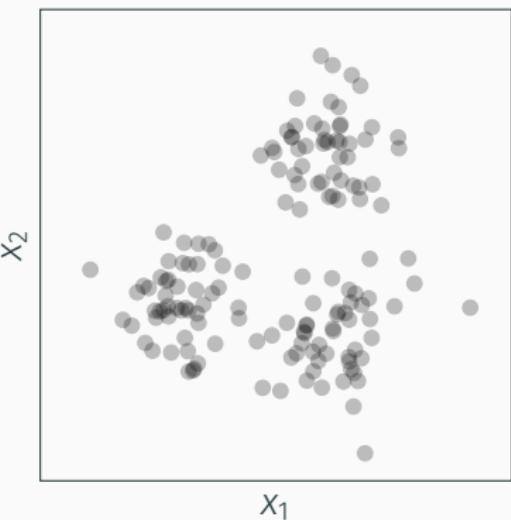
x_1	x_2
1	1
1.5	1
1.25	1.25
-1	1
-1.5	1
-1.25	1.25
0.25	0
-0.25	0
0	-0.25



Number of possible assignments: K^n

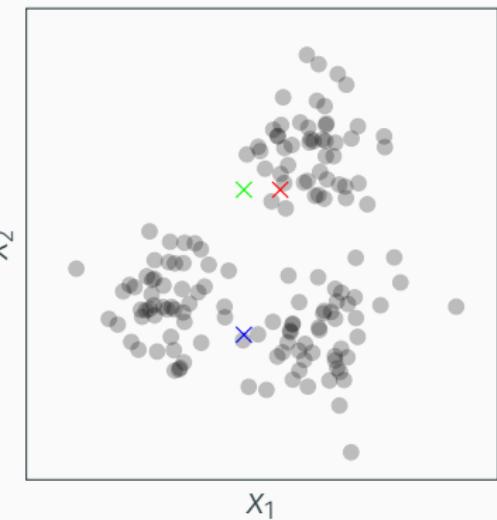


K-means clustering: Algorithm



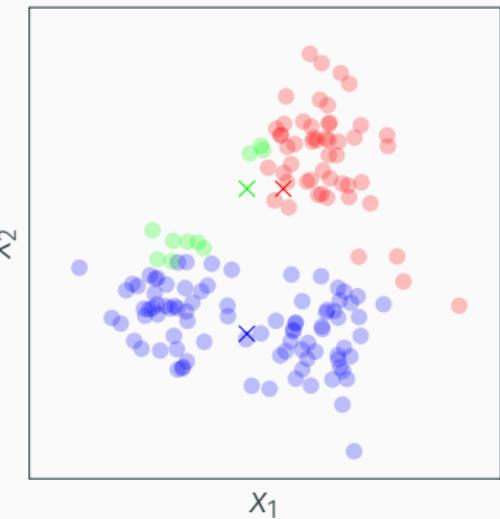
K-means clustering: Algorithm

1. Initialize k random centroids



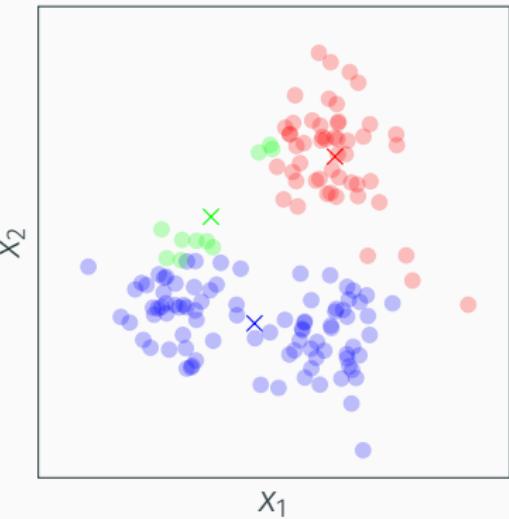
K-means clustering: Algorithm

1. Initialize k random centroids
2. Iteratively:
 - 2.1 Assign each point to the nearest centroid



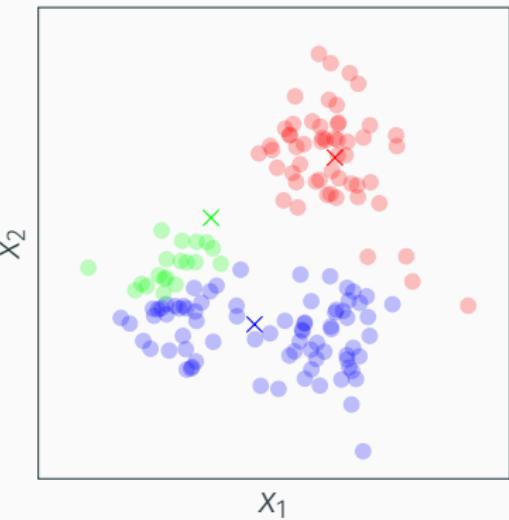
K-means clustering: Algorithm

1. Initialize k random centroids
2. Iteratively:
 - 2.1 Assign each point to the nearest centroid
 - 2.2 Update the centroids



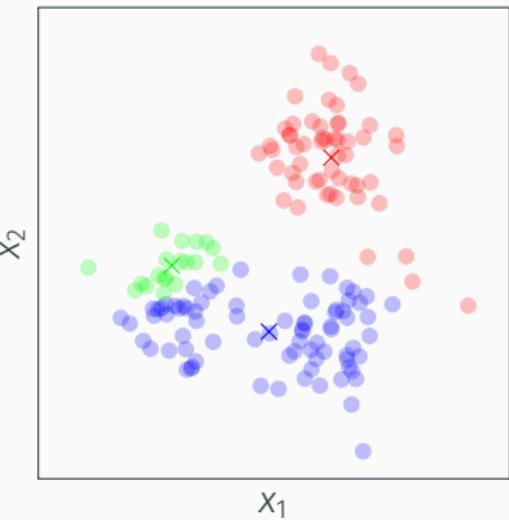
K-means clustering: Algorithm

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2. Iteratively:
 - 2.1 Assign each point to the nearest centroid
 - 2.2 Update the centroids



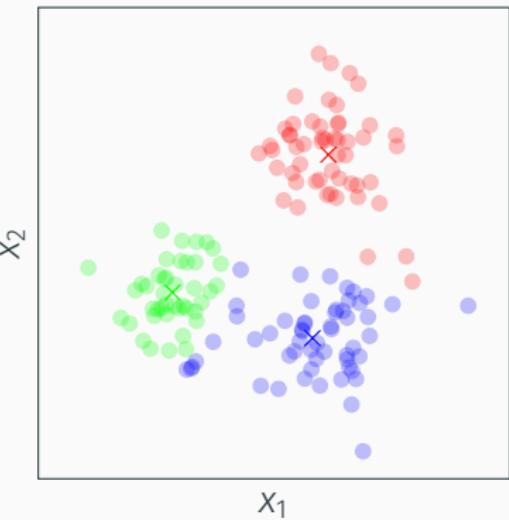
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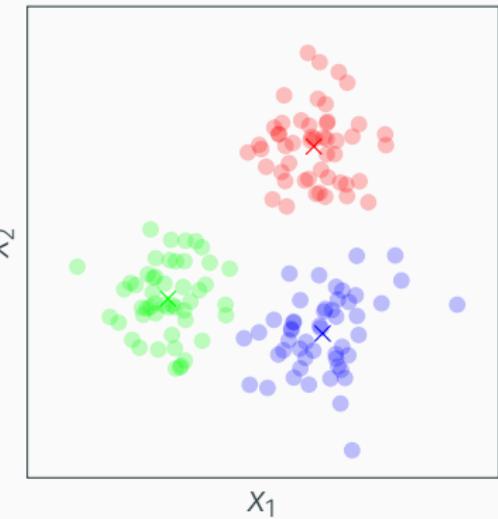
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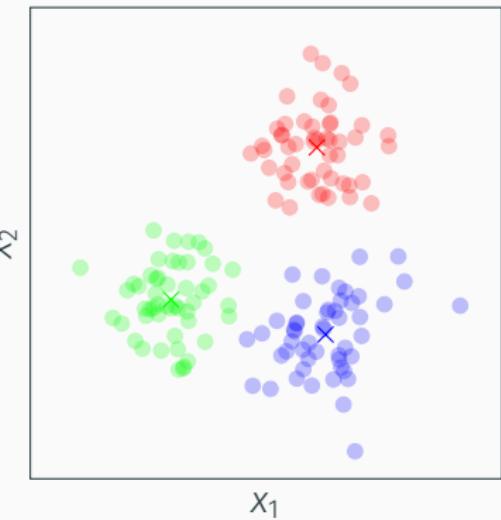
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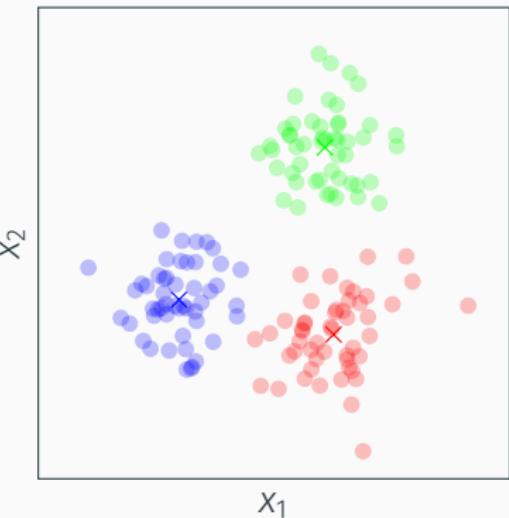
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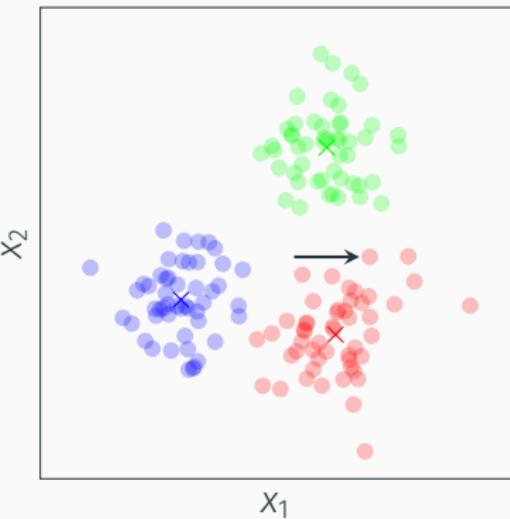
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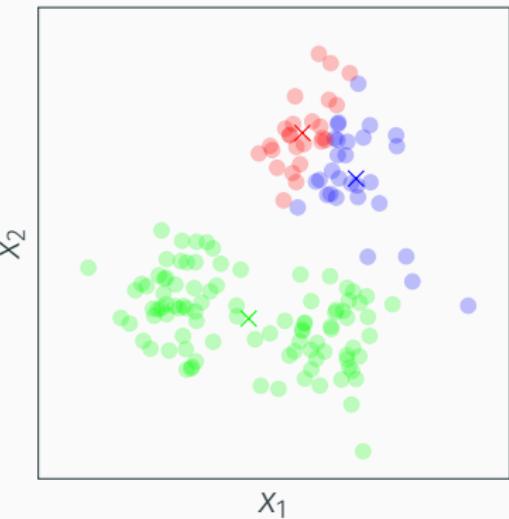
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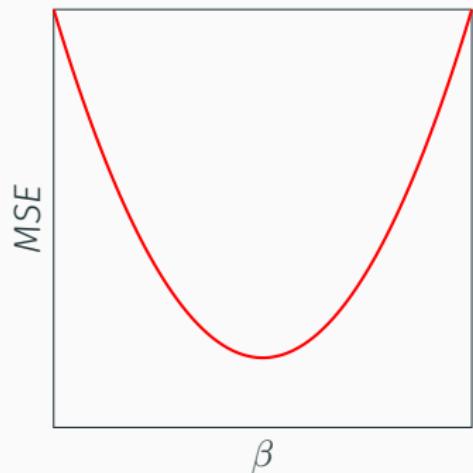


K-means clustering: Algorithm

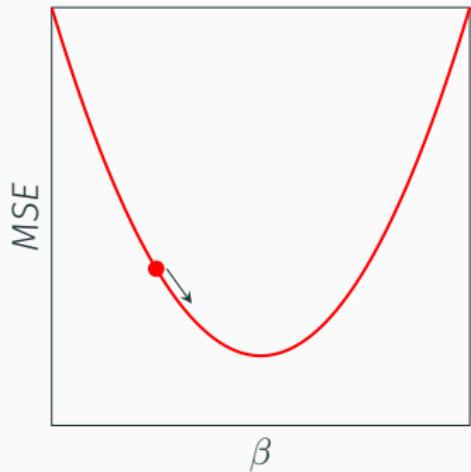
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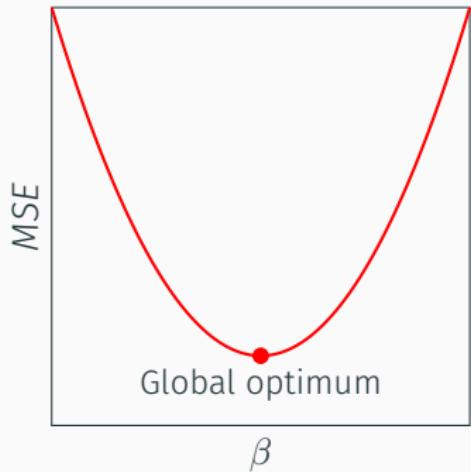
K-means clustering: Algorithm



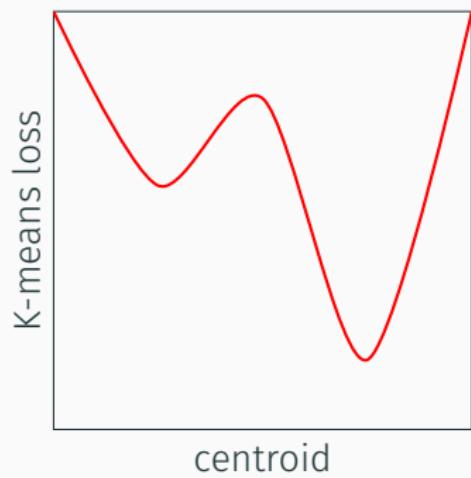
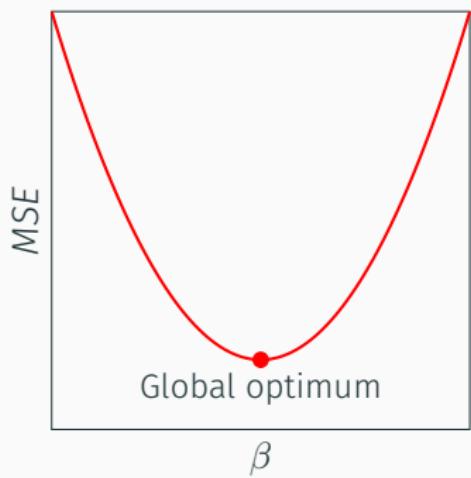
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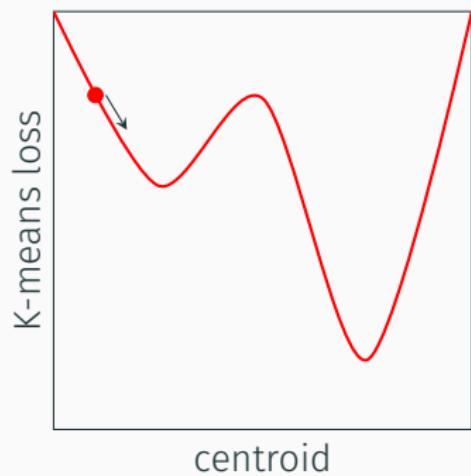
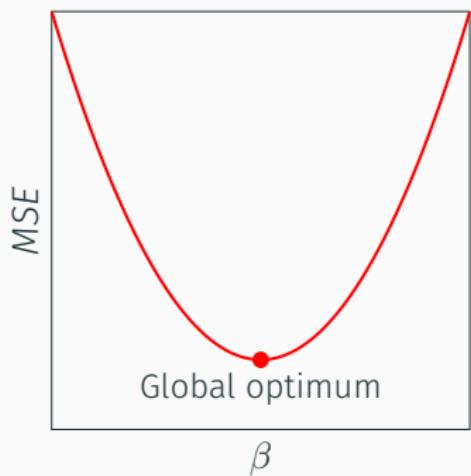
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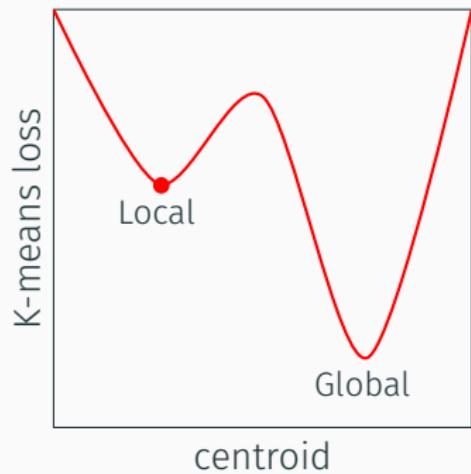
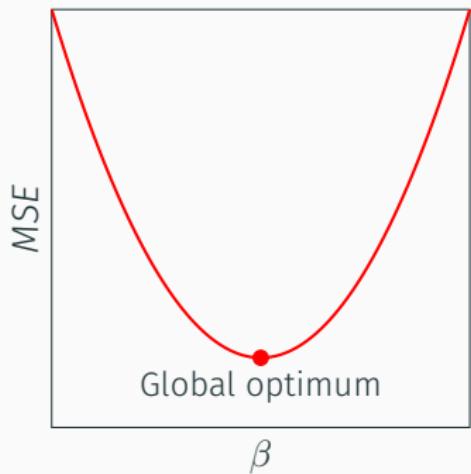
K-means clustering: Algorithm



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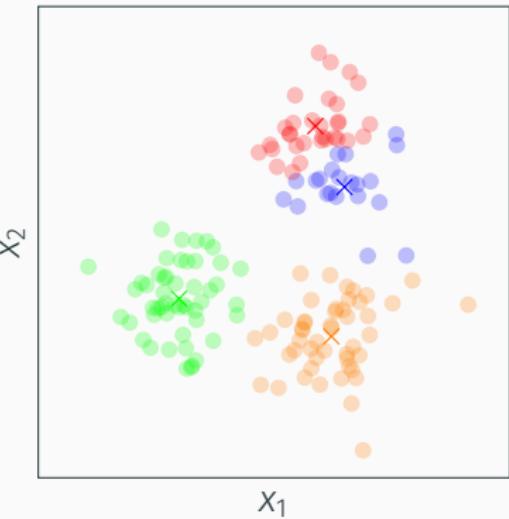


K-means clustering: Algorithm



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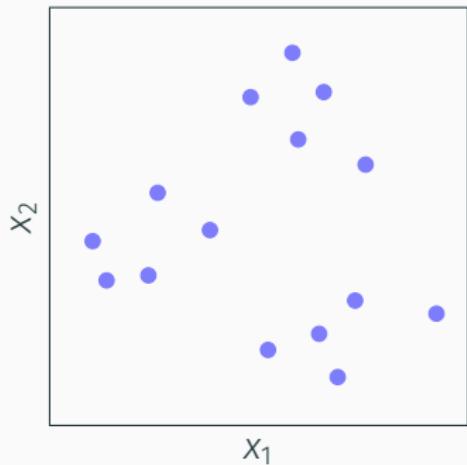
K-means clustering: Summary

K-means clustering: Finds clusters by minimizing the within-cluster variance

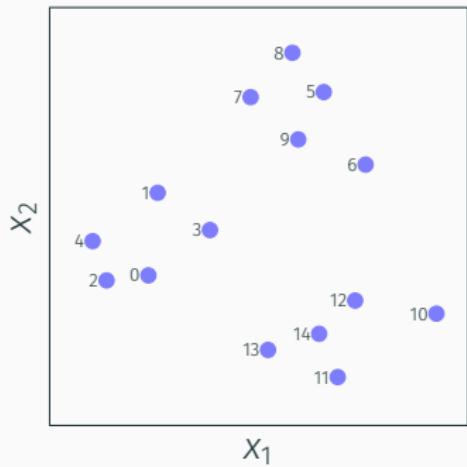
- + Intuitive way of finding clusters
- + Fast algorithm
- Dependent on knowing the number of clusters to use
- Dependent on the random initialization of centroids



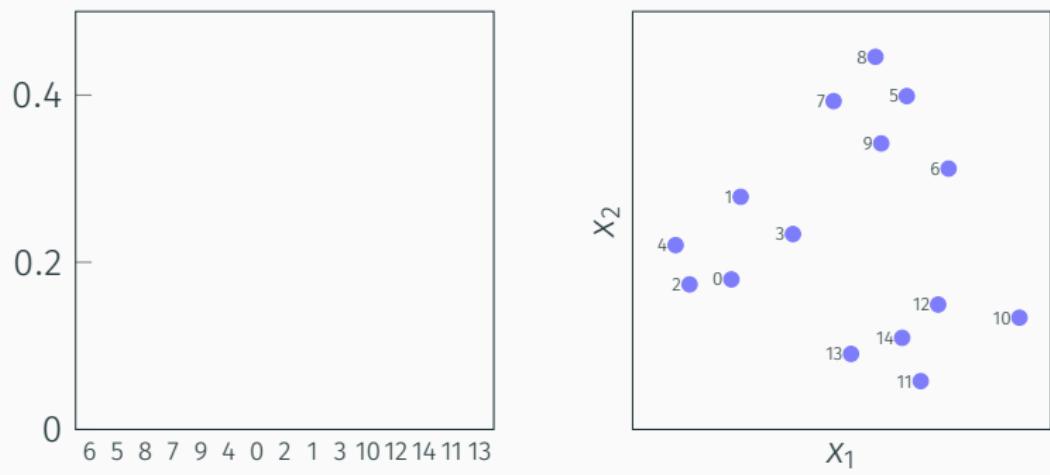
Hierarchical clustering: Algorithm



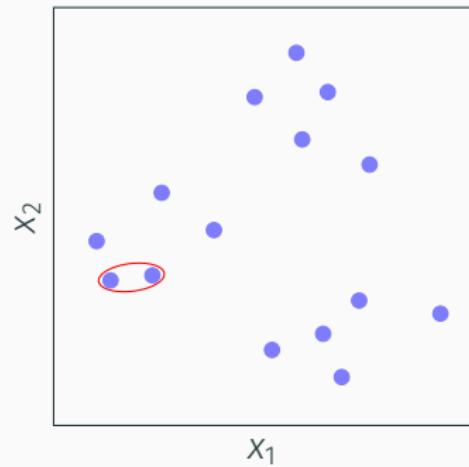
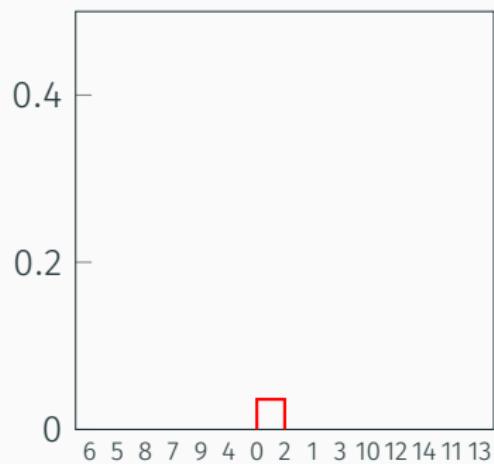
Hierarchical clustering: Algorithm



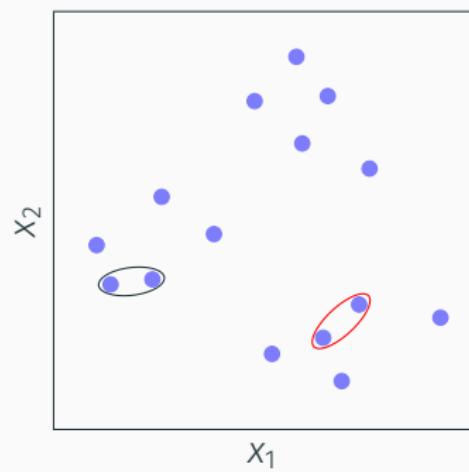
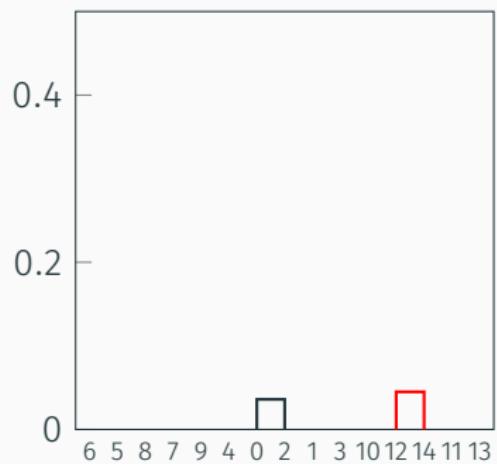
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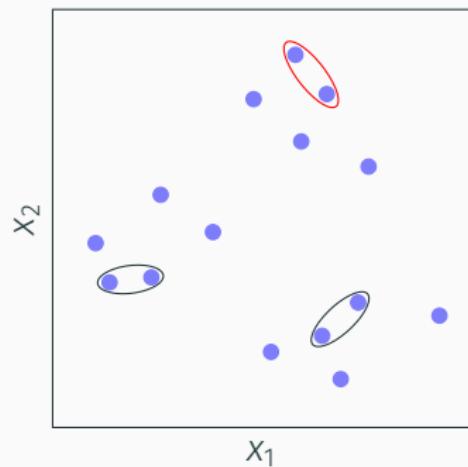
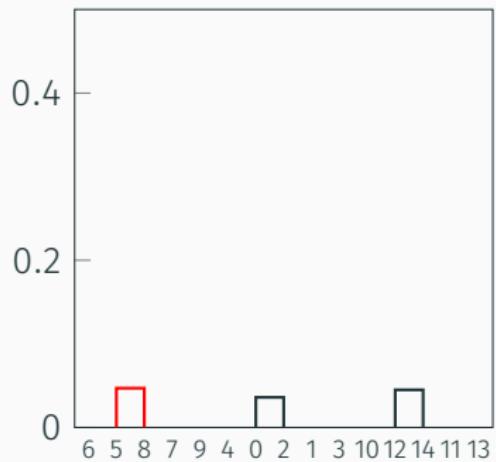
Hierarchical clustering: Algorithm



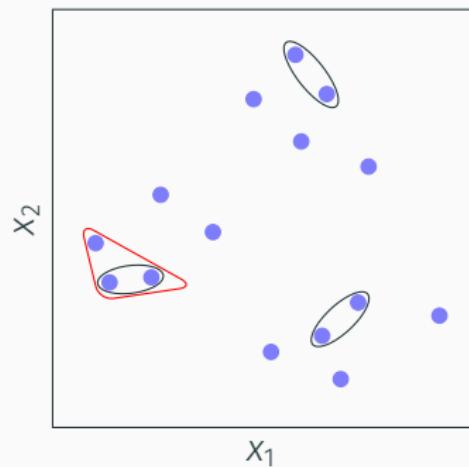
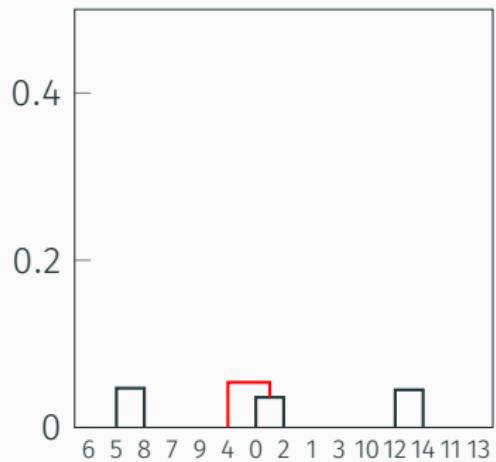
Hierarchical clustering: Algorithm



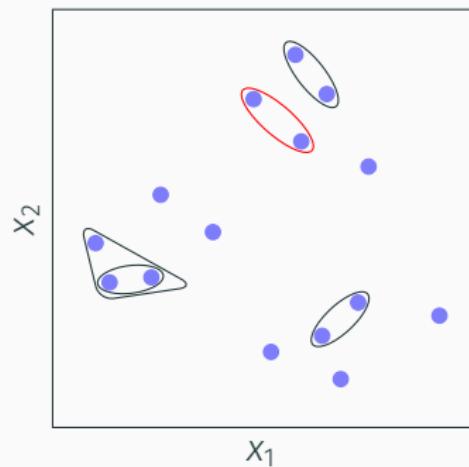
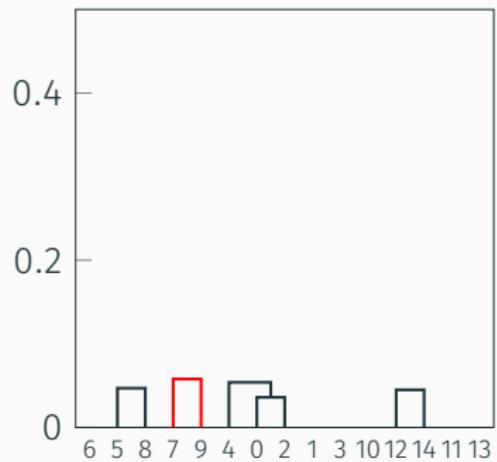
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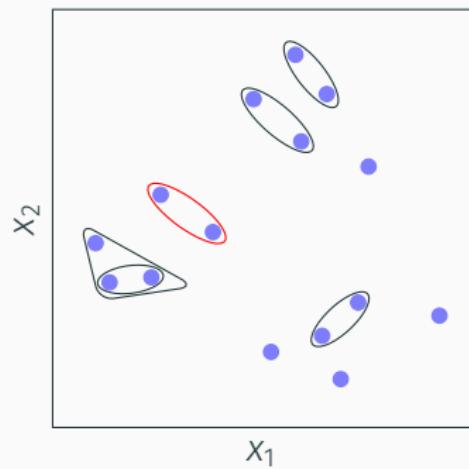
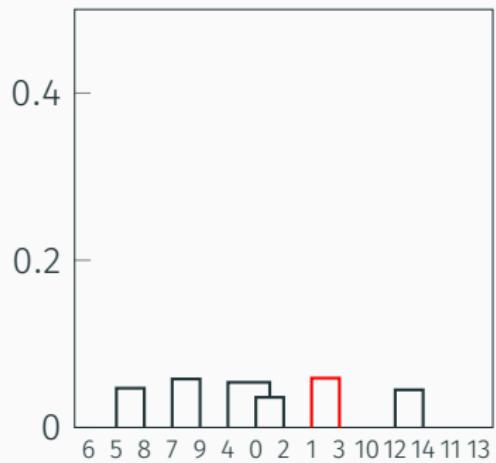
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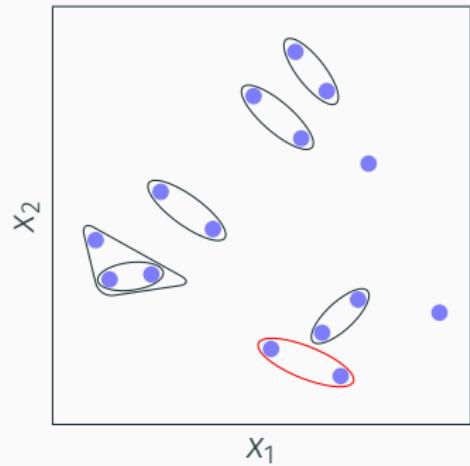
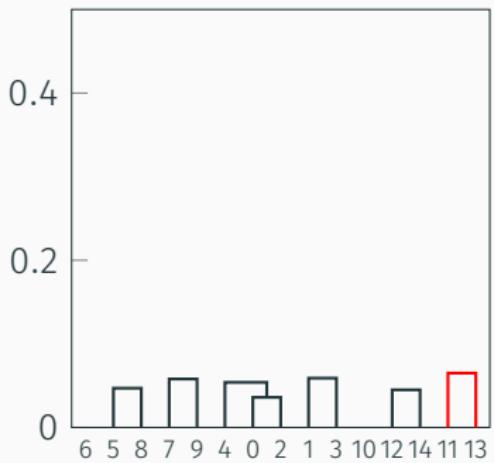
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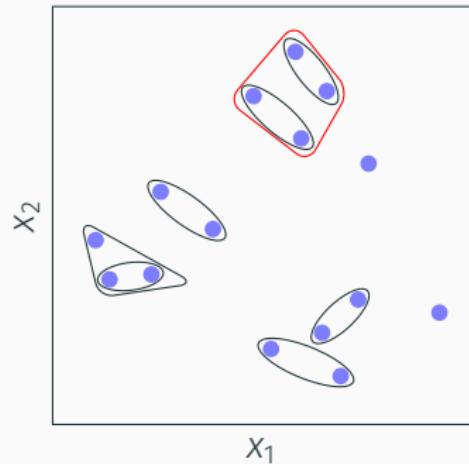
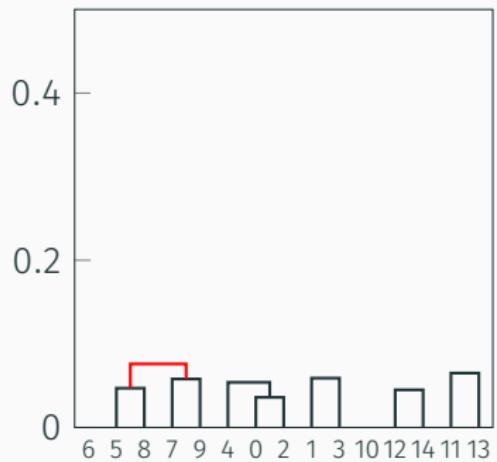
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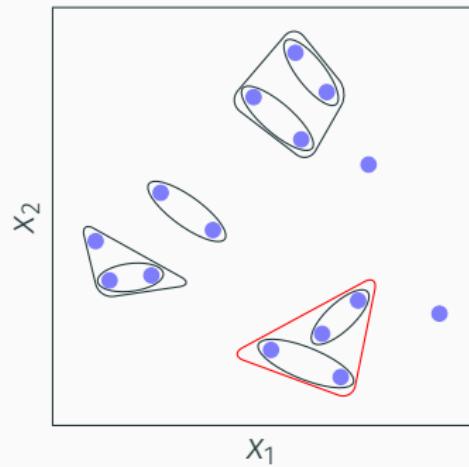
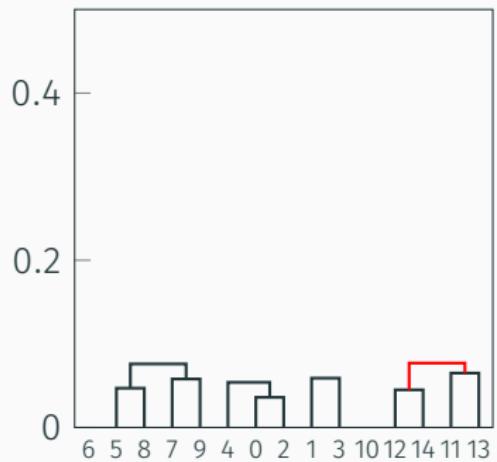
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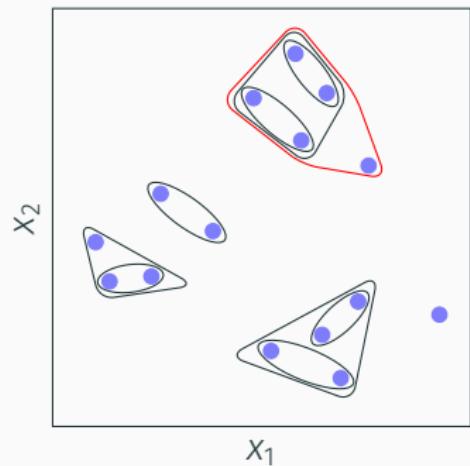
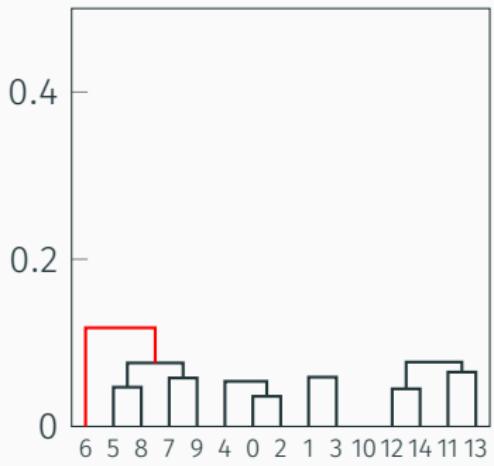
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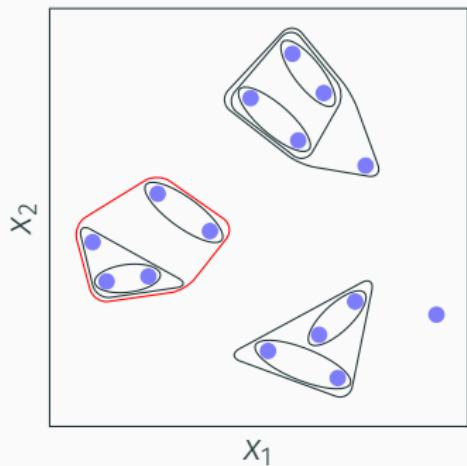
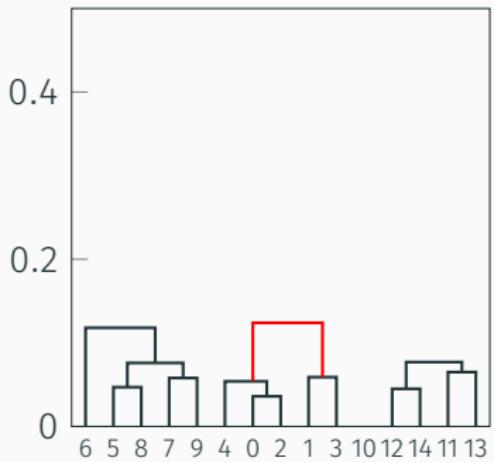
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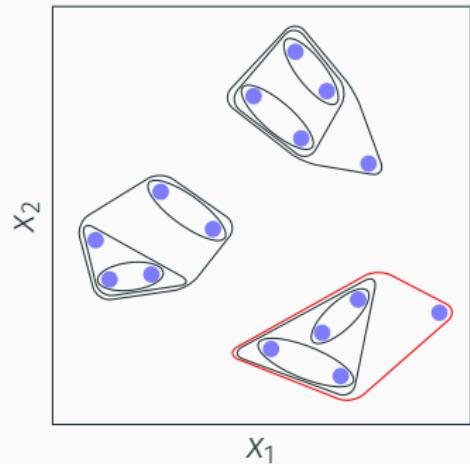
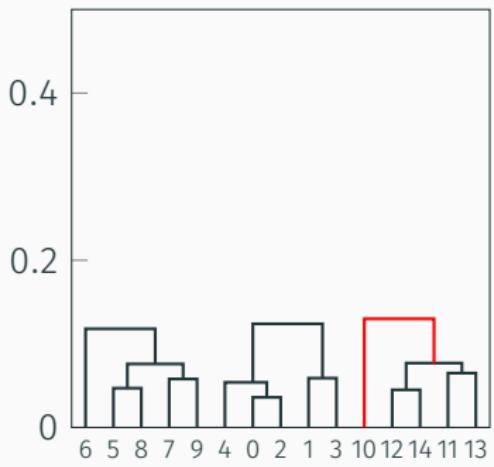
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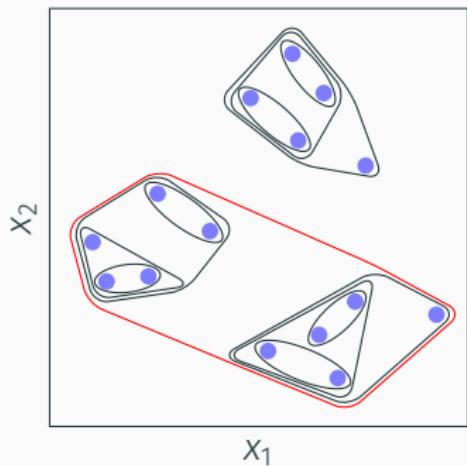
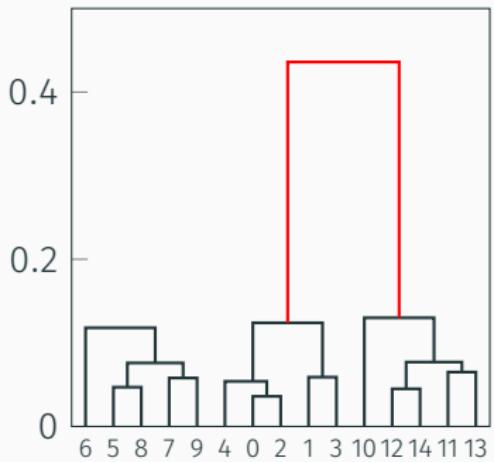
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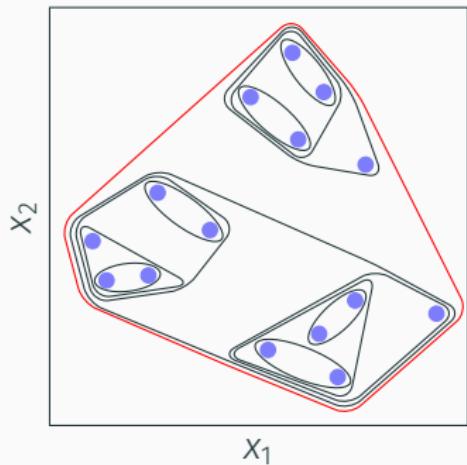
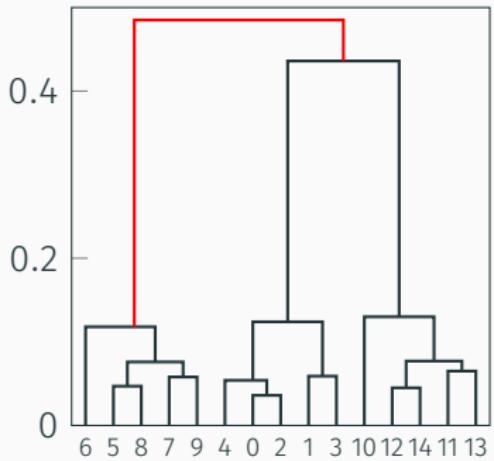
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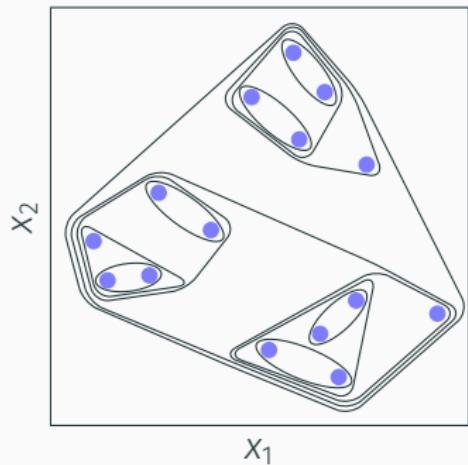
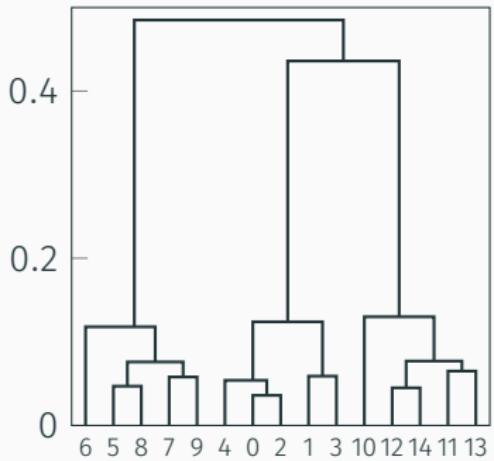
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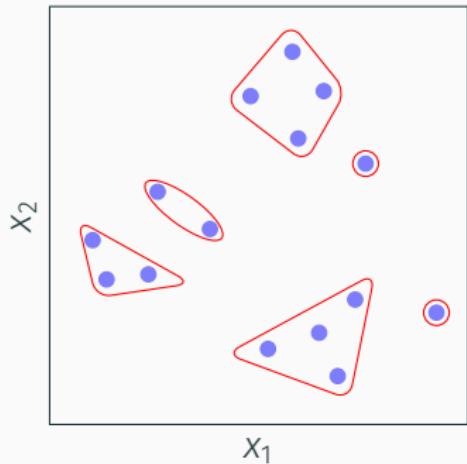
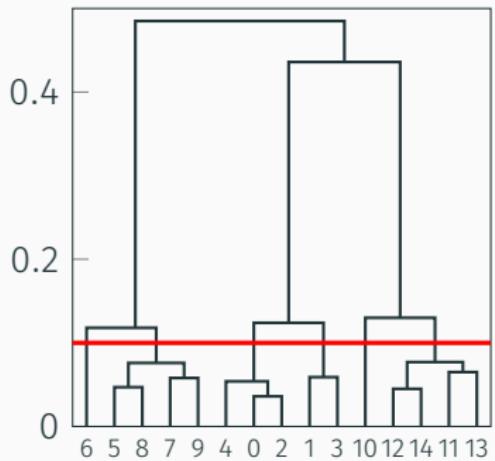
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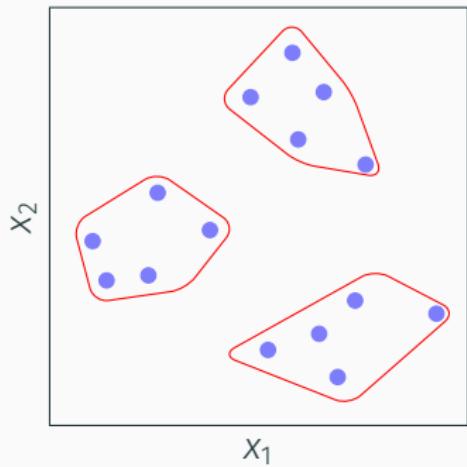
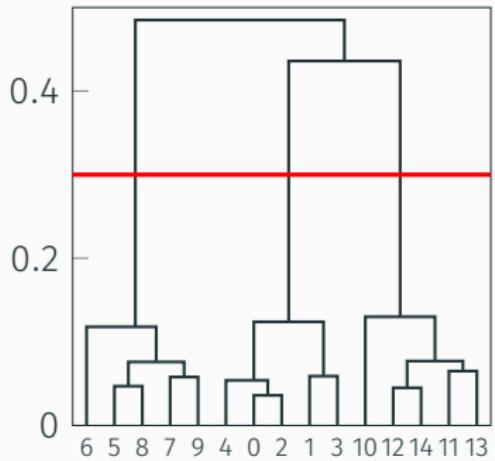
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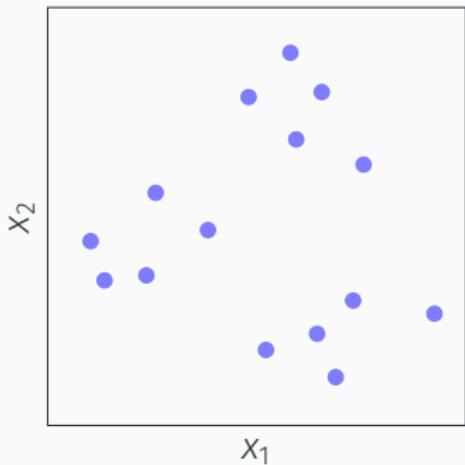
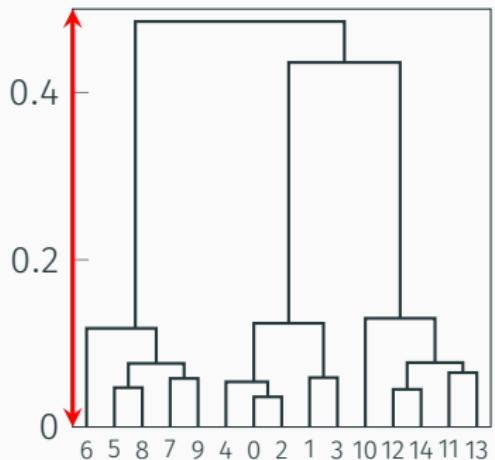
Hierarchical clustering: Interpretation



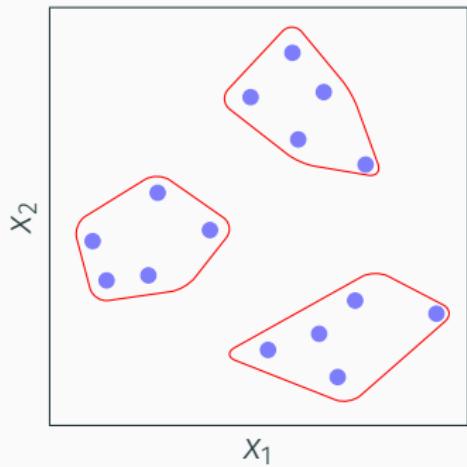
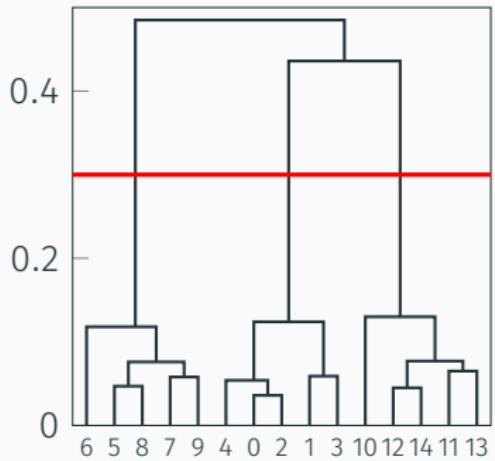
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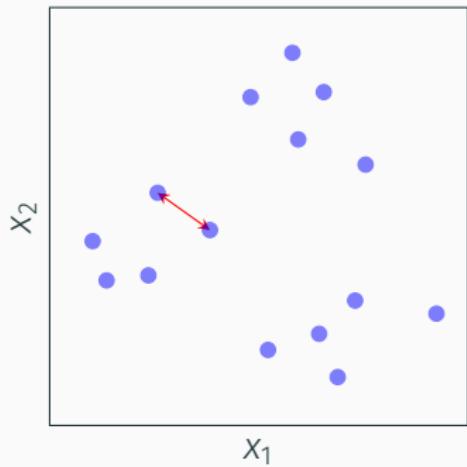
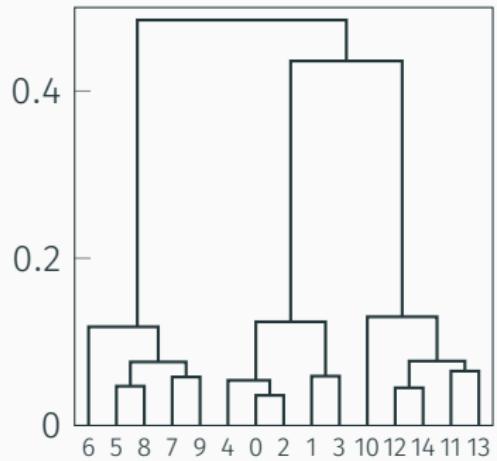
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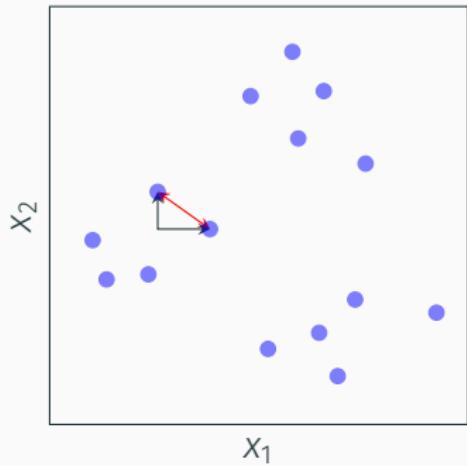
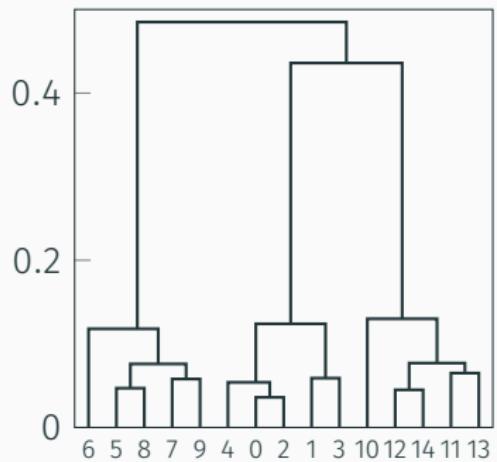
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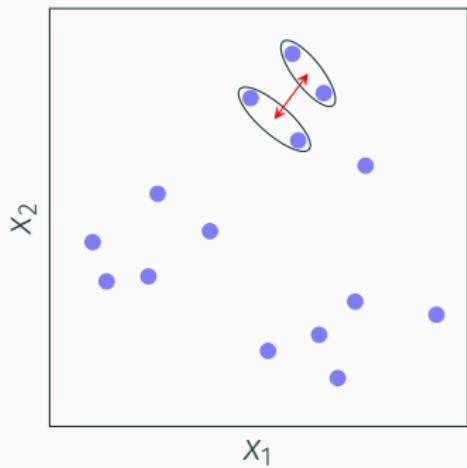
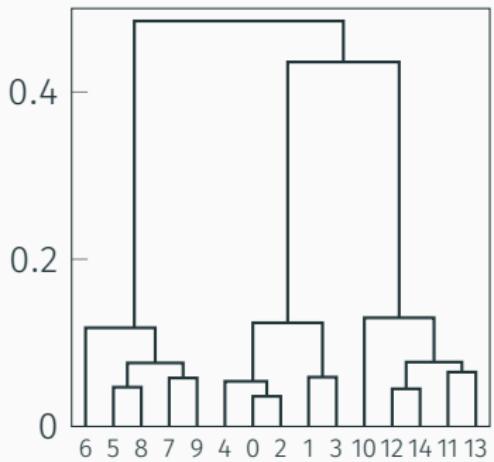
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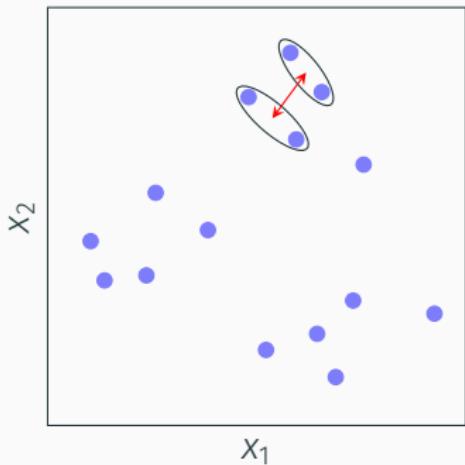
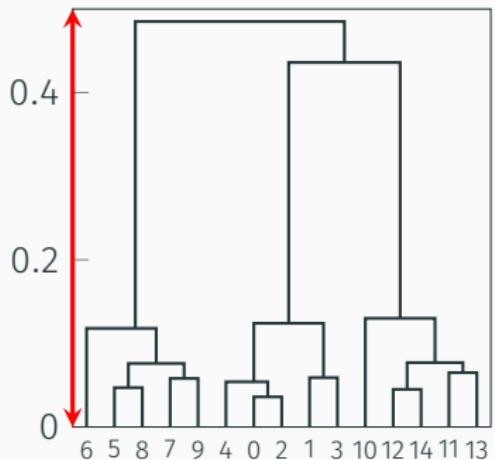
Hierarchical clustering: Interpretation



Hierarchical clustering: Interpretation



Hierarchical clustering: Interpretation



Hierarchical clustering: Interpretation

Complete	Maximal intercluster dissimilarity
Single	Minimal intercluster dissimilarity
Average	Mean intercluster dissimilarity
Centroid	Dissimilarity between the centroid for cluster A and the centroid for cluster B.



Hierarchical clustering: Interpretation

Agglomerative clustering: Iteratively merge clusters to form a hierarchy of cluster assignments.

- + Not reliant on *a priori* deciding the number of clusters
- Still relies on choices: Distance metric, linkage method, threshold



Clustering horror story



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Resting-state connectivity biomarkers define neurophysiological subtypes of depression

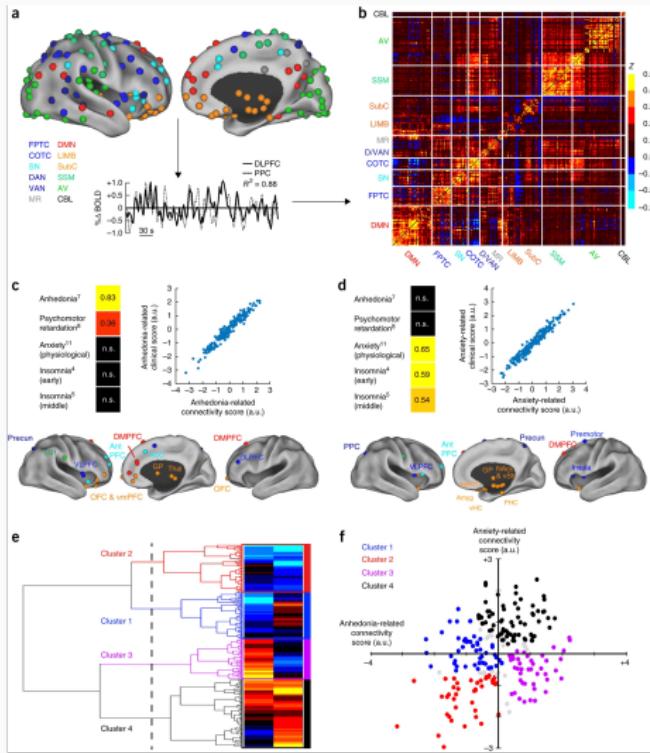
[Andrew T Drysdale](#), [Logan Grosenick](#), [Jonathan Downar](#), [Katharine Dunlop](#), [Farrokh Mansouri](#), [Yue Meng](#),
[Robert N Fetcho](#), [Benjamin Zebley](#), [Desmond J Oathes](#), [Amit Etkin](#), [Alan F Schatzberg](#), [Keith Sudheimer](#),
[Jennifer Keller](#), [Helen S Mayberg](#), [Faith M Gunning](#), [George S Alexopoulos](#), [Michael D Fox](#), [Alvaro Pascual-Leone](#), [Henning U Voss](#), [BJ Casey](#), [Marc J Dubin](#) & [Conor Liston](#) 

[Nature Medicine](#) 23, 28–38 (2017) | [Cite this article](#)

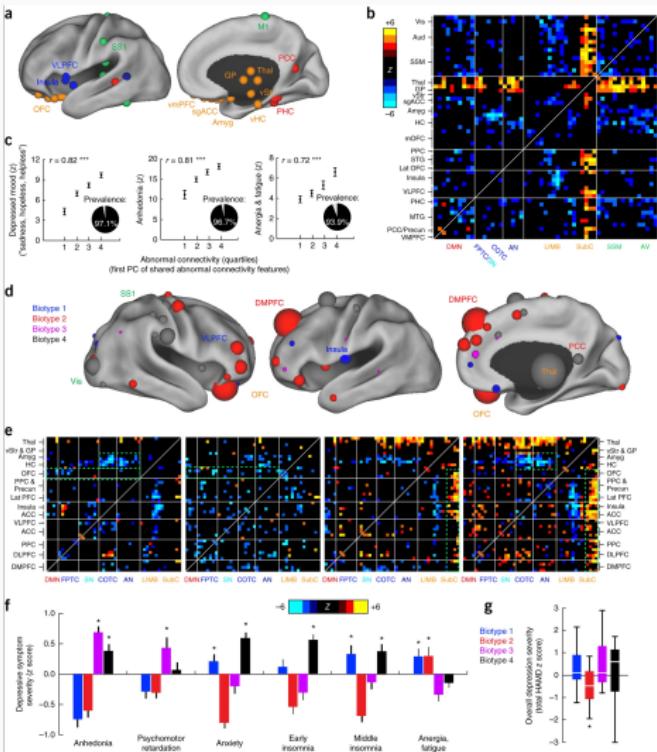
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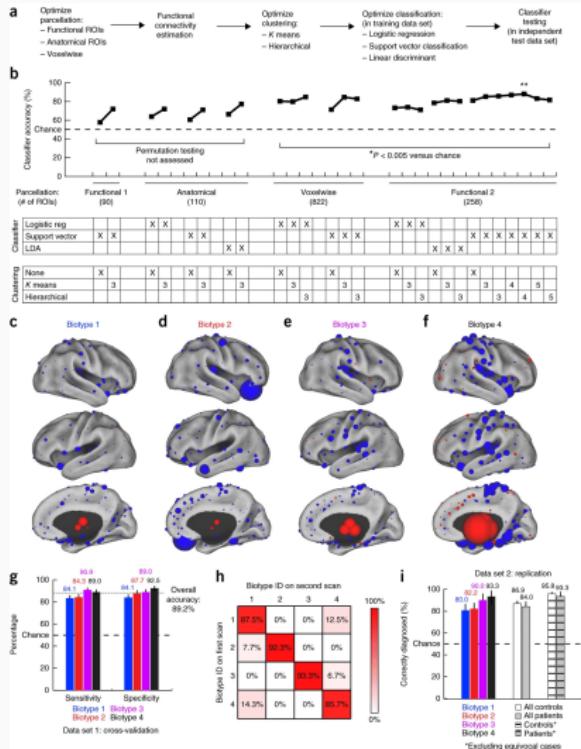
Clustering horror story



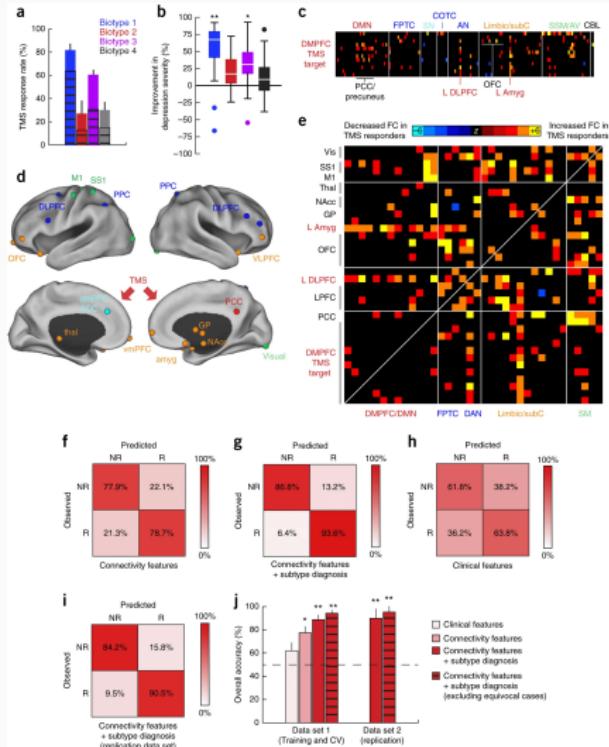
Clustering horror story



Clustering horror story



Clustering horror story





NeuroImage: Clinical
Volume 22, 2019, 101796



Evaluating the evidence for biotypes of depression: Methodological replication and extension of Drysdale et al. (2017)

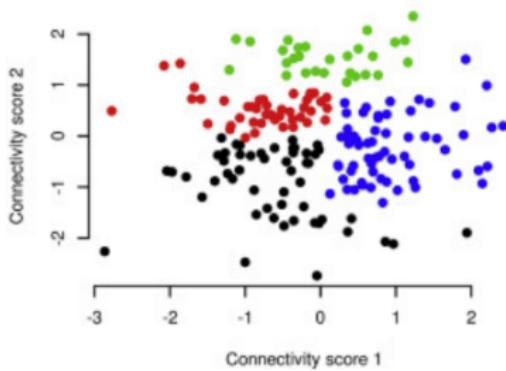
Richard Dinga ^a  , Lianne Schmaal ^{b c}, Brenda W.J.H. Penninx ^a, Marie Jose van Tol ^d,
Dick J. Veltman ^a, Laura van Velzen ^a, Maarten Mennes ^e, Nic J.A. van der Wee ^f,
Andre F. Marquand ^e



Clustering horror story



A. 4 cluster solution

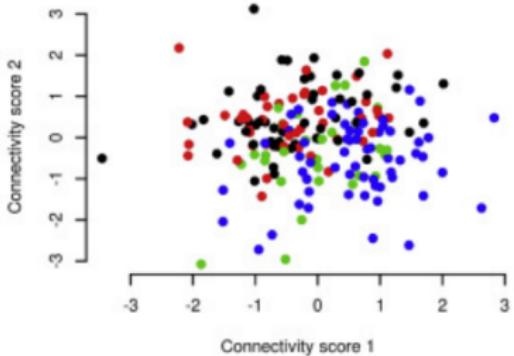




Clustering horror story



B. Cluster stability



Clustering horror story

How can we avoid ending up with a clustering nightmare? 😱

- Quantitative evaluation of our clusters (see for instance Elements of Statistical Learning)
- Test cluster stability via cross-validation, half-split tests, bootstrap etc.
- Be cautious in interpretations

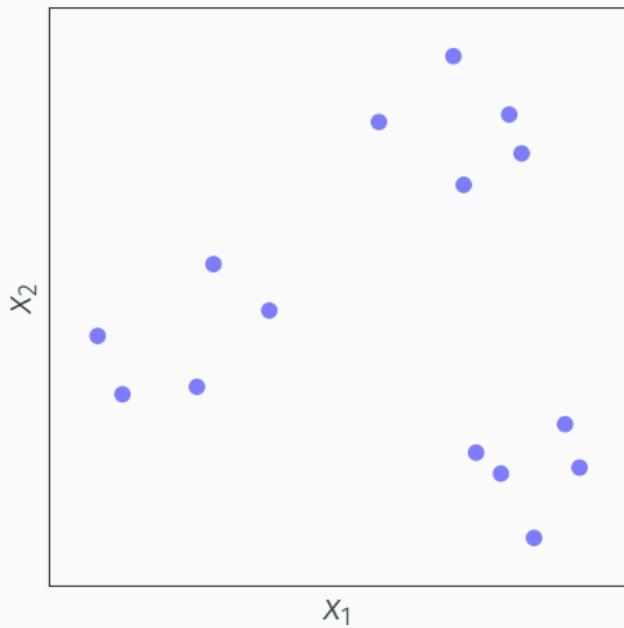


Dimensionality reduction

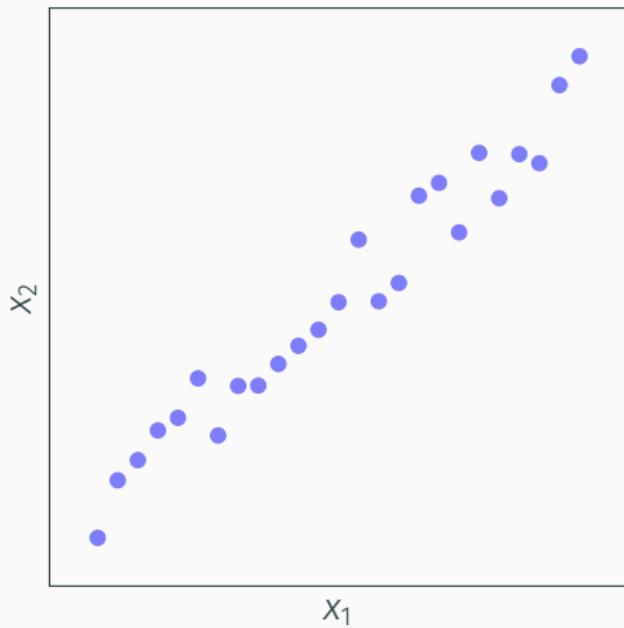


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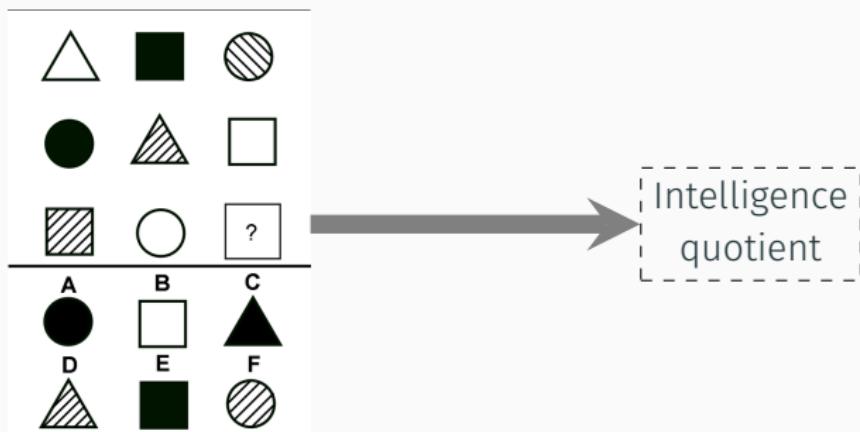
Dimensionality reduction: Motivation



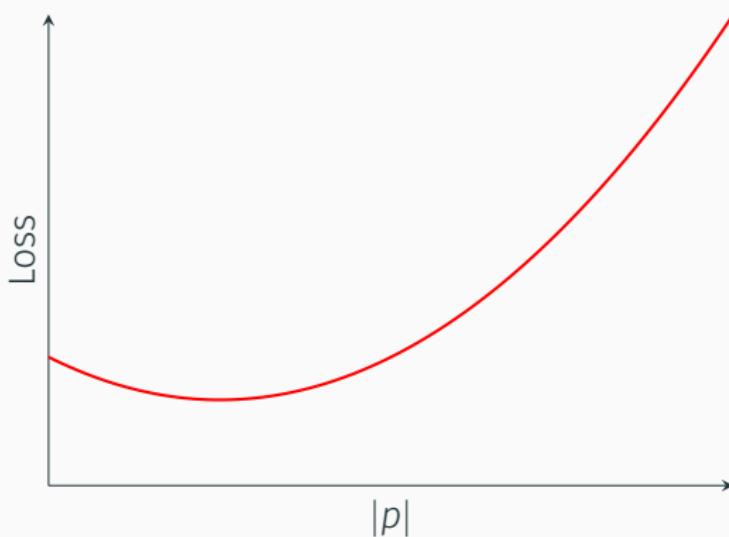
Dimensionality reduction: Motivation



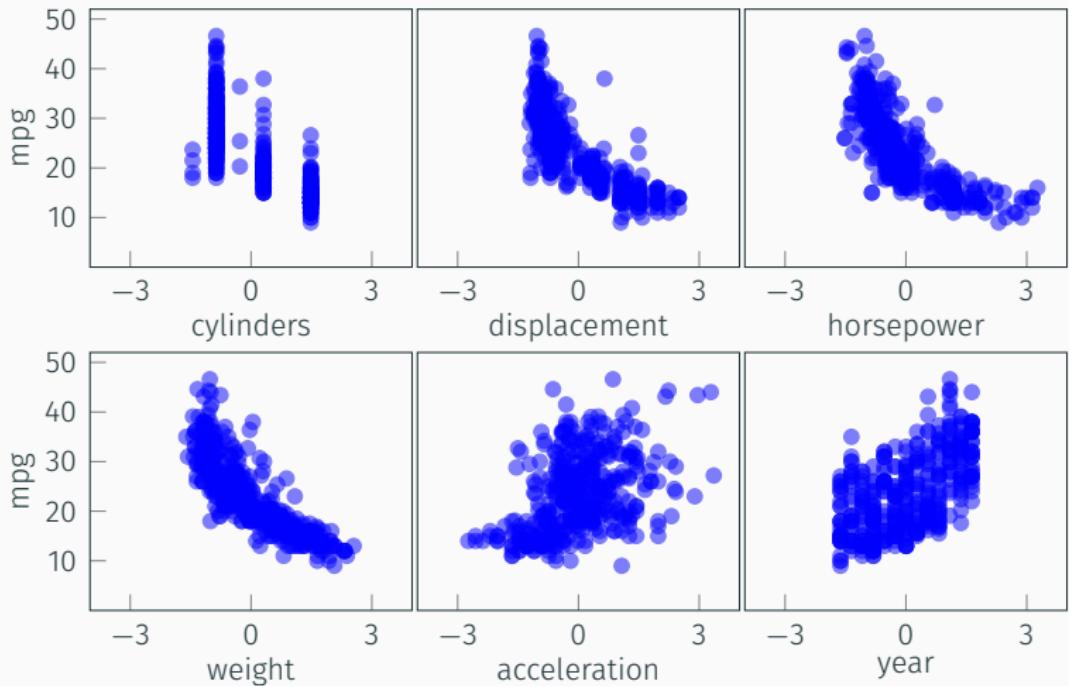
Dimensionality reduction: Motivation



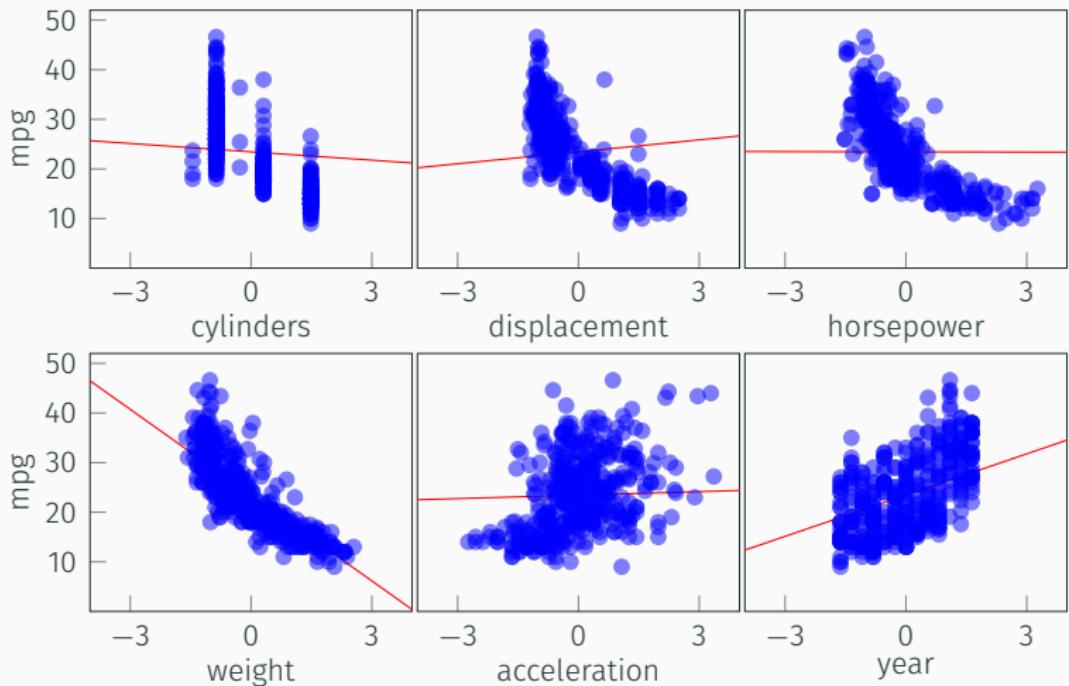
Dimensionality reduction: Motivation



Dimensionality reduction: Motivation



Dimensionality reduction: Motivation



Dimensionality reduction: Motivation

1	0.30	0.86	0.89	0.41	0.93
0.30	1	0.41	0.34	0.29	0.36
0.86	0.41	1	0.84	0.68	0.89
0.89	0.34	0.84	1	0.50	0.95
0.41	0.29	0.68	0.50	1	0.54
0.93	0.36	0.89	0.95	0.54	1

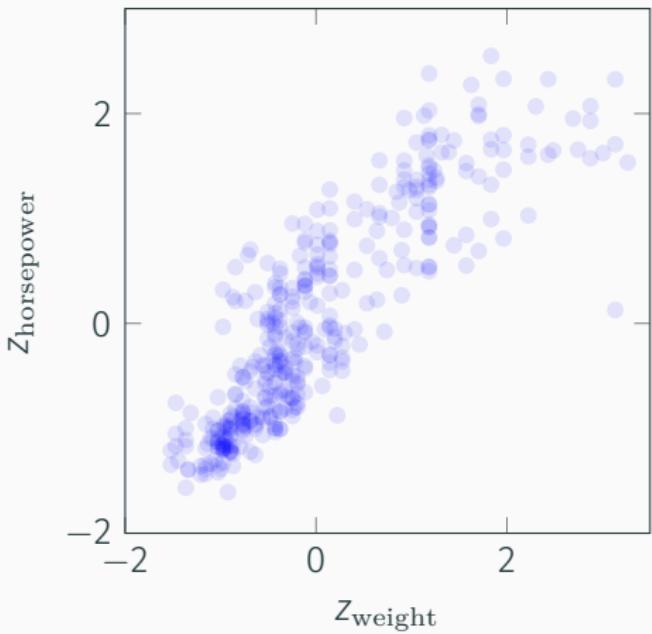


Dimensionality reduction: Motivation

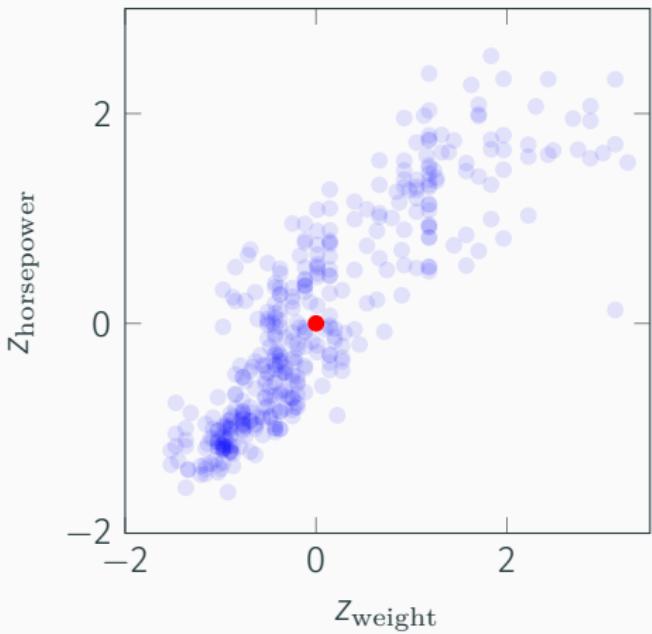
1	0.30	0.86	0.89	0.41	0.93
0.30	1	0.41	0.34	0.29	0.36
0.86	0.41	1	0.84	0.68	0.89
0.89	0.34	0.84	1	0.50	0.95
0.41	0.29	0.68	0.50	1	0.54
0.93	0.36	0.89	0.95	0.54	1



Dimensionality reduction: Principal component analysis



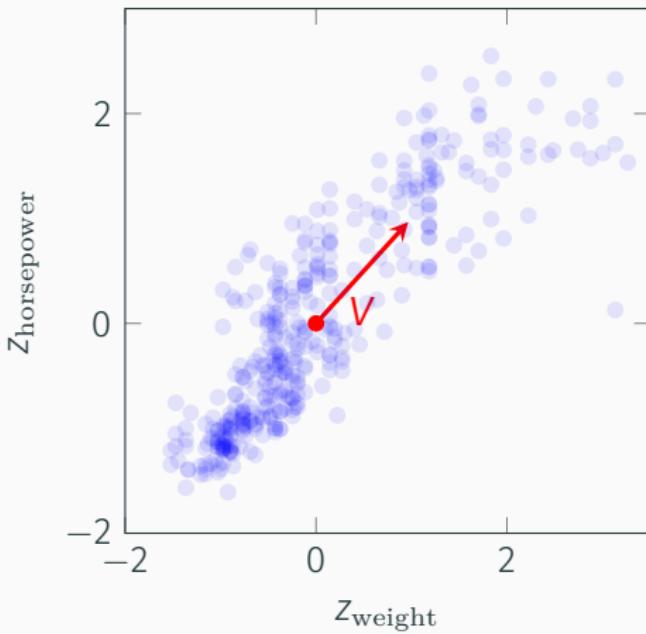
Dimensionality reduction: Principal component analysis



$c \rightarrow$ center of the data



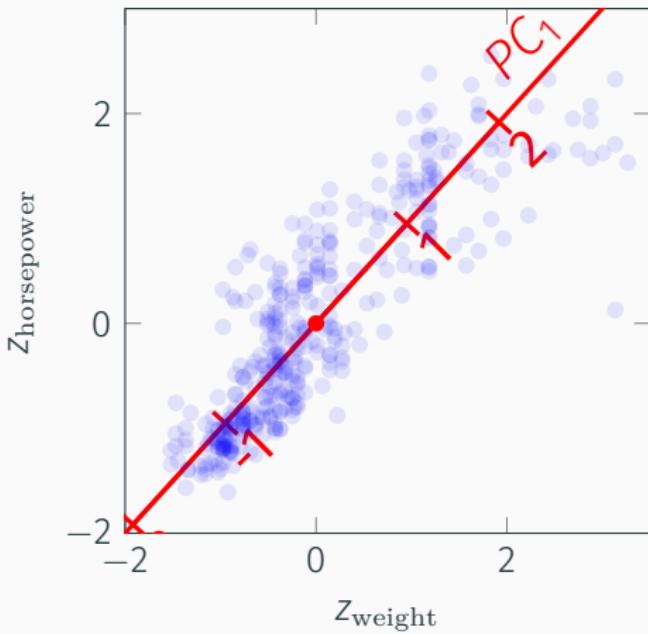
Dimensionality reduction: Principal component analysis



$v \rightarrow$ direction of maximum variance



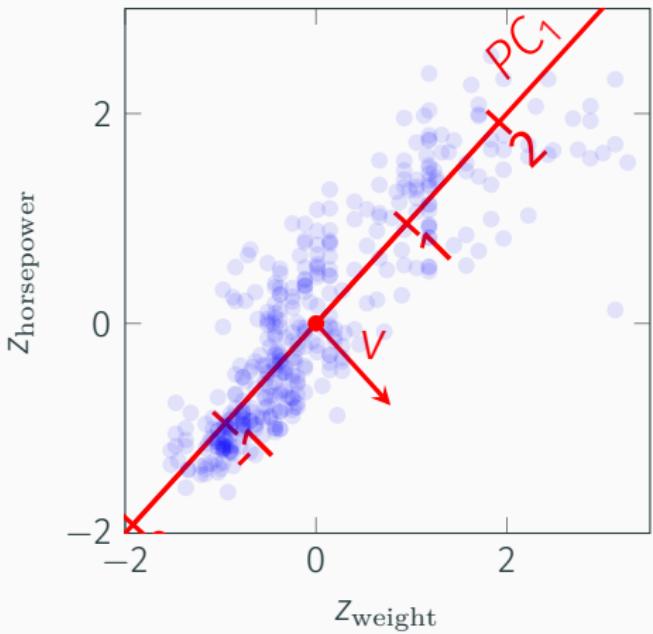
Dimensionality reduction: Principal component analysis



$$PC_1 \rightarrow 0.69 * Z_{\text{horsepower}} + 0.71 * Z_{\text{weight}}$$



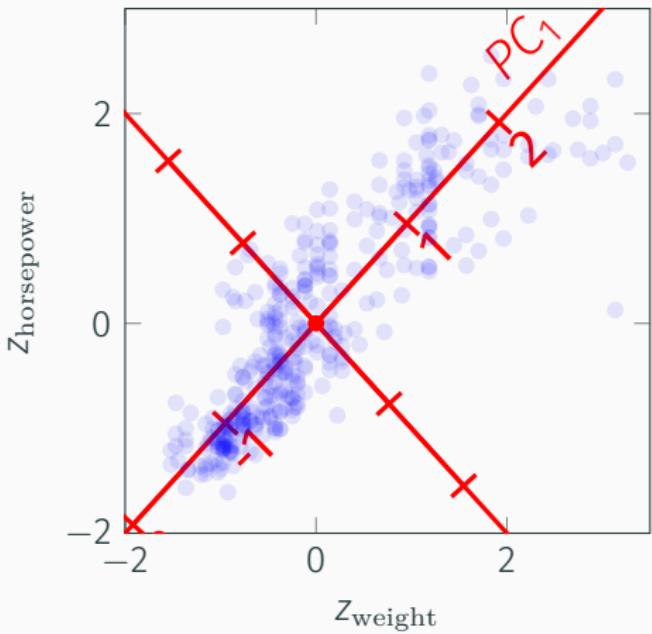
Dimensionality reduction: Principal component analysis



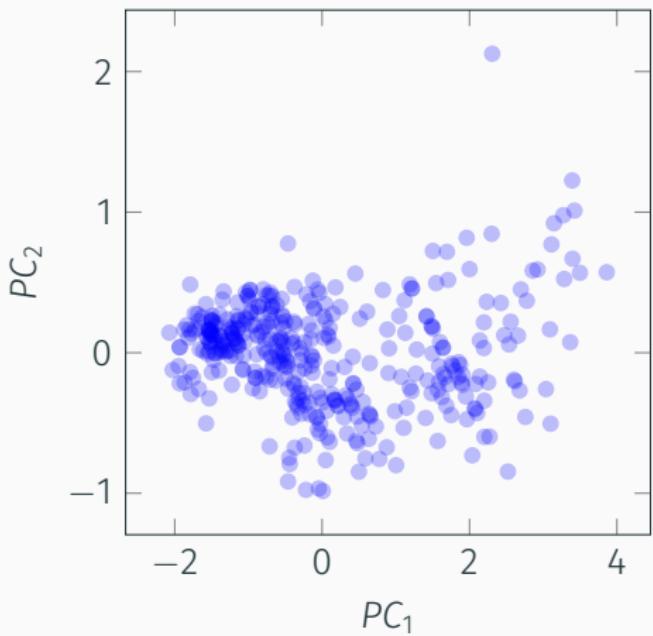
$v \rightarrow$ direction of maximum variance **orthogonal** to PC_1



Dimensionality reduction: Principal component analysis



Dimensionality reduction: Principal component analysis



Dimensionality reduction: Principal component analysis

mpg	horsepower	weight	PC1	PC2
18	130	3504	0.908	0.303
15	165	3693	1.709	0.517
18	150	3436	1.219	0.455
16	150	3433	1.217	0.457
17	140	3449	1.046	0.260
15	198	4341	2.856	0.583
14	220	4354	3.272	0.977



Dimensionality reduction: Principal component analysis

mpg	horsepower	weight	PC1	PC2
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$$PC_1 = 0.69 * z_{\text{horsepower}} + 0.71 * z_{\text{weight}}$$

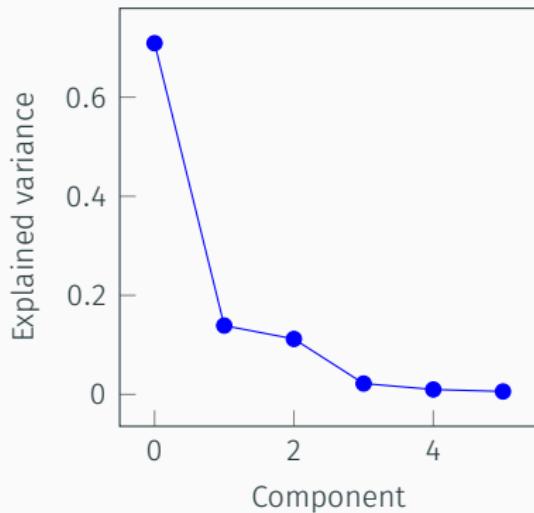


Dimensionality reduction: Principal component analysis

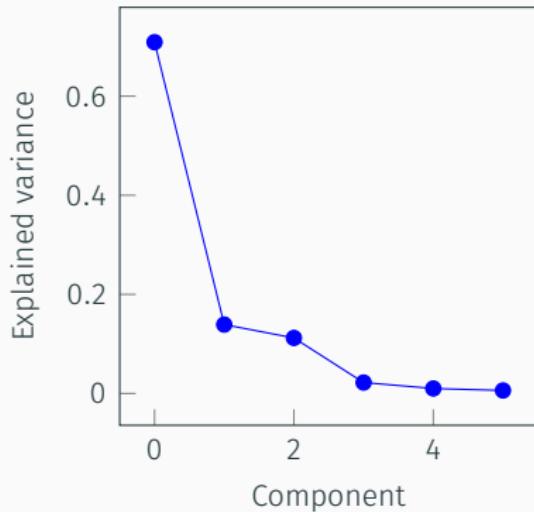
<http://localhost:8888/notebooks/notebooks%2FPCA.ipynb>



Dimensionality reduction: Principal component analysis



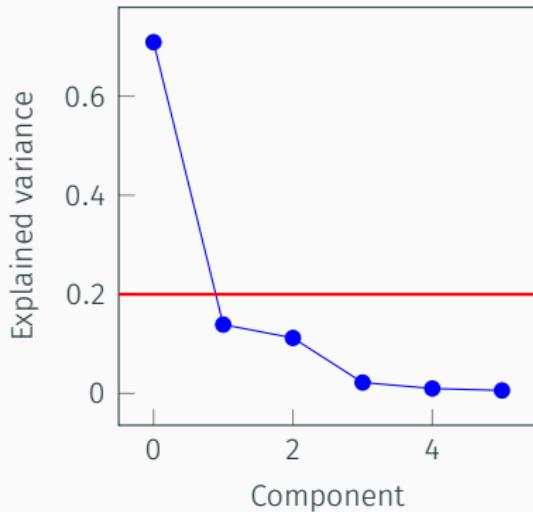
Dimensionality reduction: Principal component analysis



$$\hat{y} = \beta_0 + \sum_{i=0}^n \beta_i PC_i$$



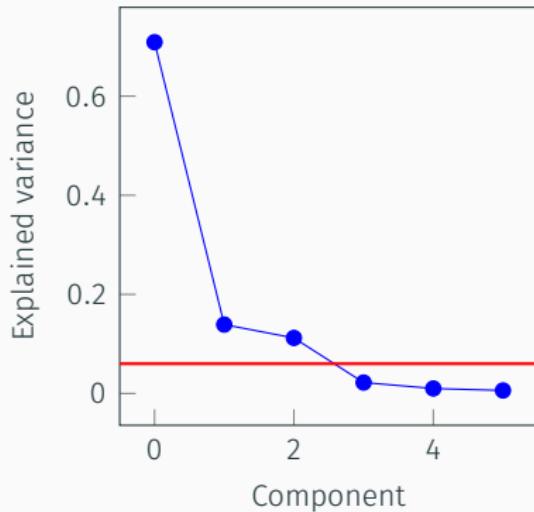
Dimensionality reduction: Principal component analysis



$$\hat{y} = \beta_0 + \sum_{i=1}^1 \beta_i PC_i$$



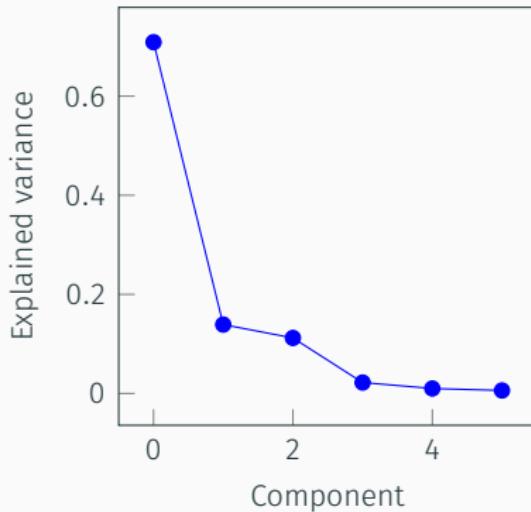
Dimensionality reduction: Principal component analysis



$$\hat{y} = \beta_0 + \sum_{i=1}^3 \beta_i PC_i$$



Dimensionality reduction: Principal component analysis



$$\hat{y} = \beta_0 + \sum_{i=0}^n \beta_i PC_i$$

n decided via a validation set, tested in a **held-out test set**



Dimensionality reduction: Principal component analysis

Principal component analysis: Transforms our dataset by computing *principal components* to replace our original variables.

- Principal components are:
 - Linear combinations of the original variables
 - Orthogonal to each other, meaning that they capture different signals in our data (linearly uncorrelated)
- They can be useful for:
 - (Qualitatively) understanding the signal in our data
 - Reducing the number of predictors for modelling



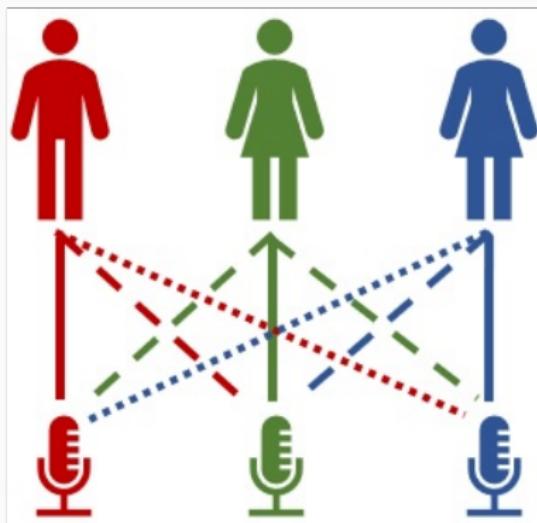
Dimensionality reduction: Principal component analysis

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 - (Qualitatively) understanding the signal in our data
 - Reducing the number of predictors for modelling



Dimensionality reduction: Independent component analysis



Dimensionality reduction: Independent component analysis

Principal component analysis: Create orthogonal components that are linear combinations of our variables:

$$PC_0 = \beta_0x_0 + \beta_1x_1 + \dots + \beta_nx_n,$$

$$PC_1 = \gamma_0x_0 + \gamma_1x_1 + \dots + \gamma_nx_n,$$

$PC_0 \perp PC_1$ (e.g. no linear correlation)

Independent component analysis: Represent each of our original variables as a linear combination of underlying sources:

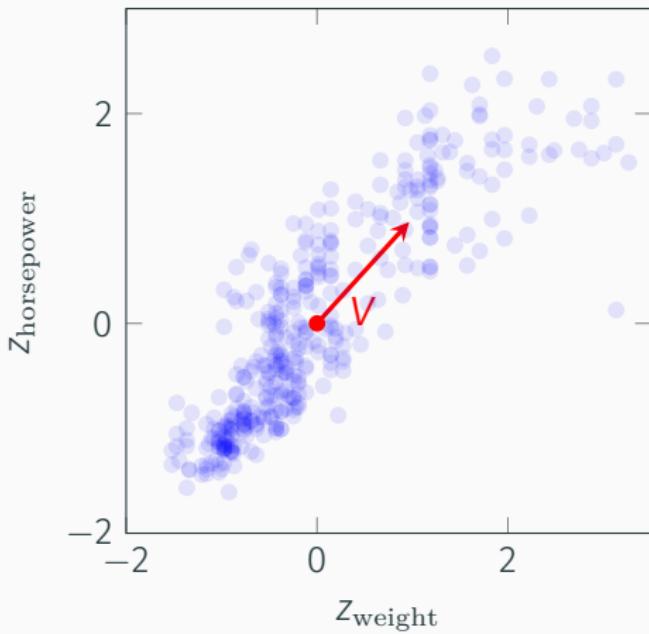
$$x_0 = \alpha_{00}s_0 + \alpha_{01}s_1 + \dots + \alpha_{0n}s_n,$$

$$x_1 = \alpha_{10}s_0 + \alpha_{11}s_1 + \dots + \alpha_{1n}s_n,$$

$s_0 \perp\!\!\!\perp s_1$ (e.g. statistically independent)



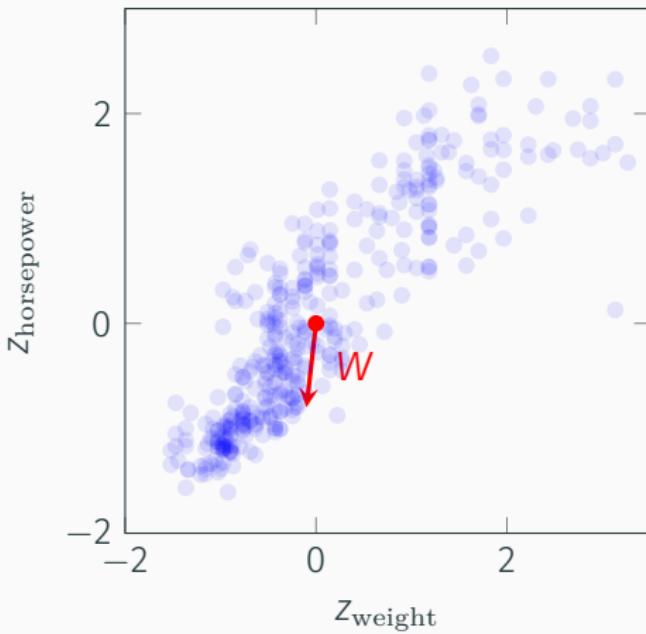
Dimensionality reduction: Independent component analysis



$v \rightarrow$ direction of greatest variance



Dimensionality reduction: Independent component analysis



$w \rightarrow$ direction that maximizes the non-Gaussianity of $w^T X$



Dimensionality reduction: Independent component analysis

https://scikit-learn.org/dev/auto_examples/decomposition/plot_ica_blind_source_separation.html#sphx-glr-auto-examples-decomposition-plot-ica-blind-source-separation-py

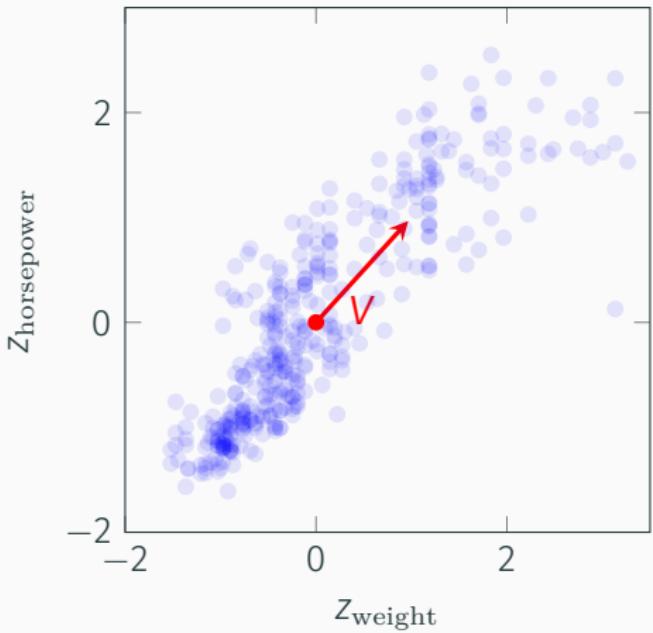


Dimensionality reduction: Independent component analysis

<https://PMC7162660>



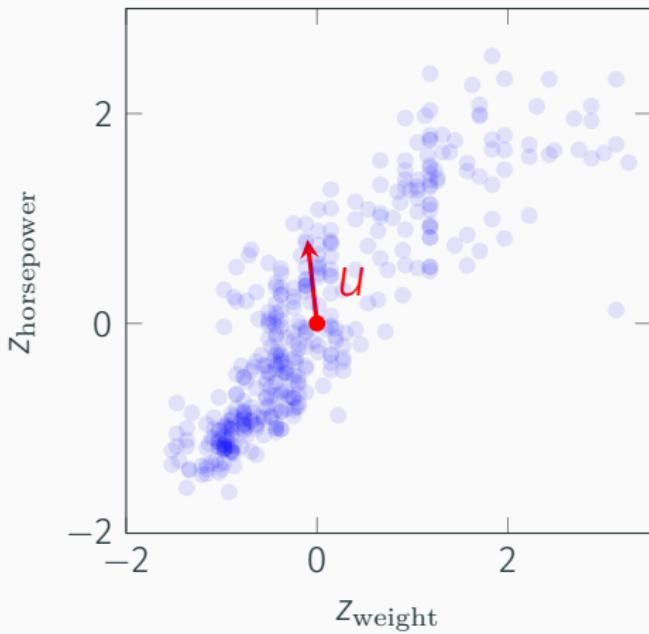
Dimensionality reduction: Partial least squares



$v \rightarrow$ direction of maximum variance



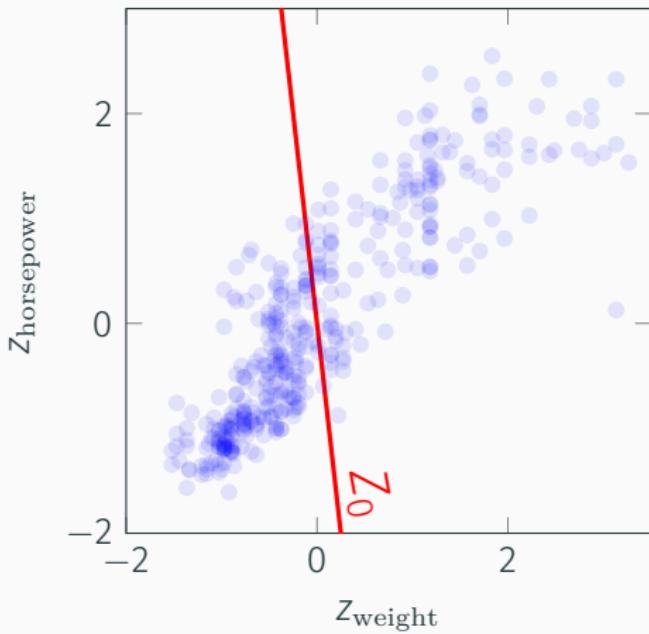
Dimensionality reduction: Partial least squares



$u \rightarrow$ direction of greatest covariance between X and y



Dimensionality reduction: Partial least squares



Dimensionality reduction: Partial least squares

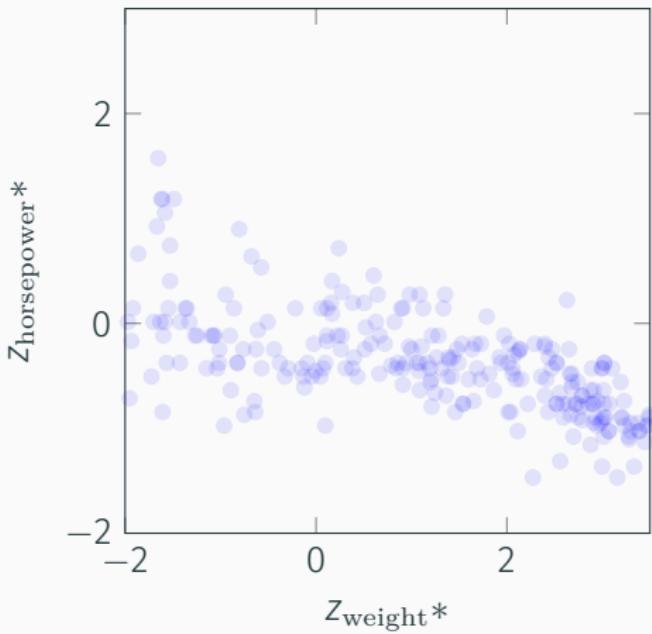
$$z_{\text{horsepower}*} = z_{\text{horsepower}} - Z_0$$

$$z_{\text{weight}*} = z_{\text{weight}} - Z_0$$

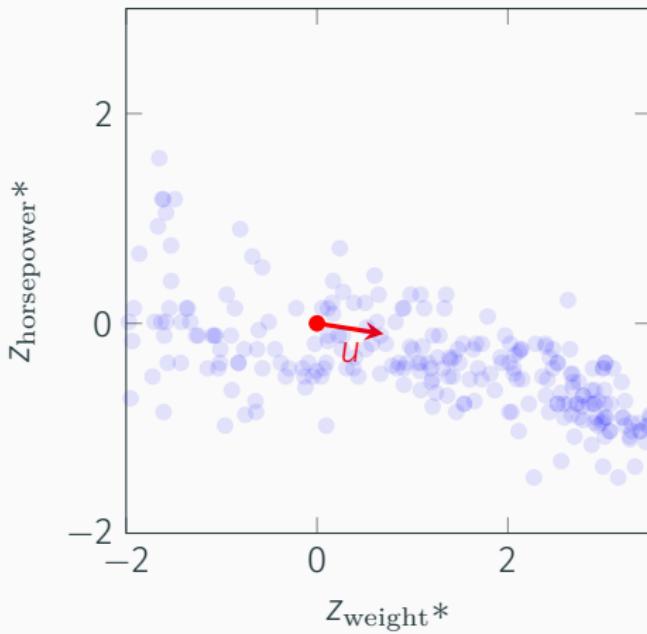
$$y* = y - Z_0$$



Dimensionality reduction: Partial least squares



Dimensionality reduction: Partial least squares



$u \rightarrow$ direction of greatest covariance between X^* and y^*



Dimensionality reduction: Partial least squares

Principal component analysis: Create orthogonal components that are linear combinations of our variables:

$$PC_0 = \beta_0x_0 + \beta_1x_1 + \dots + \beta_nx_n,$$

$$PC_1 = \gamma_0x_0 + \gamma_1x_1 + \dots + \gamma_nx_n,$$

$PC_0 \perp PC_1$ (e.g. no linear correlation),

that maximize the variance of X

Partial least squares: Create orthogonal components that are linear combinations of our variables:

$$Z_0 = \beta_0x_0 + \beta_1x_1 + \dots + \beta_nx_n,$$

$$Z_1 = \gamma_0x_0 + \gamma_1x_1 + \dots + \gamma_nx_n,$$

$Z_0 \perp PC_1$ (e.g. no linear correlation),

that maximize the covariance between X and y



Dimensionality reduction: Summary

Dimensionality reduction techniques allow us to reduce the number of variables in our dataset to either aid interpretation, or improve our models through implicit regularization.

- Principal component analysis (PCA): Finds components that are orthogonal and maximize variance
- Independent component analysis (ICA): Finds components that are non-Gaussian and statistically independent
- Partial least squares (PLS): Finds components that are orthogonal and maximize covariance between X and y

