Urban Informatics

Fall 2017

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@fedhere

XI: Clustering

Recap:

- Good practices with data: falsifiability, reproducibility
- Basic data retrieving and munging: APIs, Data formats
- SQL
- Basic statistics: distributions and their moments
- Hypothesis testing: *p*-value, statistical significance
- Statistical and Systematic errors
- Goodness of fit tests
- Likelihood
- OLS
- Topics in (time) series analysis
- Visualizations
- Geospatial analysis
- Topics in time series analysis

Today:

- Clusters

machine learning

algorithms that can learn from and make predictions on data.

machine learning

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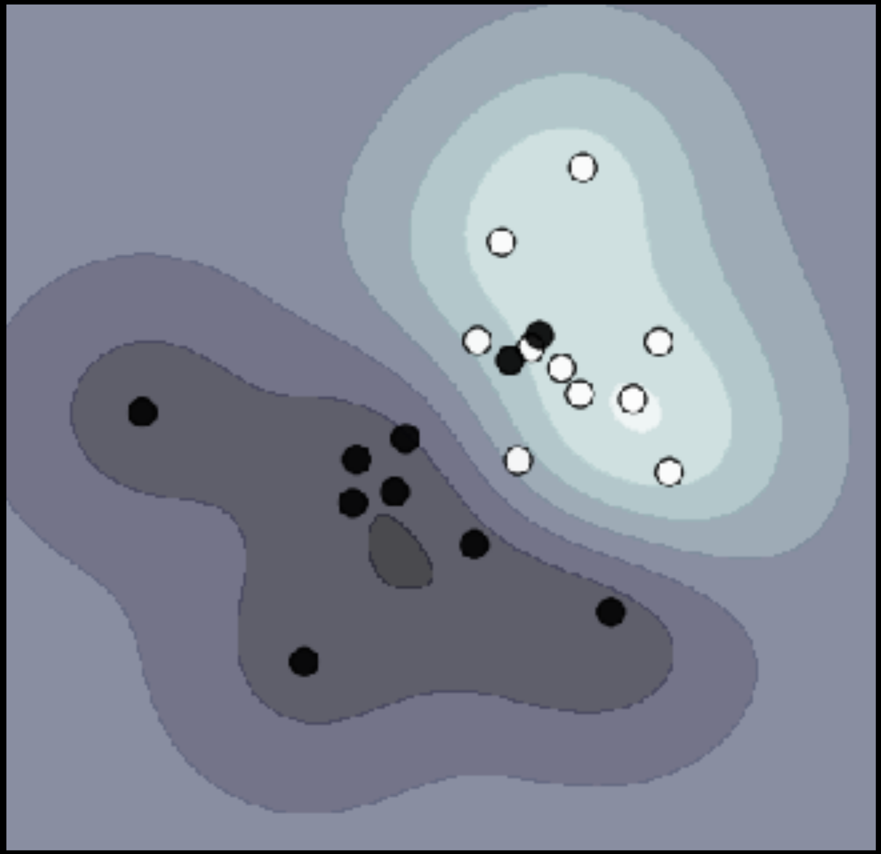
supervised learning

extract features and create models that allow prediction where the correct answer is known for a subset of the data



machine learning

algorithms that can learn from and make predictions on data.

supervised learning

extract features and create models that allow prediction where the correct answer is known for a subset of the data

unsupervised learning

identify features and create models that allow to understand structure in the data

machine learning

algorithms that can learn from and make predictions on data.

supervised methods

classification

prediction

unsupervised methods

understanding structure

organizing + compressing data

(classification, feature learing)

machine learning

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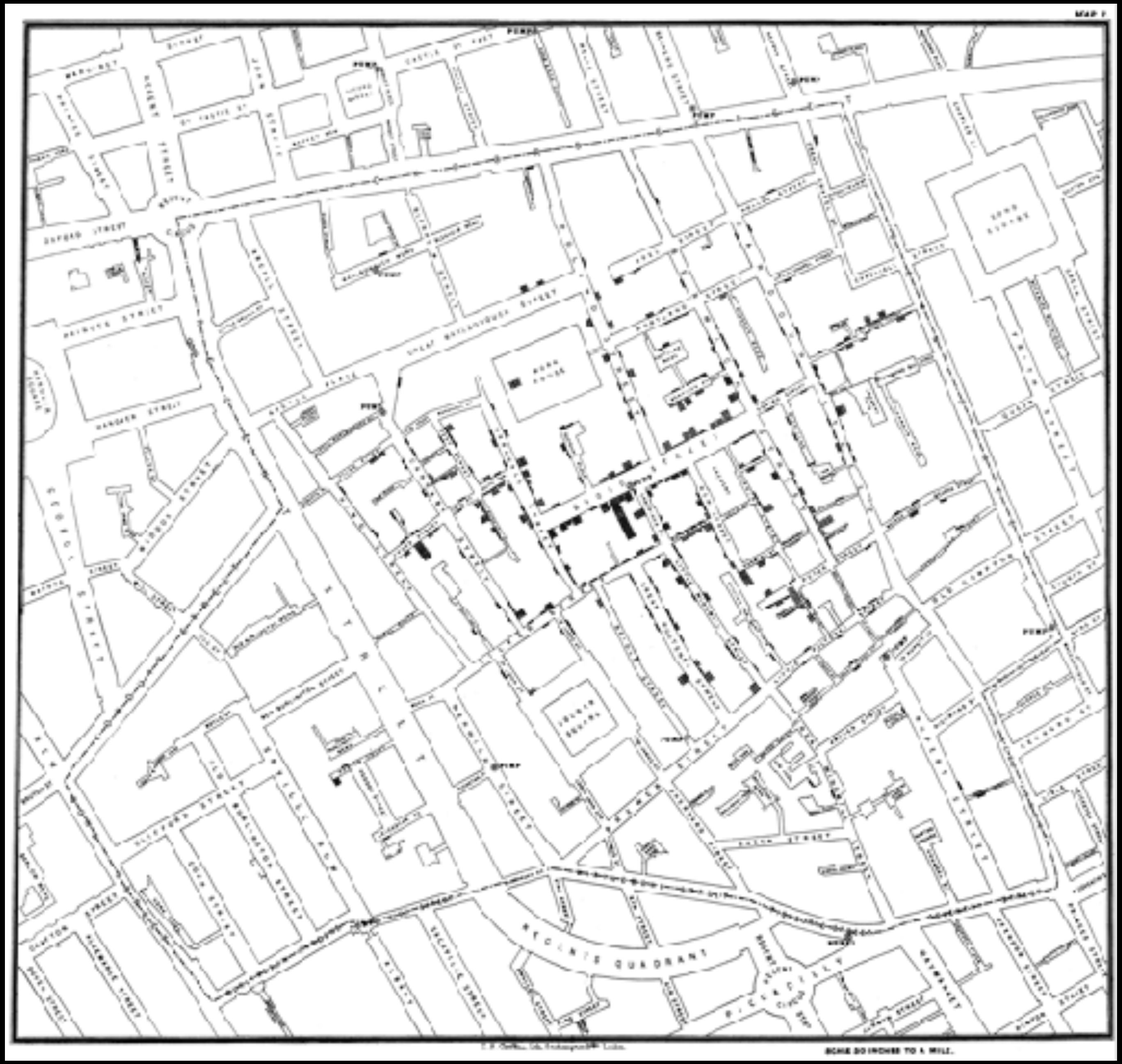
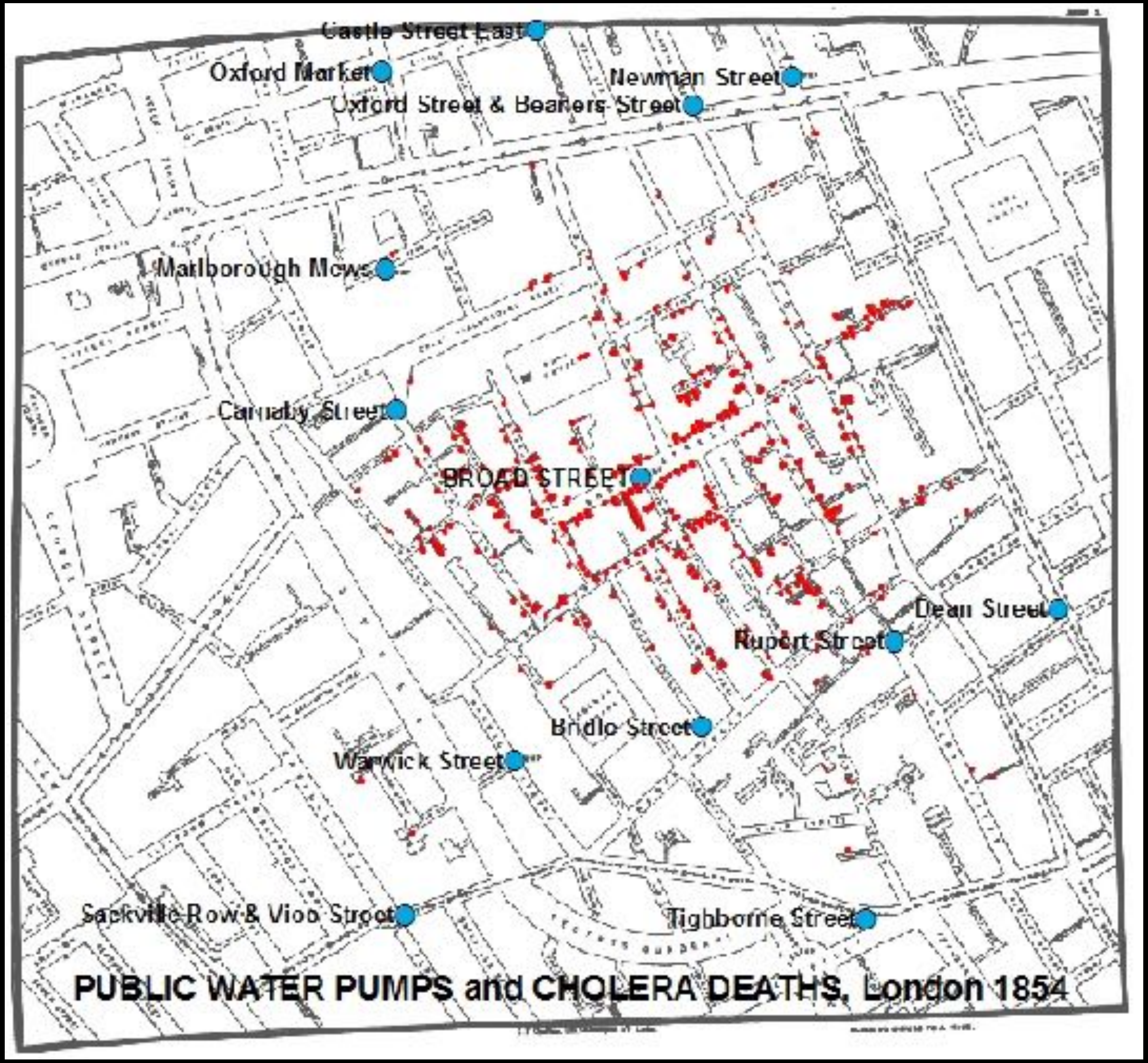
What is clustering?

Dr. John Snow September 1854 cholera outbreak map



Steven Johnson's 2006 book *The Ghost Map: the Story of London's Most Terrifying Epidemic, and How it Changed Science*.

Dr. John Snow September 1854 cholera outbreak map



digitization by John Mackenzie, University of Delaware
https://www1.udel.edu/johnmack/frec682/cholera/cholera2.html

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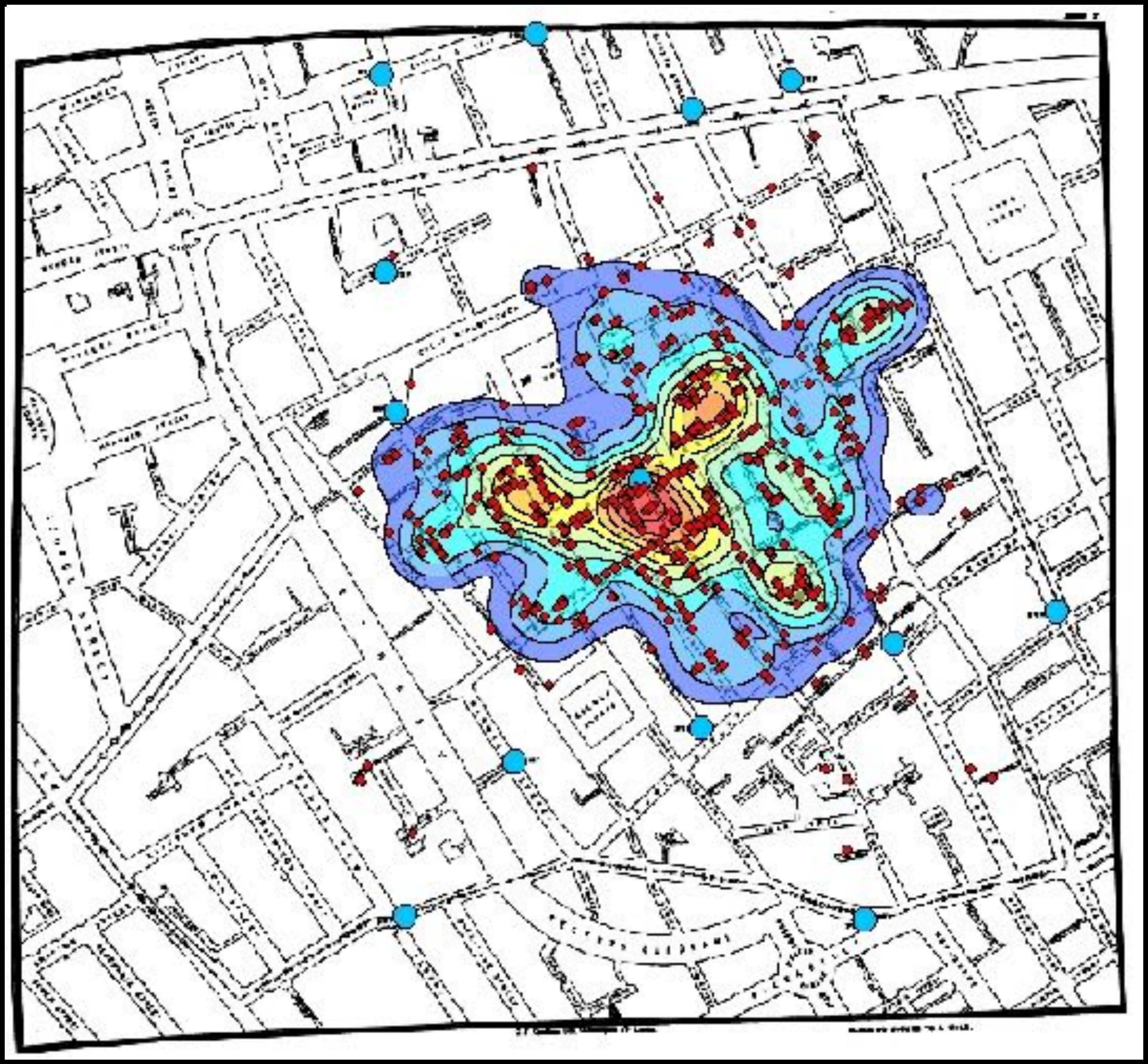

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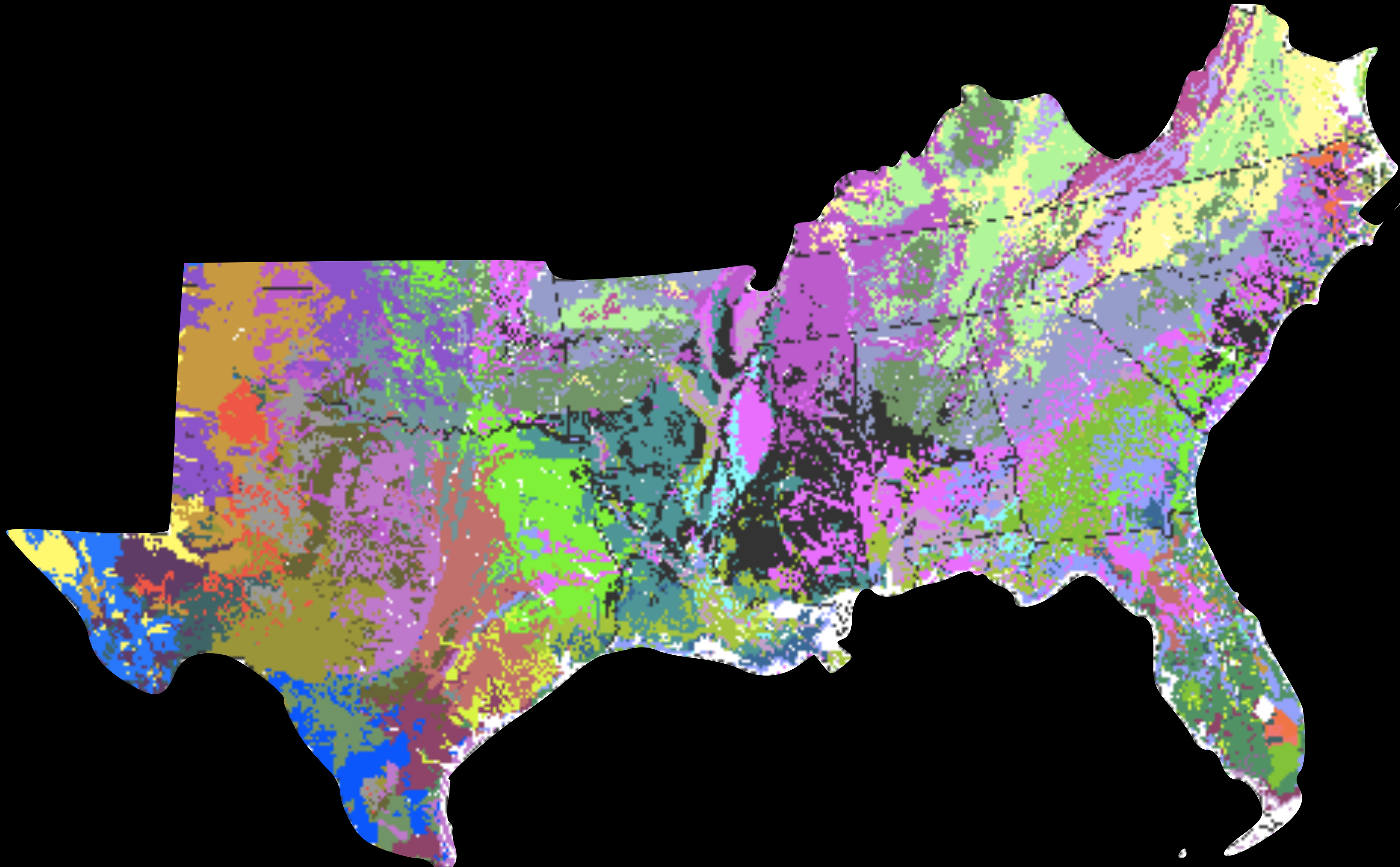


A Spatial Clustering Technique for the Identification of Customizable Ecoregions

William W. Hargrove and Robert J. Luxmoore

50-year mean monthly **temperature**, 50-year mean monthly ***precipitation***, **elevation**, total plant-available **water content of soil**, total **organic matter in soil**, and total Kjeldahl **soil nitrogen**

XI: Clustering

machine learning

supervised methods

classification
prediction

unsupervised methods

understanding structure

organizing + compressing data

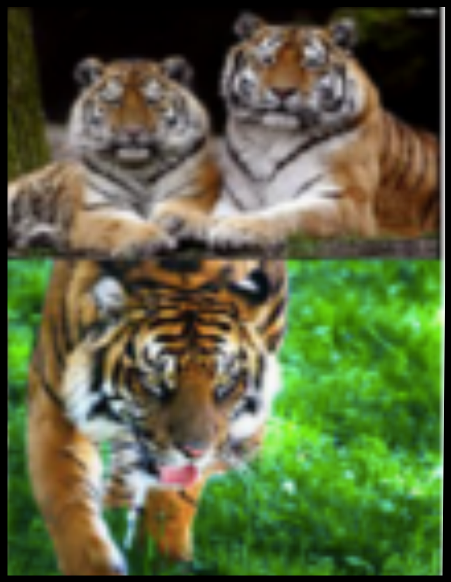
GOAL:
partitioning data in *maximally homogeneous*, *maximally distinguished* subsets.

machine learning

http://www-bcf.usc.edu/~soltanol/Applications.html

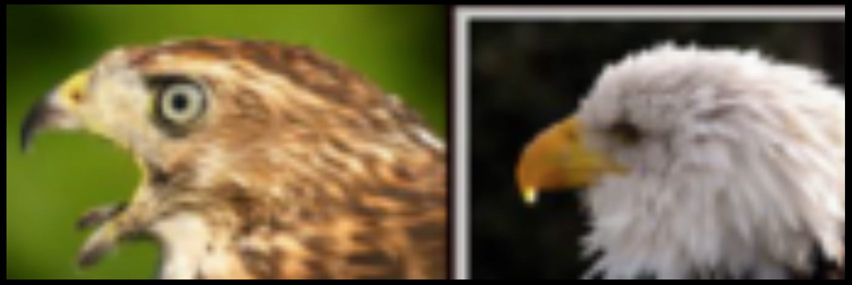
what is a cluster?

- **internal criterion:** members of the cluster should be similar to each other **(intra cluster compactness)**



tigers

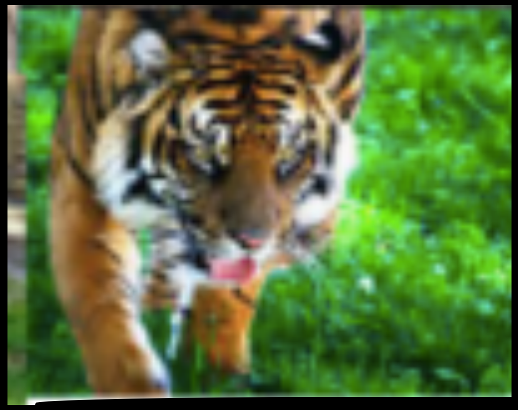
whales



eagles

what is a cluster?

- **internal criterion:** members of the cluster should be similar to each other
- **external criterion:** objects outside the cluster should be dissimilar from the objects inside the cluster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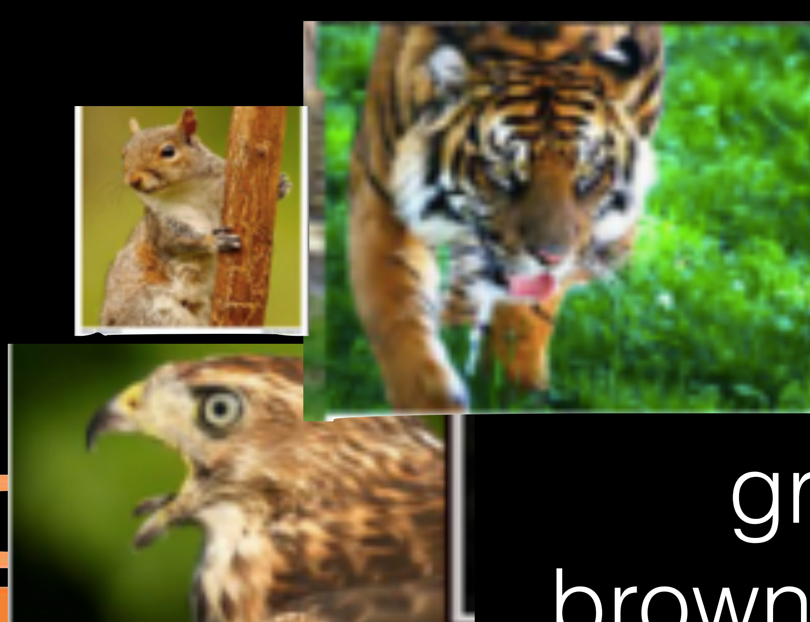
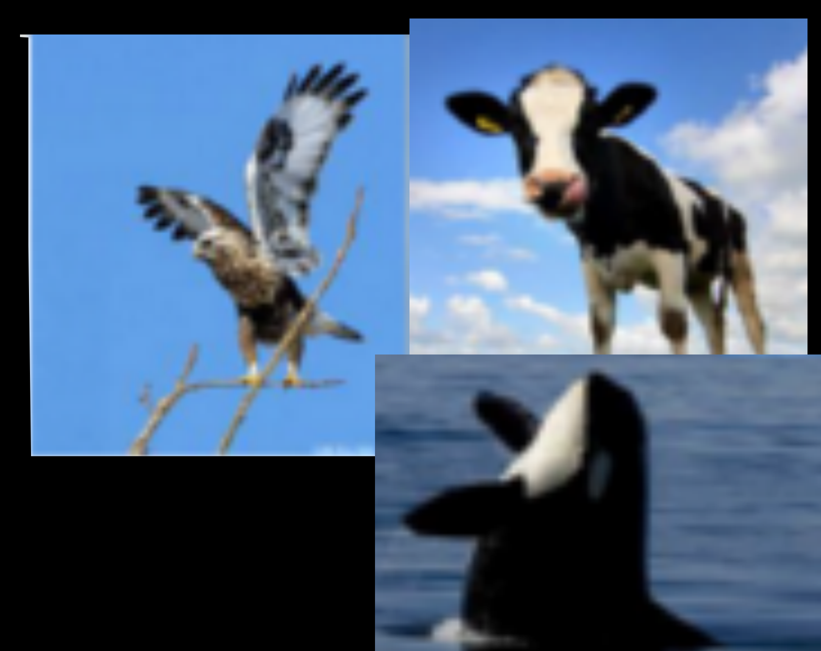


green
brown & white

blue
black
&
white



https://github.com/fedhere/UInotebooks/blob/master/cluster/imageProcessingKmeans.ipynb

https://github.com/fedhere/UInotebooks/blob/master/cluster/clusteringCUSPfaces.ipynb

https://github.com/fedhere/UInotebooks/blob/master/cluster/hardVSsoftClustering.ipynb

The ideal clustering algorithm:

- Scalability (naive algorithms are Np hard)
- Ability to deal with different types of attributes
- Discovery of clusters with arbitrary shapes
- Minimal requirement for domain knowledge
- Deals with noise and outliers
- Insensitive to order
- Allows incorporation of constraints
- Interpretable

Defining the distance

Distance Metrics   Continuous variables

Minkowski family of distances

$$D(i,j) = \sqrt[p]{|x_{i1}-x_{j1}|^p+|x_{i2}-x_{j2}|^p+\ldots+|x_{iN}-x_{jN}|^p}$$

Distance Metrics Continuous variables

Minkowski family of distances

$$D(i,j) = \sqrt[p]{\sum_{k=1}^{N} |x_{ik}-x_{jk}|^p}$$

N features (dimensions)

Distance Metrics Continuous variables

Minkowski family of distances

$$D(i,j) = \sqrt[p]{\sum_{k=1}^{N} |x_{ik} - x_{jk}|^p}$$

N features (dimensions)

$$D(i,j) > 0$$

$$D(i,i) = 0$$

$$D(i,j) = D(j,i)$$

$$D(i,j) <= D(i,k) + D(k,j)$$

Distance Metrics Continuous variables

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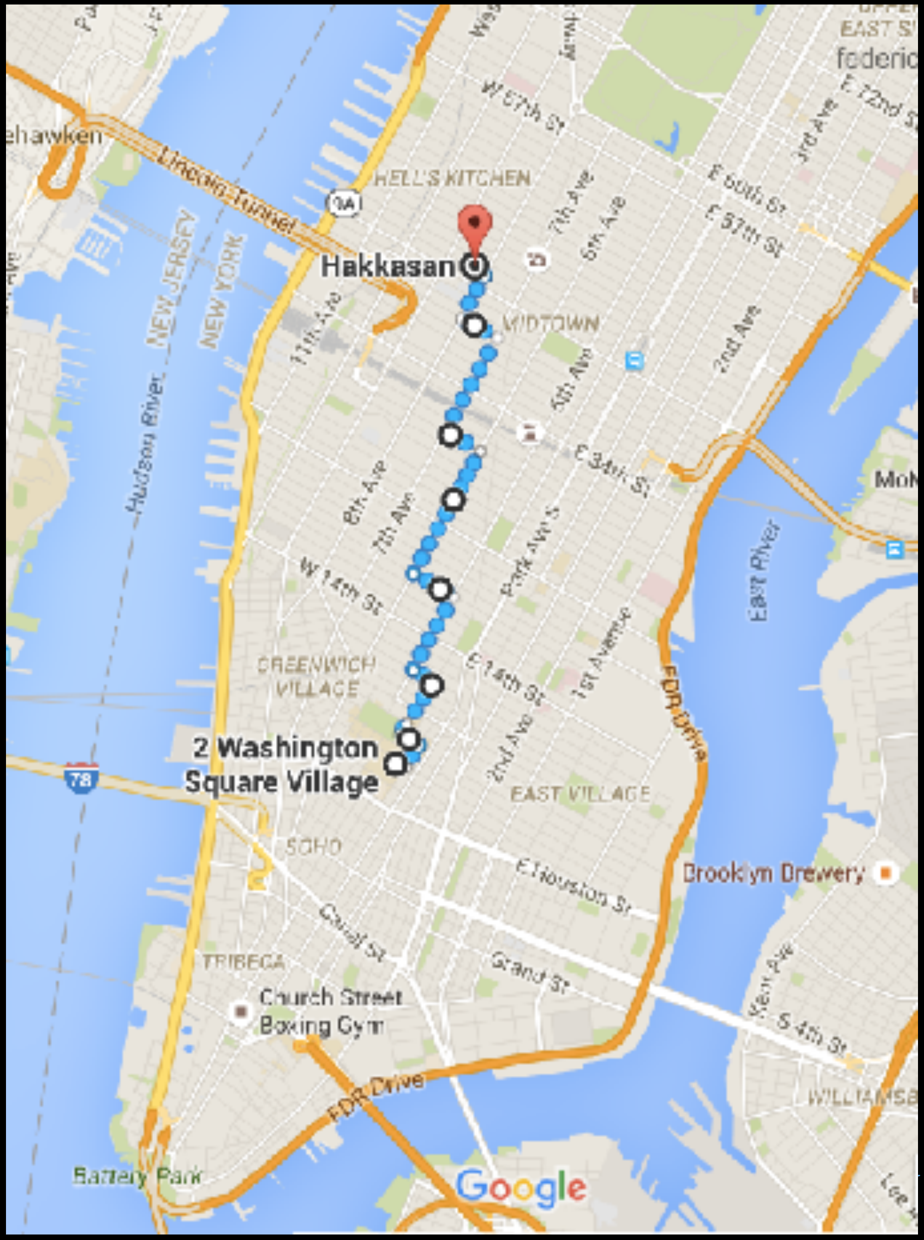
N features (dimensions)



Manhattan: p = 1

$$D_{Man}(i,j) = \sum_{k=1}^{N} |x_{ik} - x_{jk}|$$

stering

Distance Metrics Continuous variables

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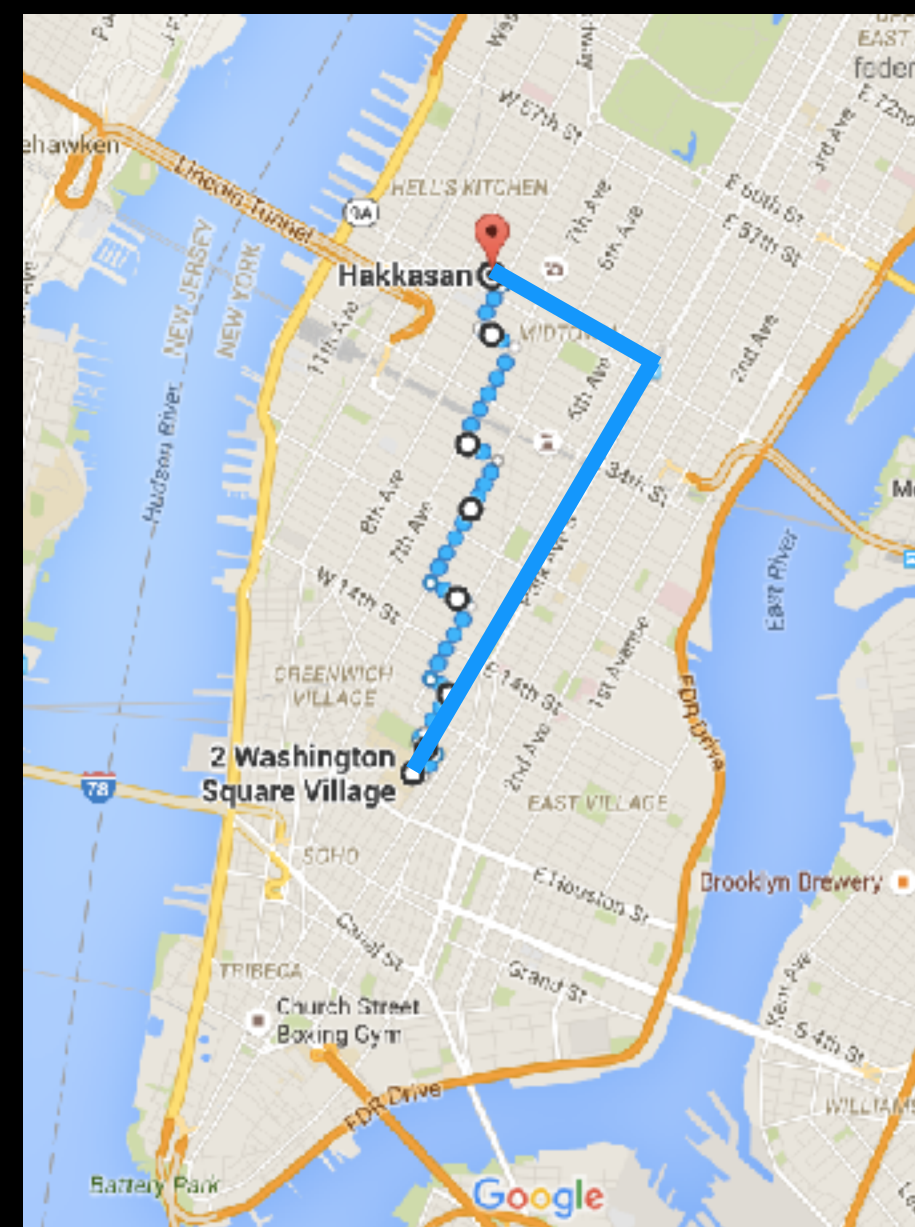

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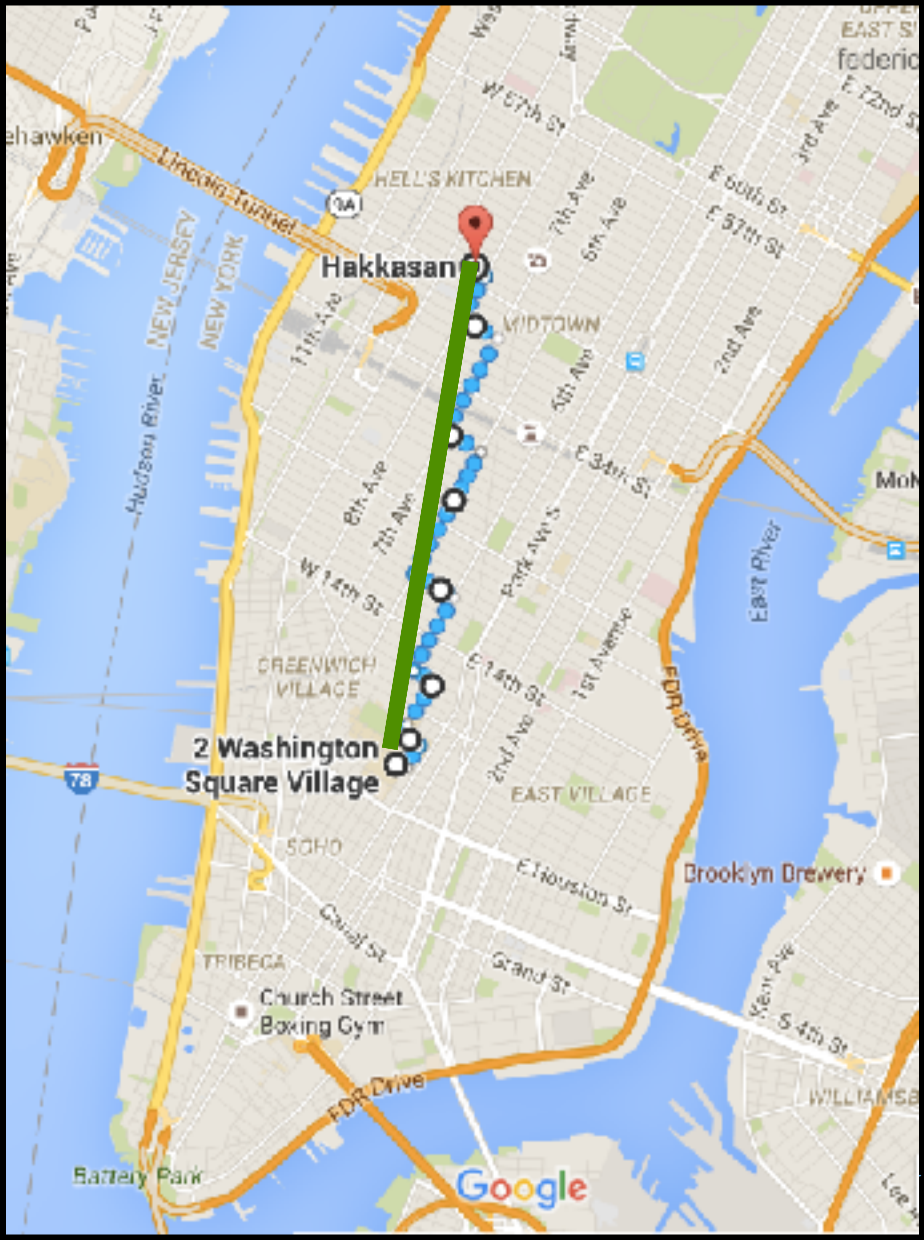


Euclidean: p = 2

$$D_{Euc}(i,j) = \sqrt{\sum_{k=1}^{N} |x_{ik}-x_{jk}|^2}$$

stering

Distance Metrics   Continuous variables

Minkowski family of distances

$$D(i,j) = \sqrt[p]{\sum_{k=1}^{N} |x_{ik} - x_{jk}|^p}$$

Great Circle distances: $\phi_i, \lambda_i, \phi_j, \lambda_j$

geographical latitude and longitude

$$D(i,j) = R \arccos\left(\sin\phi_i \cdot \sin\phi_j + \cos\phi_i \cdot \cos\phi_j \cdot \cos(\Delta\lambda) \right)$$

Distance Metrics Continuous variables

Minkowski family of distances

$$D(i,j) = \sqrt[p]{\sum_{k=1}^{N} |x_{ik}-x_{jk}|^p}$$

N features (dimensions)

Weighted distances:

$$D(i,j) = \sqrt[p]{w_1|x_{ik}-x_{jk}|^p + w_2|x_{i2}-x_{j2}|^p + \ldots + w_N|x_{iN}-x_{jN}|^p}$$

Distance Metrics   Binary variables

Uses presence/absence data in two samples

Simple similarity coefficient *SMC*

$$S_{ij} = \frac{M_{i=0j=0} + M_{i=1j=1}}{M_{00} + M_{01} + M_{10} + M_{11}}$$

Distance Metrics Binary variables

	1	0	sum
1	a	b	$a+b$
0	c	d	$c+d$
sum	$a+c$	$b+d$	p

Uses presence/absence data in two samples

Simple similarity coefficient *SMC*

$$S_{ij} = \frac{b+c}{a+b+c+d}$$

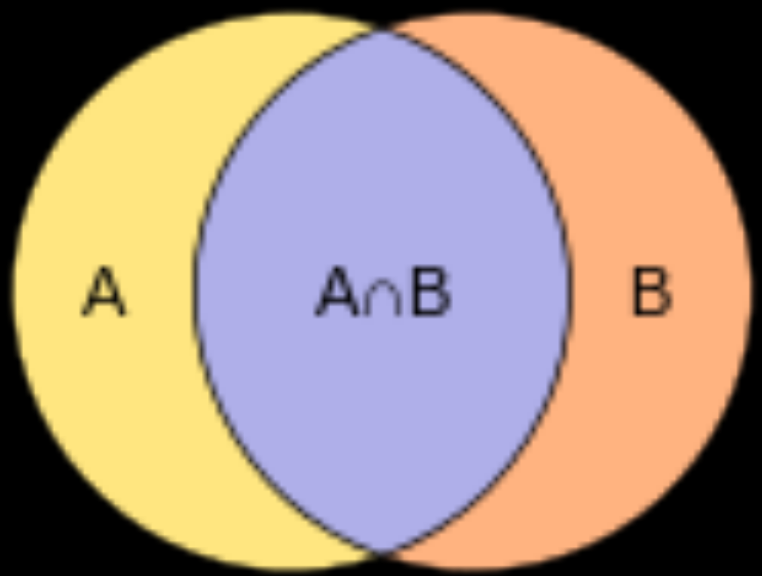
a = number of items in common,
b = number of items unique to the first set
c = number of items unique to the second set

Distance Metrics Sets variables

Uses presence/absence data

Jaccard similarity coefficient *S_j*

$$S_j = \frac{a}{a+b+c}$$



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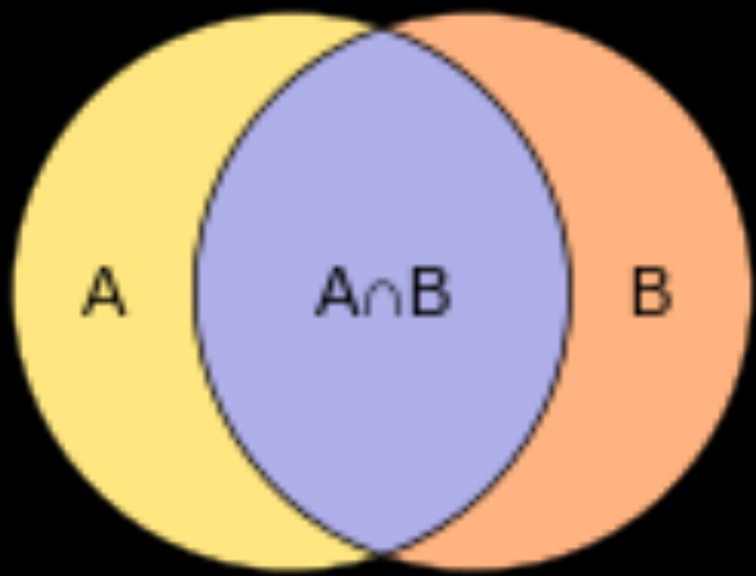
Jaccard similarity coefficient S_j

$$S_j = \frac{A \bigcap B}{A \bigcup B}$$



a = number of items in common,
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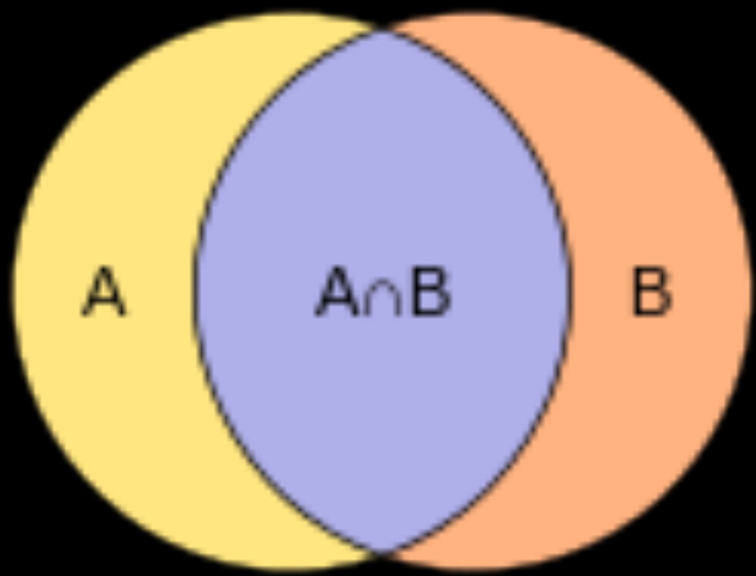
c = number of items unique to the second set

Distance Metrics   Sets variables

Uses presence/absence data

Jaccard distance *D_j = 1- S_j*

$$S_j = \frac{A \bigcap B}{A \bigcup B}$$



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jupyter

https://github.com/fedhere/UInotebooks/blob/master/cluster/categoricalDistance.ipynb

jupyter

https://github.com/fedhere/UInotebooks/blob/master/cluster/thanksgivingClustering.ipynb

How clustering works

Clustering methods

- **Partitioning**

  Hard clustering

  K-means (McQueen '67)
  K-medoids (Kaufman & Rausseeuw '87)

  Soft Clustering
  Expectation Maximization (Dempster,Laird,Rubin '77)

- **Hirarchical**
  agglomerative

  devisive

- **also:**
  - **Density based**
  - **Grid based**
  - **Model based**

Clustering methods

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K-means:

1. **Choose N "centers" guesses:** random points in the data space

2. **Calculate which center each datapoint is closest to:** these are the N clusters

3. **Calculate the new centers as means of the assigned clusters**: these are the new N centers

4. **Iterate 2&3 till convergence**: when clusters no longer change

K-means:

Minimizes the intra cluster gaussian

Order: #clusters #dimensions #iterations #datapoints
O(KdN)

works on minimizing the aggregate distance within the cluster if the distance is Euclidean this is the same am minimizing the variance

Its non-deterministic: the result depends on the (random) starting point

It only works where the mean is defined: alternative is K-medoids which represents the cluster by its central member, rather than by the mean

Must declare the number of clusters upfront

https://github.com/fedhere/UInotebooks/blob/master/cluster/thanksgivingClustering.ipynb

jupyter

https://github.com/fedhere/UInotebooks/blob/master/cluster/kmeans.ipynb

K-means:

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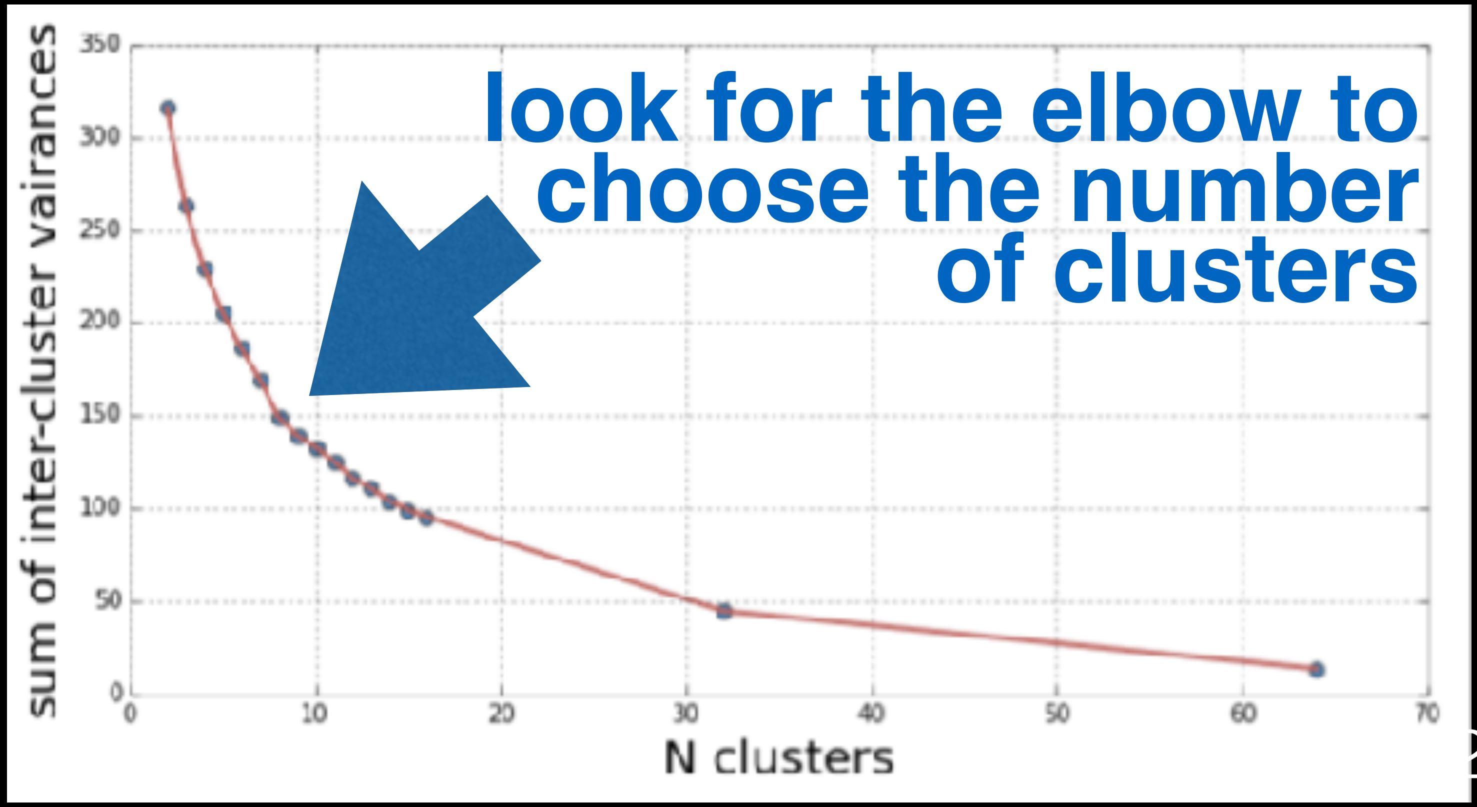

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Clustering methods

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DBSCAN
(Ester,Kriegel,Sander,Xu '96) **A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise**
(11,000+ citations)

Clustering methods

- **Partitioning**

  Hard clustering

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- **Hirarchical**
  agglomerative

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- **also:**
  - **Density based**
  - **Grid based**
  - **Model based**

Hard Clustering:

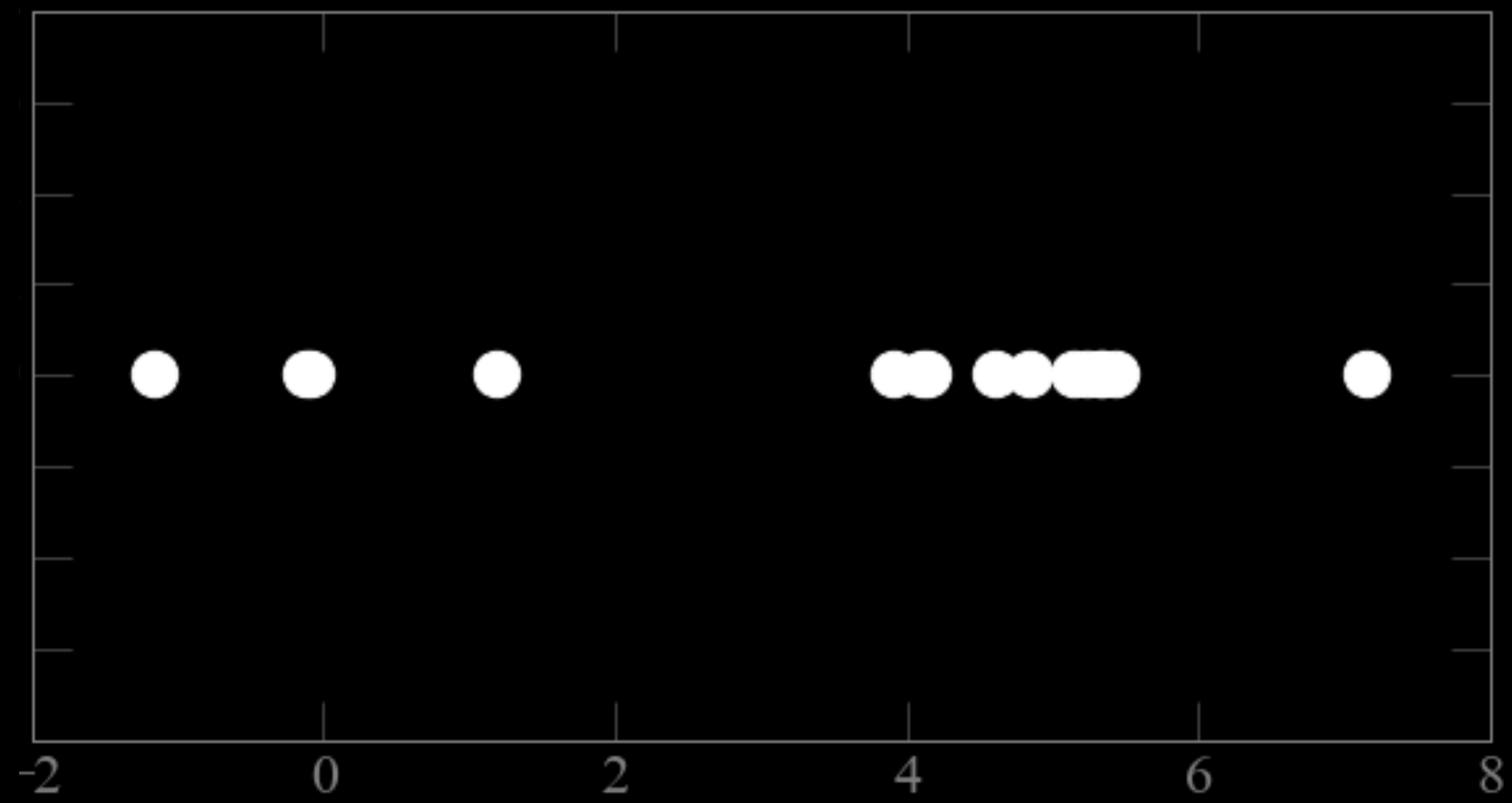
each object in the sample belongs to only 1 cluster

Soft Clustering:

to each object in the sample we assign a degree of belief that it belongs to a cluster

Mixture models

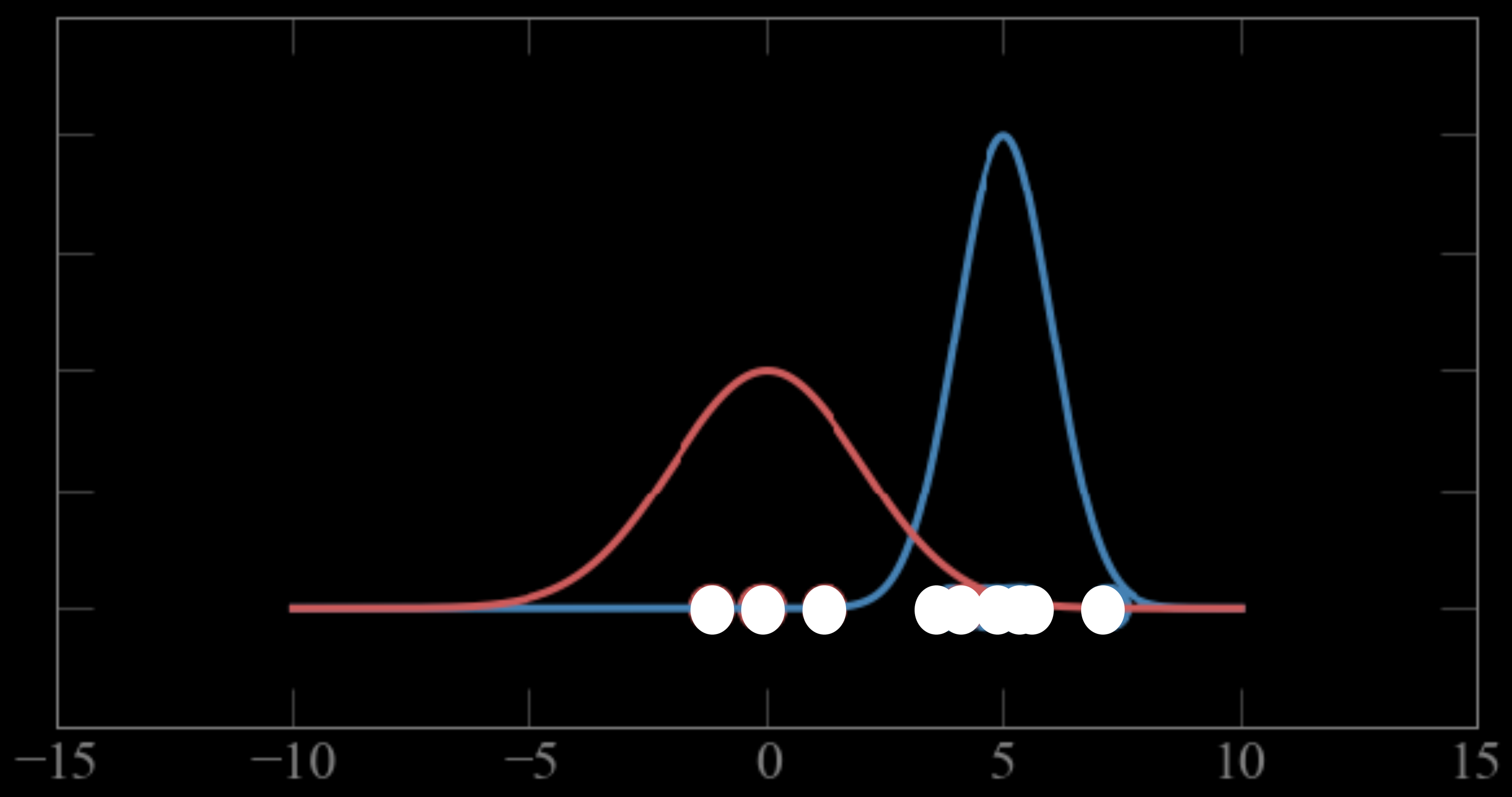
A probabilistic way to do soft clustering



I have a series of points and I know they come from
2 gaussians generative processes
if i know which point comes from which gaussian

Mixture models

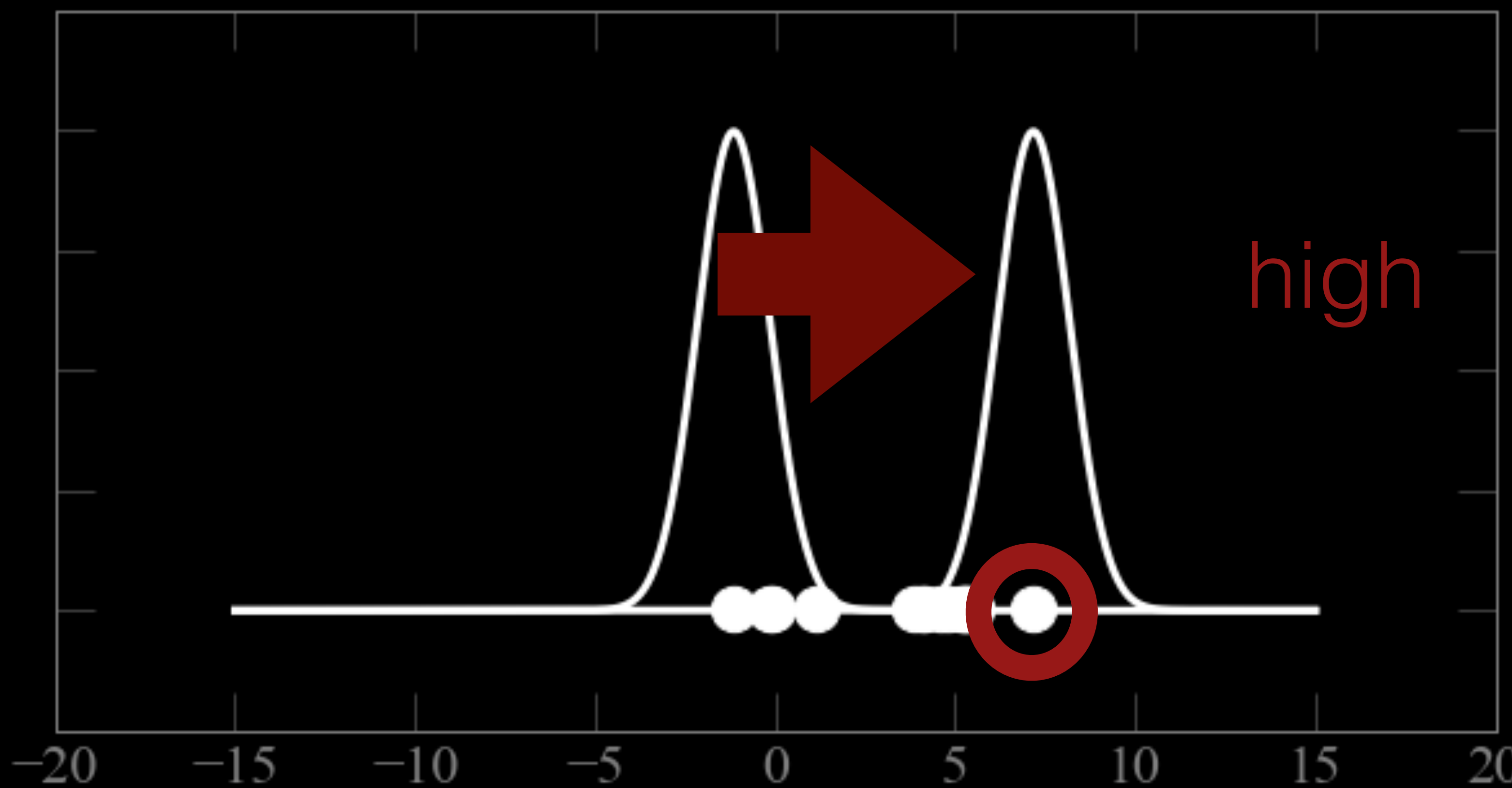
A probabilistic way to do soft clustering



if i know which the parameters *(μ,σ)* of the gaussians i can figure out which gaussian each point is most likely to come from

EM

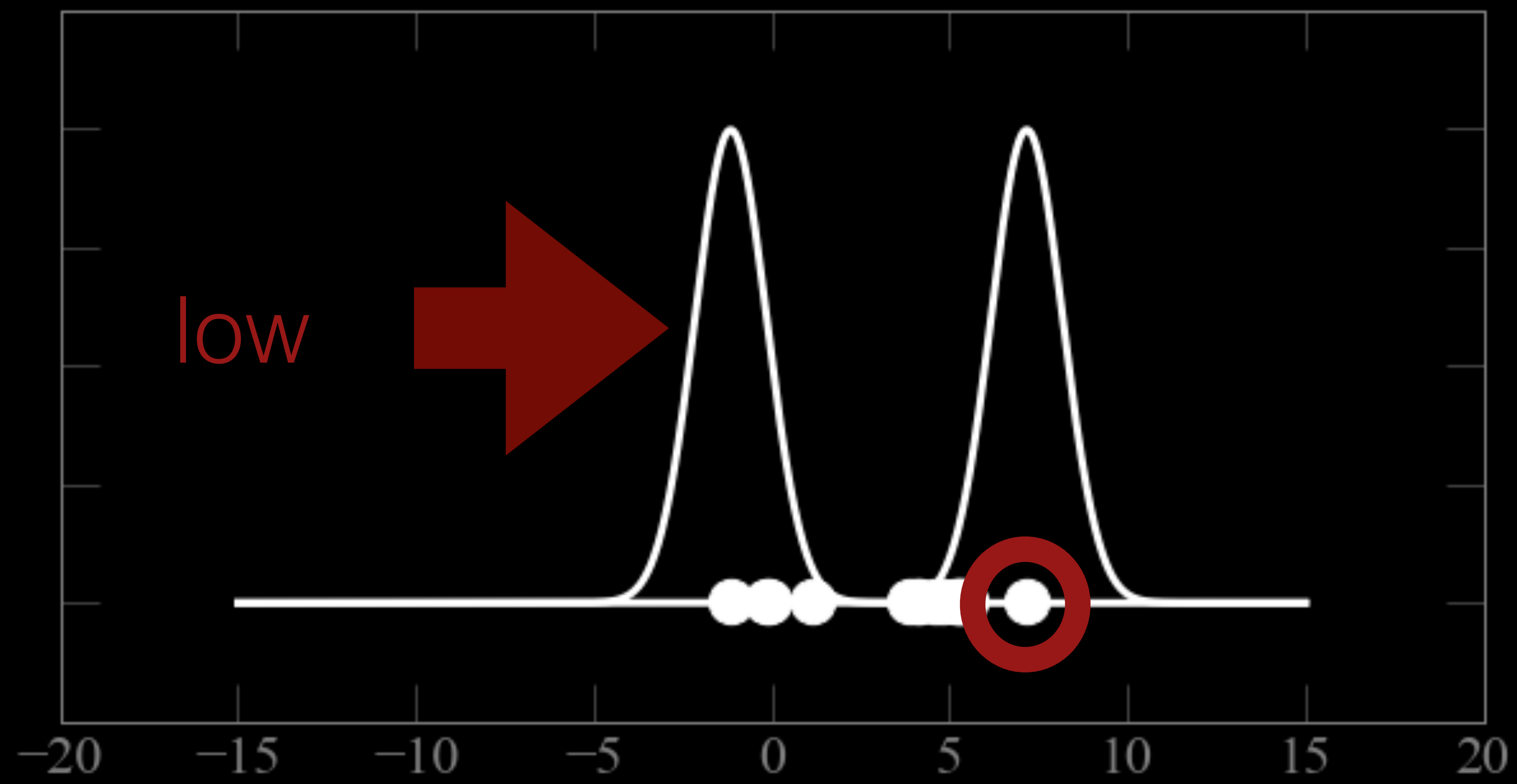
$$P(x_i | \mu_j, \sigma_j) = \frac{1}{\sqrt{2\pi\sigma_j^2}} exp\left(- \frac{x_i - \mu_j}{2\sigma_j^2} \right)$$



for every point calculate the probability it comes from either gaussian

EM

$$P(x_i \mid \mu_j, \sigma_j) = \frac{1}{\sqrt{2\pi\sigma_j^2}} exp\left(- \frac{x_i - \mu_j}{2\sigma_j^2} \right)$$

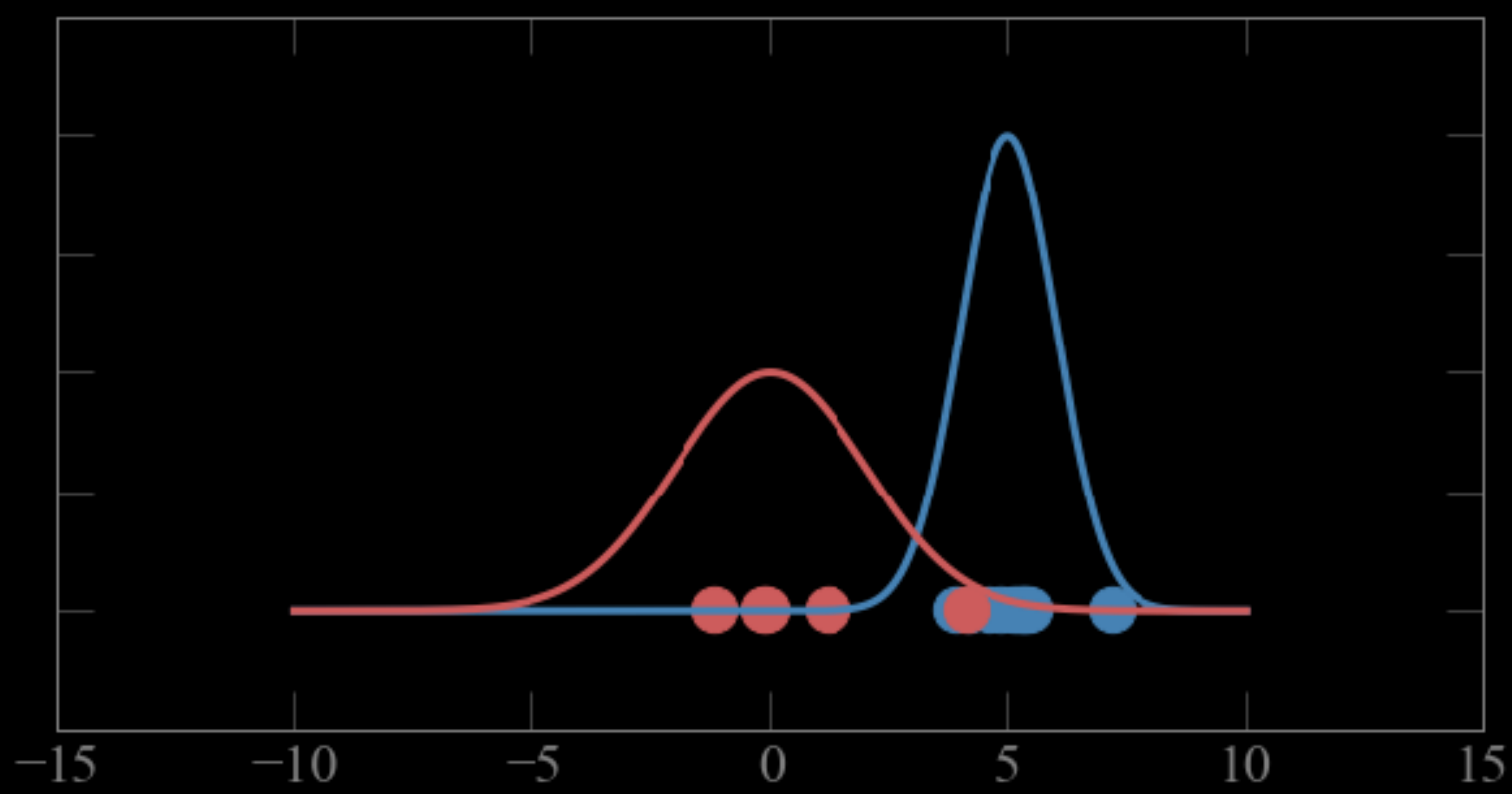


for every point calculate the probability it comes from either gaussian

Mixture models

A probabilistic way to do soft clustering

$$P(x_i) = \mathcal{N}(\mu,\lambda)$$

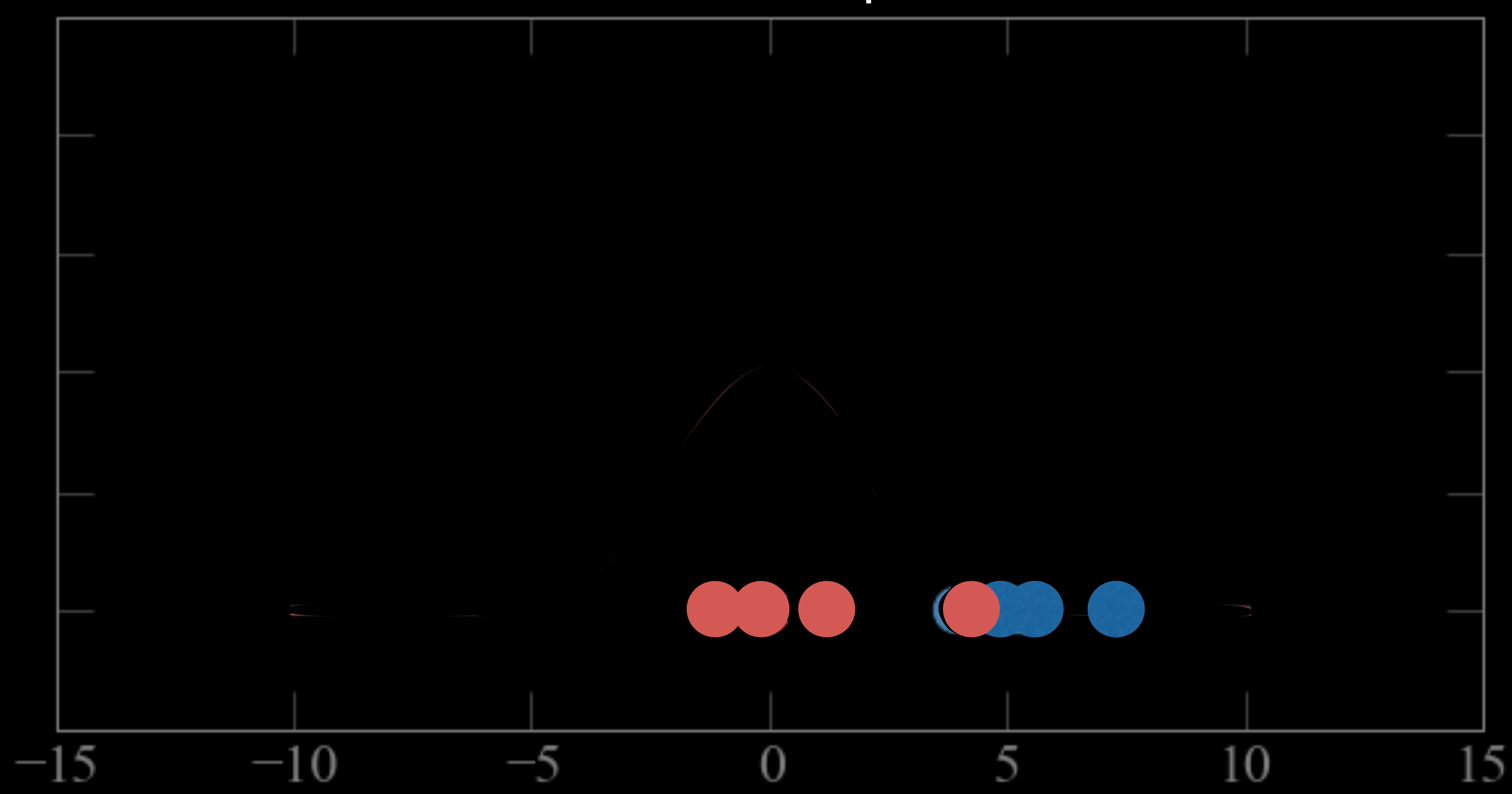


if i know which the parameters (μ,σ) of the gaussians i can figure out which gaussian each point is most likely to come from **(calculate probability)**

Mixture models

A probabilistic way to do soft clustering

$$P(\mu,\lambda \mid \vec{x})$$



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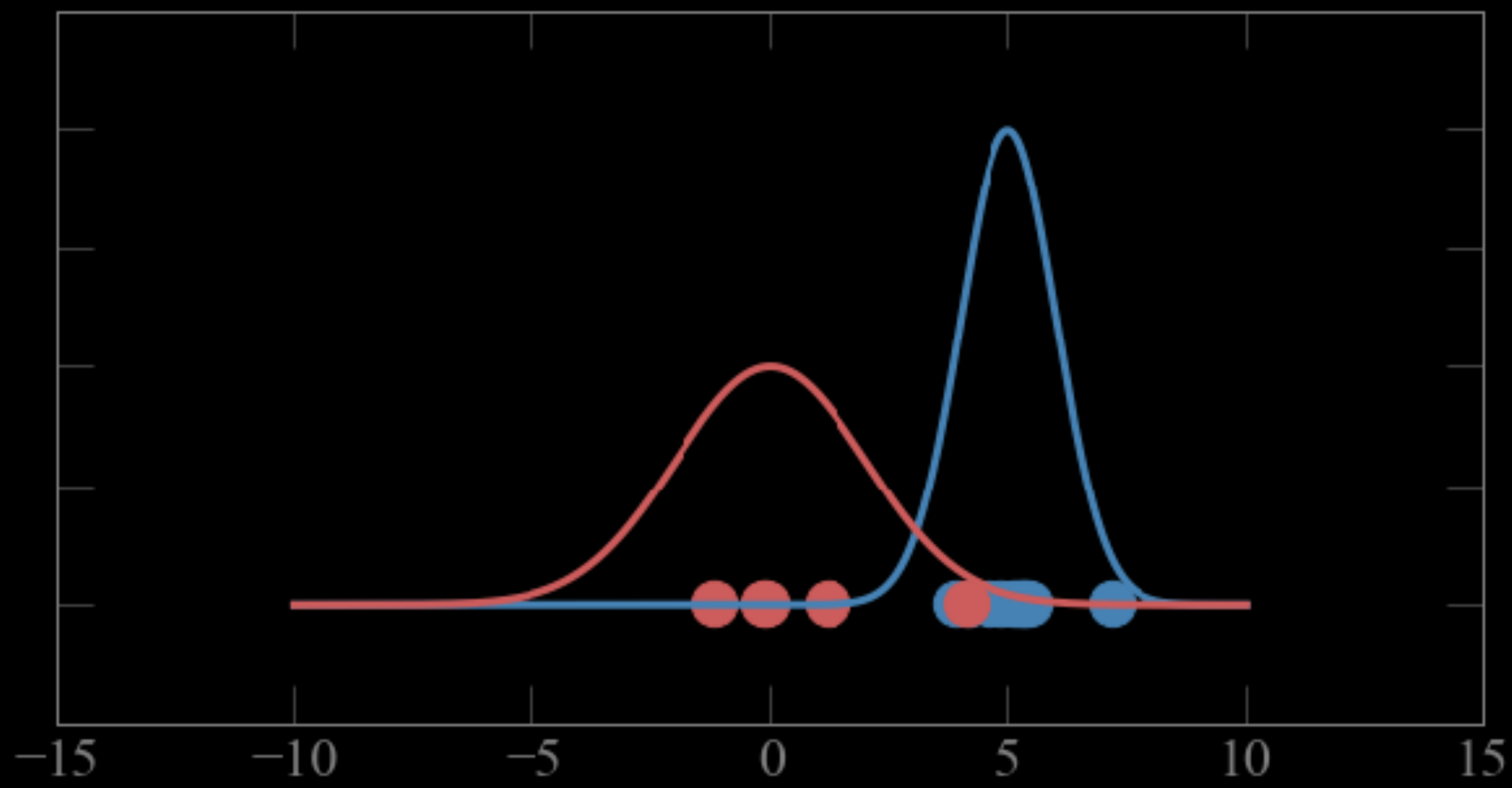
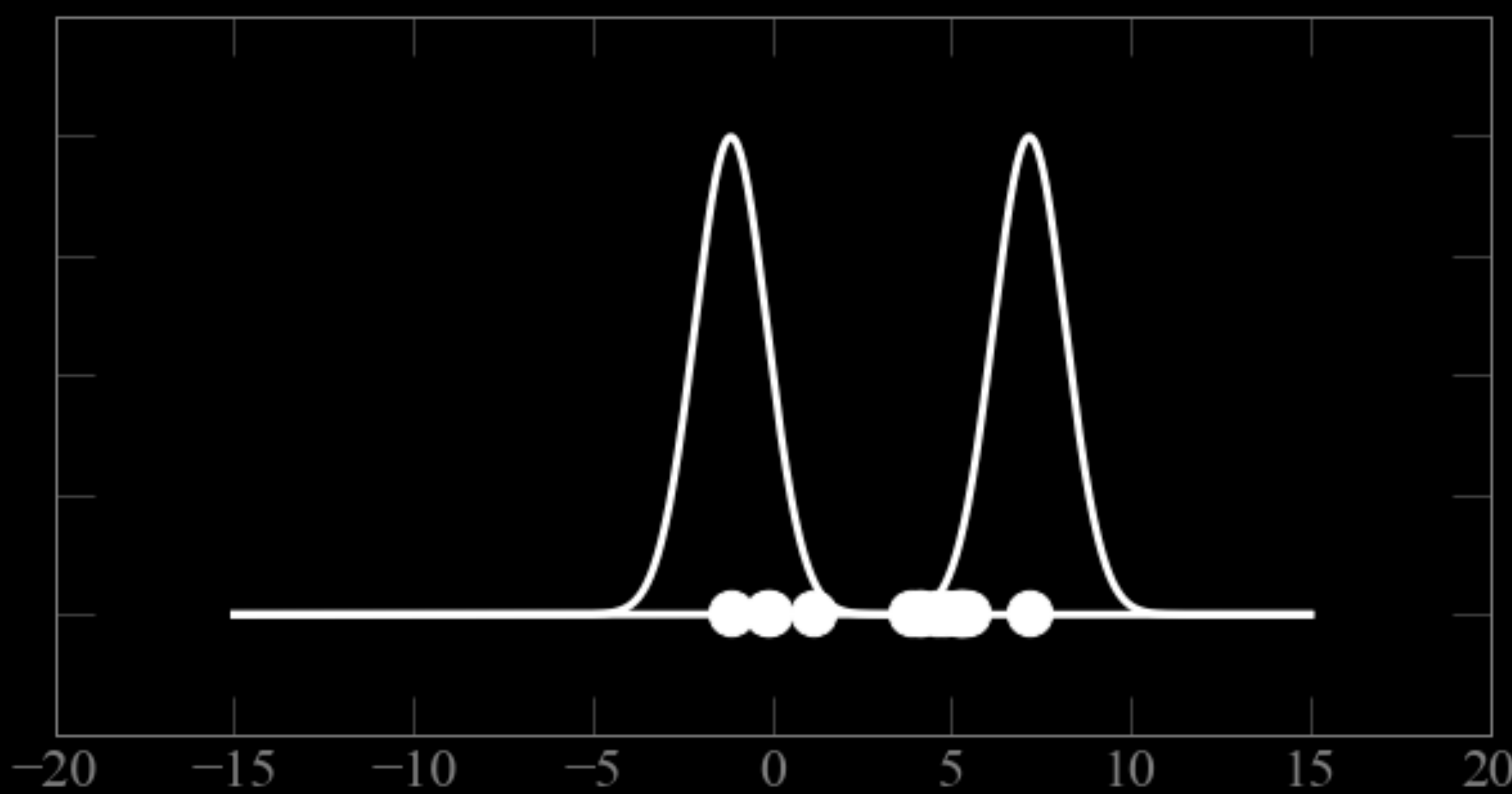


if i know which point comes from which gaussian
i can solve for the parameters of the gaussian
(e.g. maximizing likelihood)

EM

$$P(x_i \mid \mu_j, \sigma_j) = \frac{1}{\sqrt{2\pi\sigma_j^2}} exp\left(- \frac{x_i - \mu_j}{2\sigma_j^2} \right)$$



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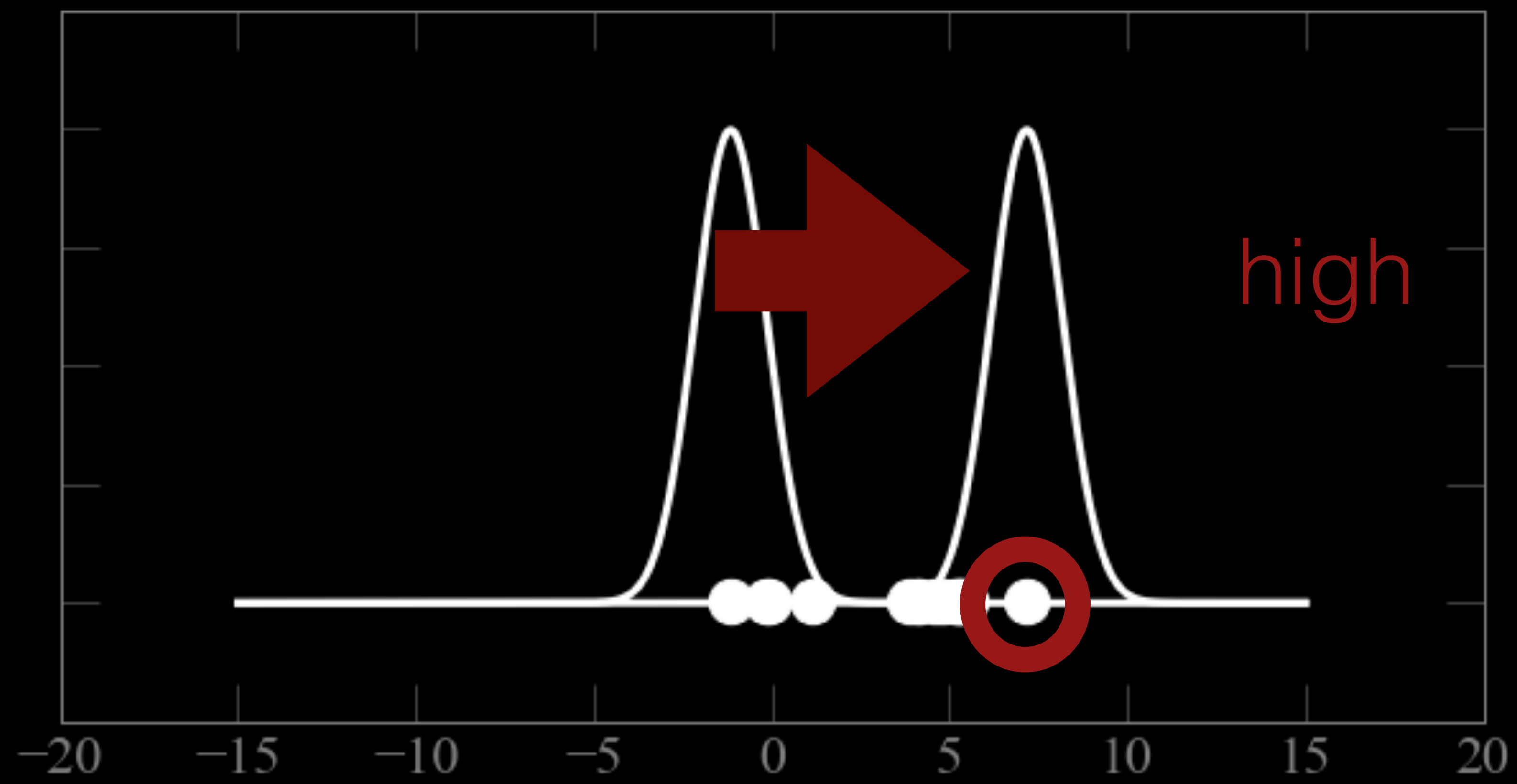

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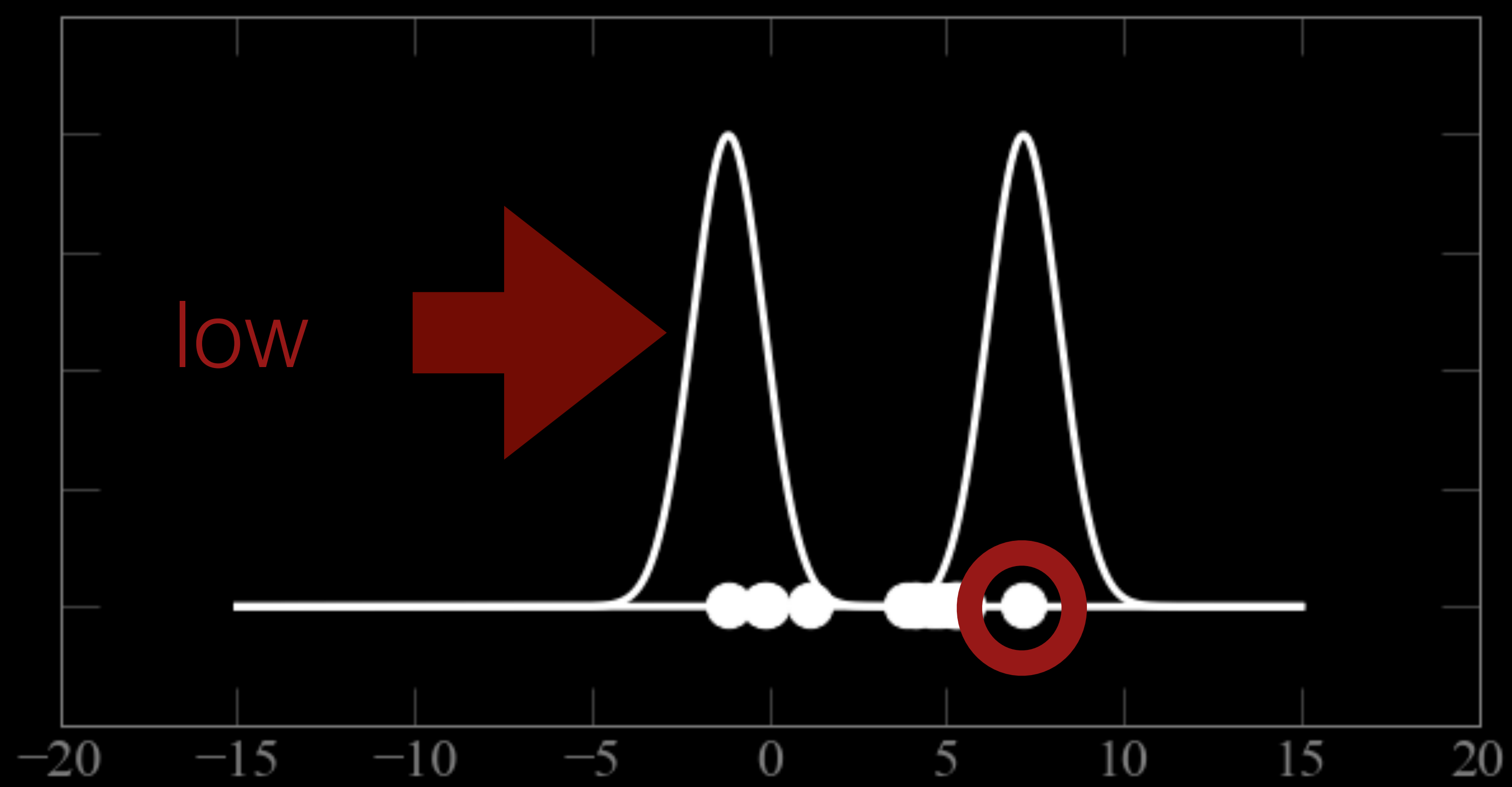

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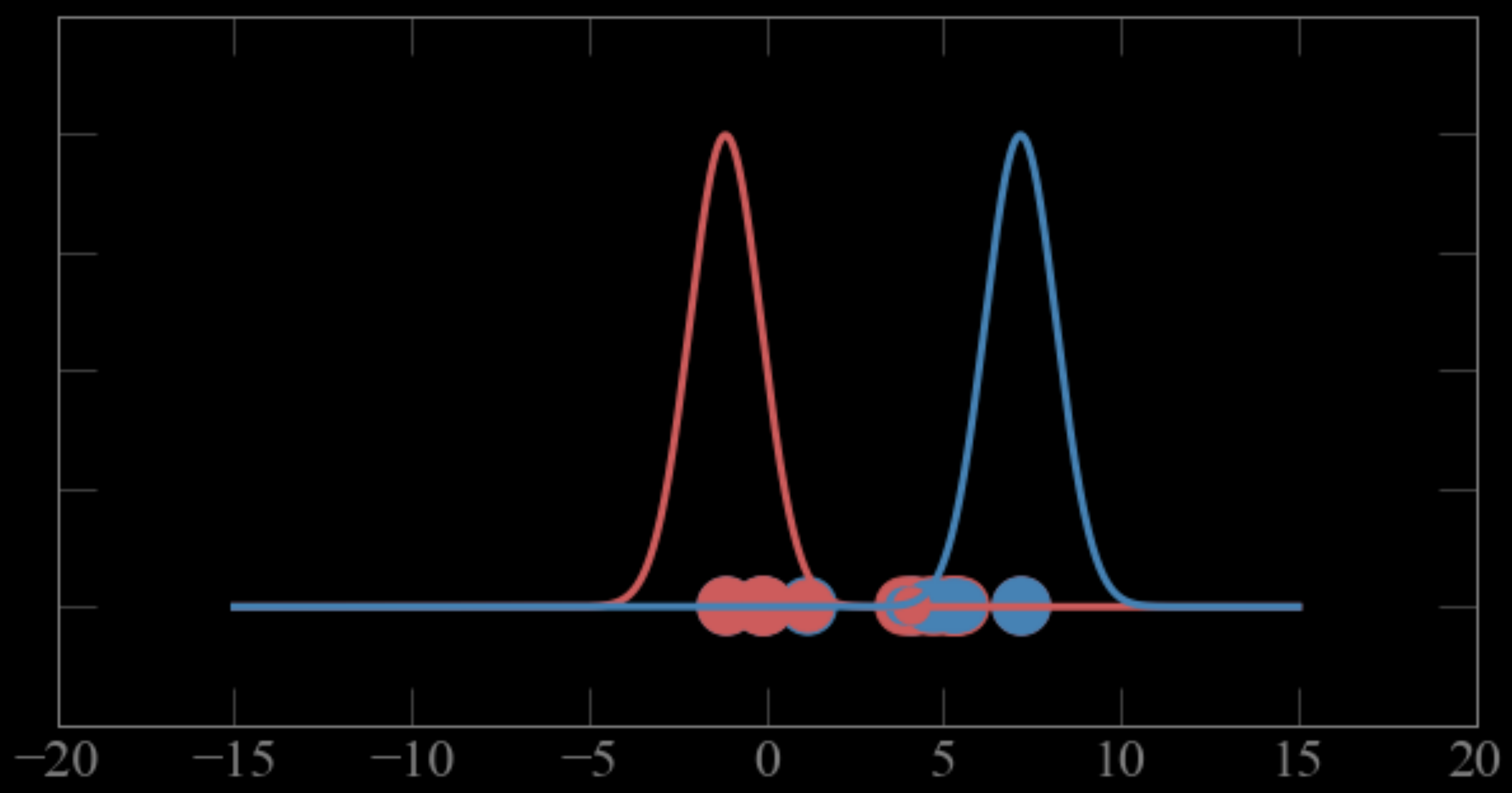
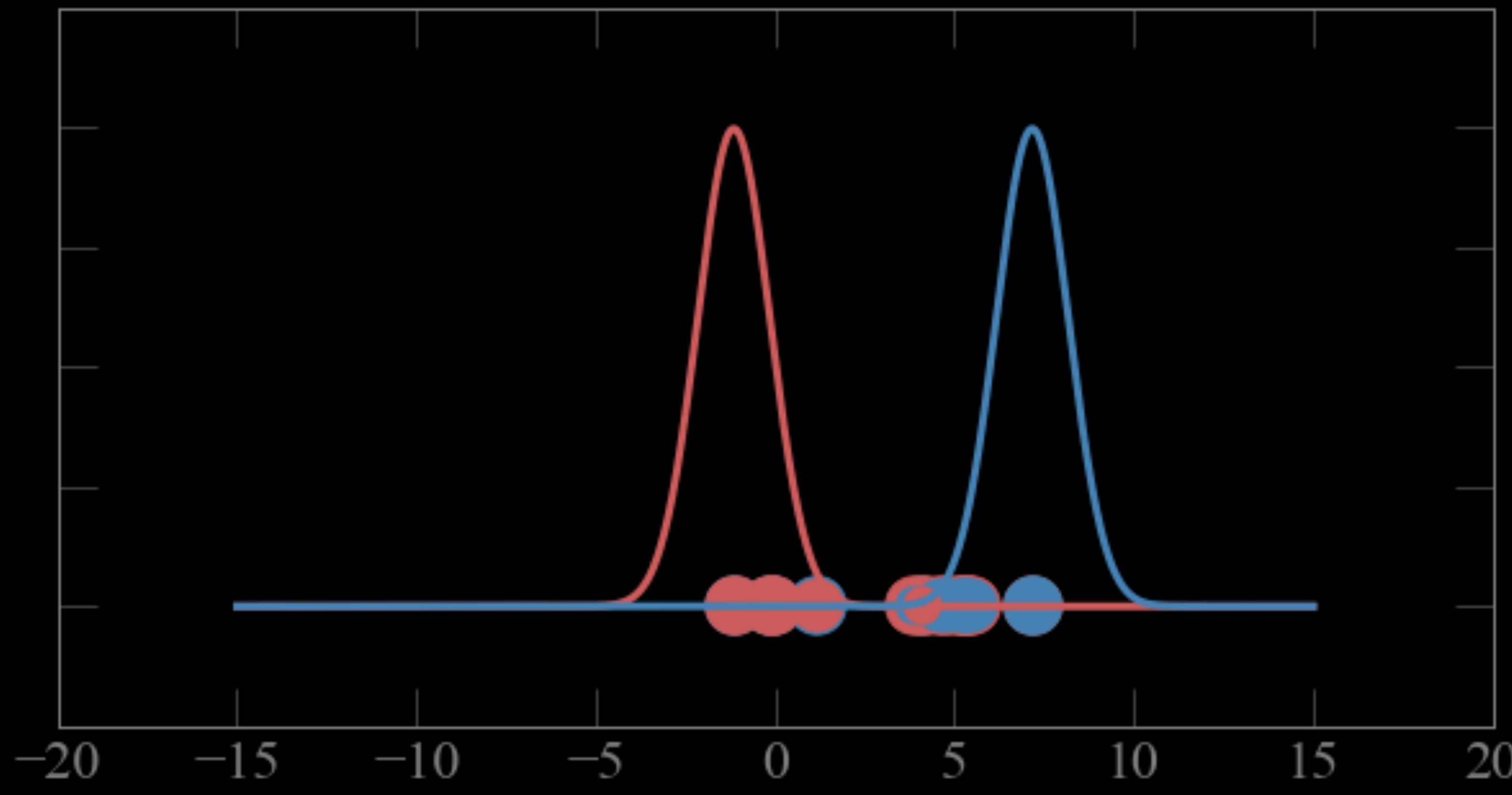


for every point calculate the probability it comes from either gaussian

EM

$$P(x_i|\mu_j,\sigma_j) = \frac{1}{\sqrt{2\pi\sigma_j^2}} exp\left(-\frac{x_i-\mu_j}{2\sigma_j^2}\right)$$

$$P(\mu_1,\sigma_1|x_i) = \frac{P(x_i|\mu_1,\sigma_1)P(\mu_1,\sigma_1)}{P(x_i|\mu_1,\sigma_1)P(\mu_1,\sigma_1)+P(x_i|\mu_2,\sigma_2)P(\mu_2,\sigma_2)}$$

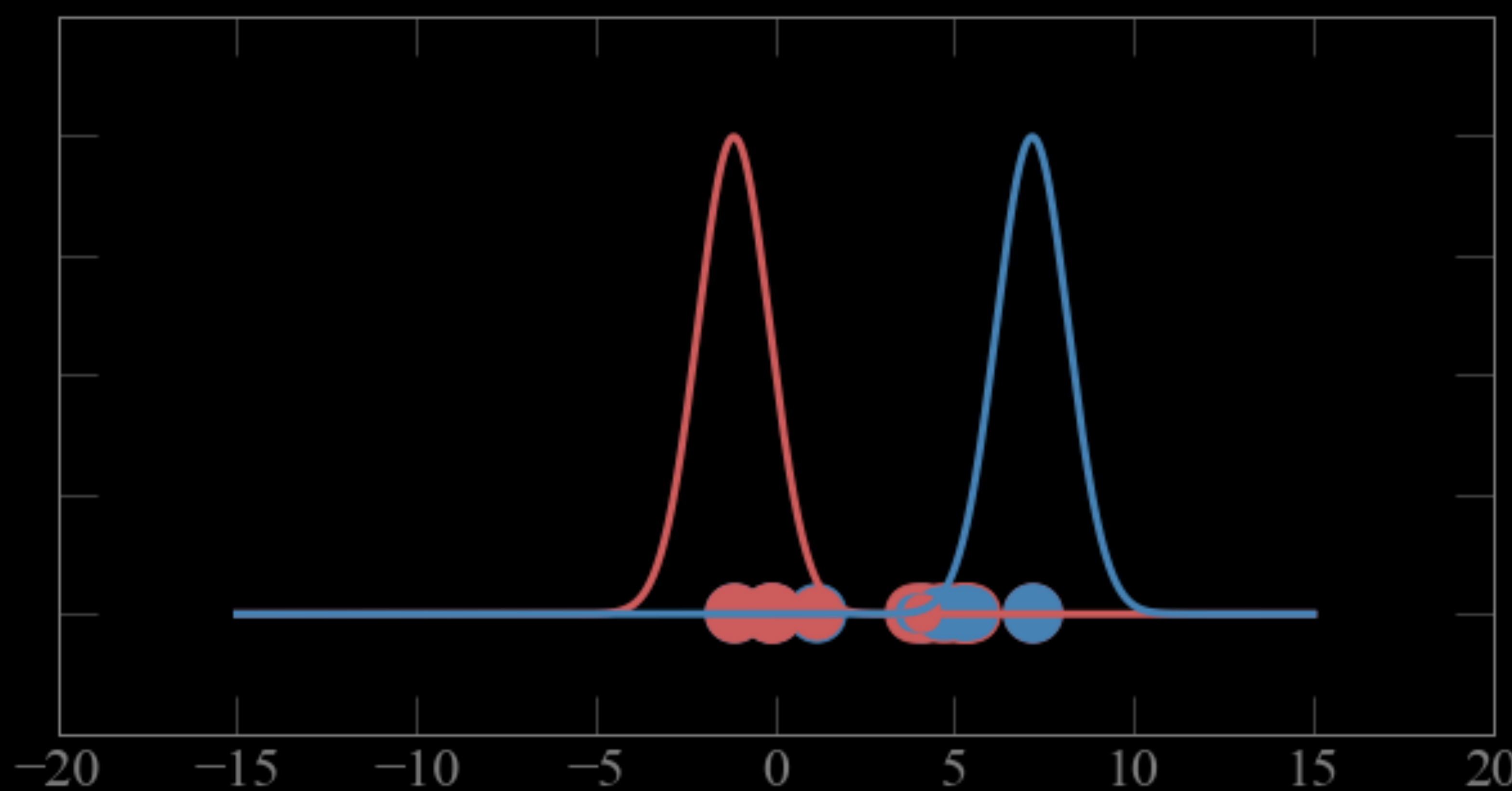


for every point calculate the probability it comes from either gaussian

EM

$$P(x_i|\mu_j,\sigma_j) = \frac{1}{\sqrt{2\pi\sigma_j^2}} exp\left(-\frac{x_i-\mu_j}{2\sigma_j^2}\right)$$

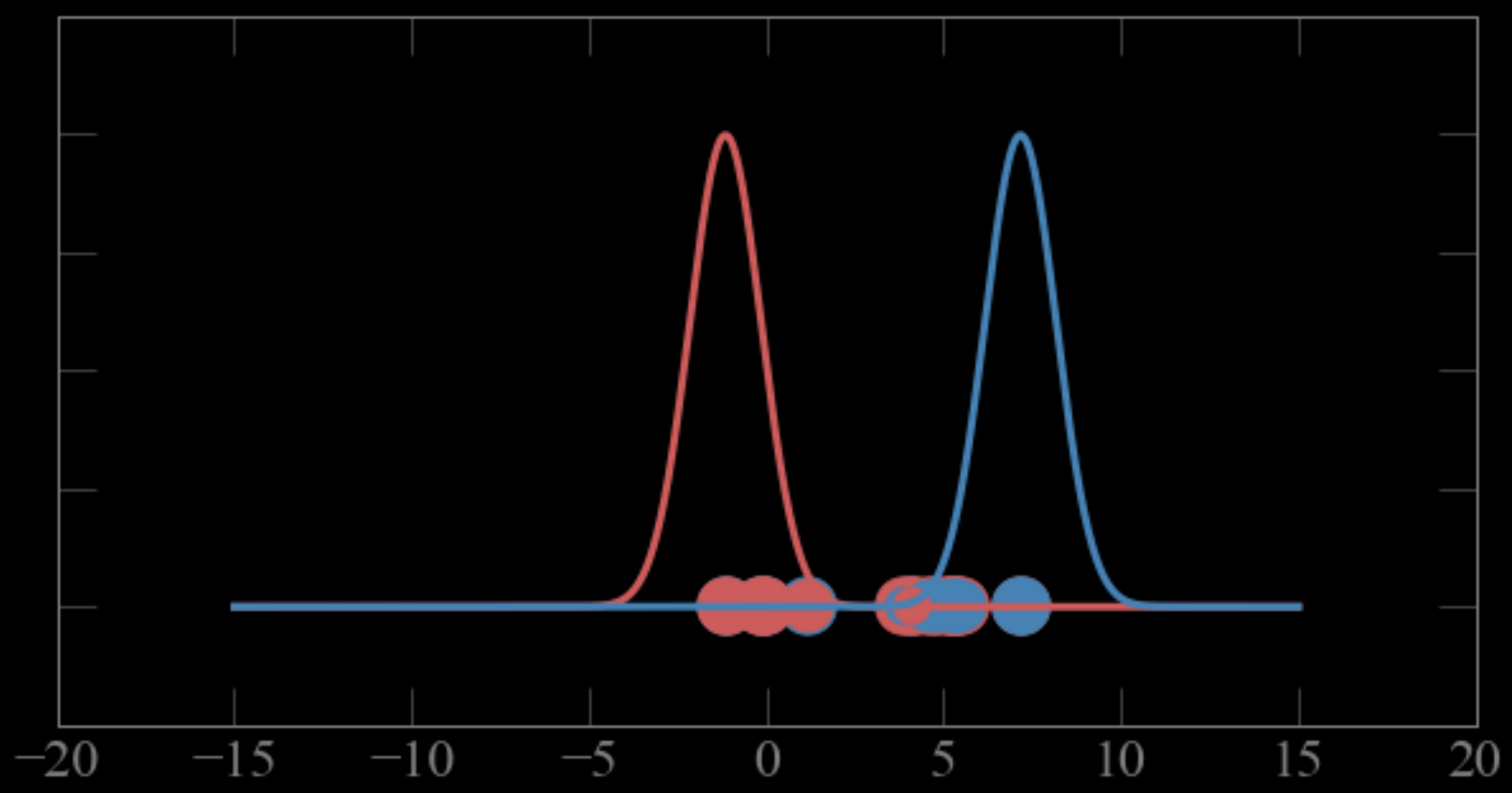
$$P(g_1|x_i) = \frac{P(x_i|g_1)P(g_1)}{P(x_i|g_1)P(g_1)+P(x_i|g_2)P(g_2)}$$



for every point calculate the probability it comes from either gaussian

Bayes Theorem!

$$P(x|\alpha)P(\alpha) \;=\; P(x|\beta)P(\beta)$$



for every point calculate the probability it comes from either gaussian

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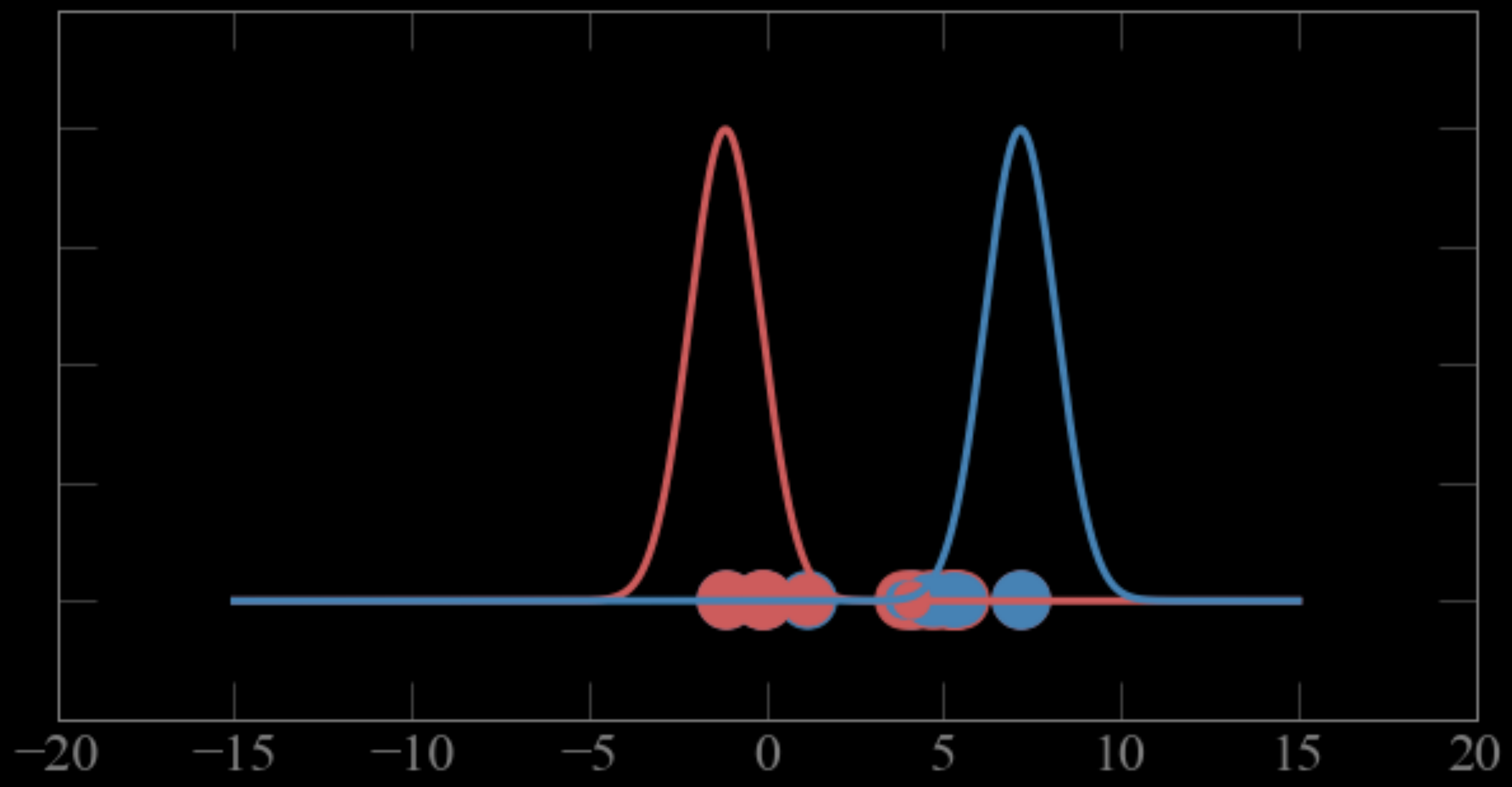
$$P(x_i | \mu_j, \sigma_j) = \frac{1}{\sqrt{2\pi\sigma_j^2}} exp\left(- \frac{x_i - \mu_j}{2\sigma_j^2} \right)$$

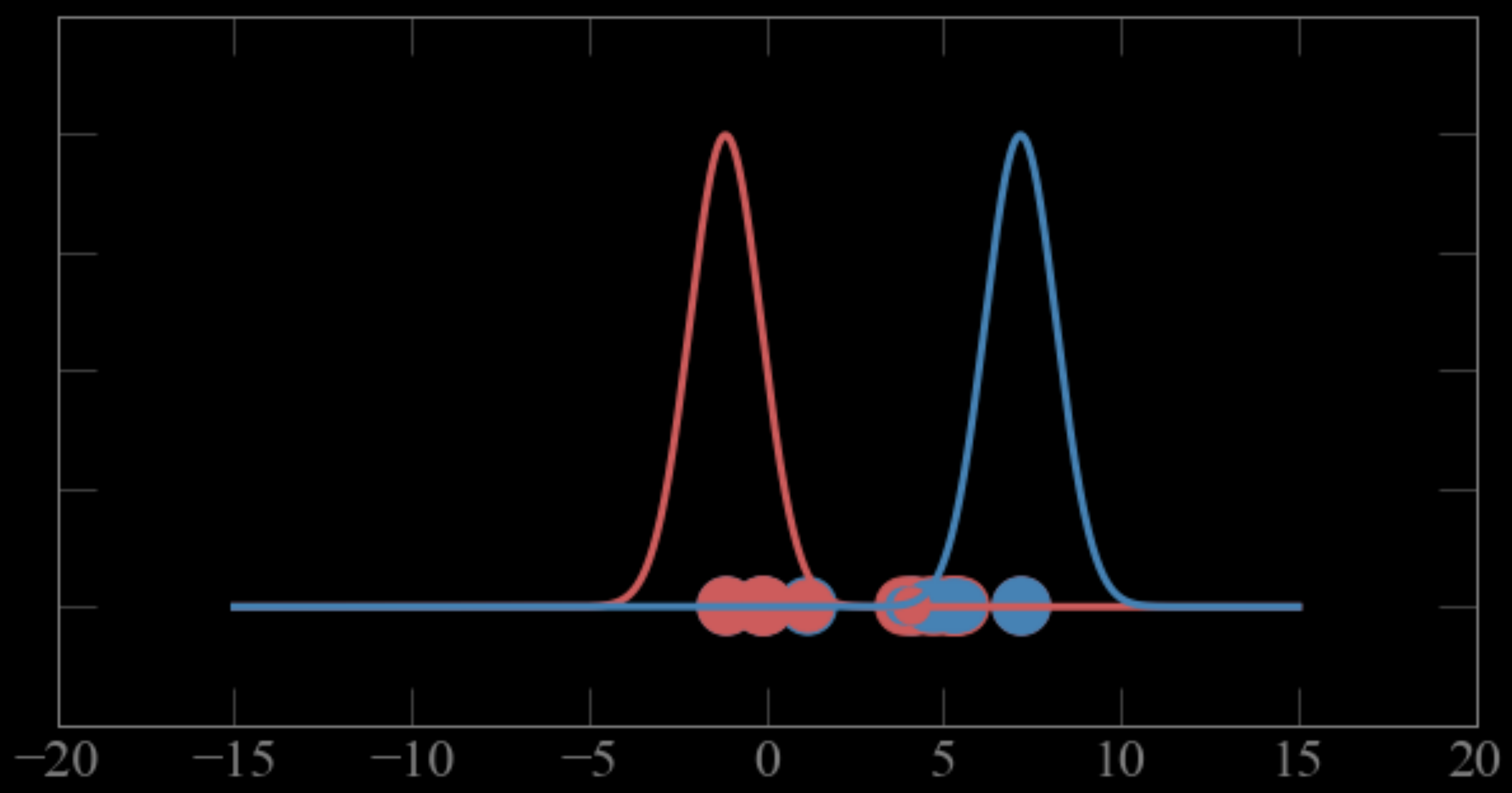
p_ji = $P(g_1 | x_i) = \dfrac{P(x_i | g_1) P(g_1)}{P(x_i | g_1) P(g_1) + P(x_i | g_2) P(g_2)}$



calculate the weighted mean of the cluster, weighted by the p_ji

EM

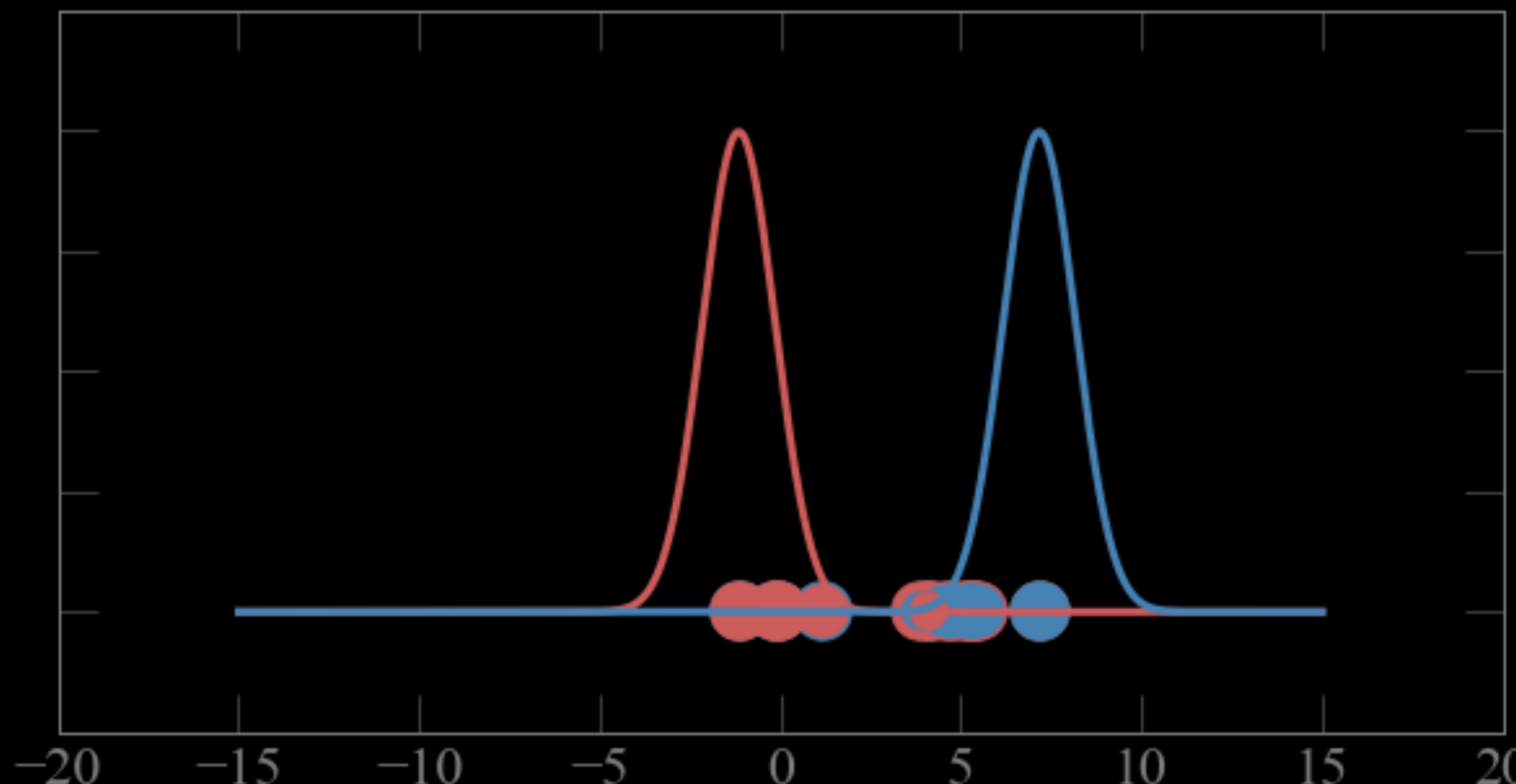
$$\mu_i = \frac{\sum_j P(g_i|x_j)x_j}{\sum_j P(g_i|x_j)}$$



calculate the weighted mean of the cluster, weighted by the p_ji

EM

$$\mu_i = \frac{\sum_j P(g_i|x_j)x_j}{\sum_j P(g_i|x_j)} \qquad \sigma\_j = \frac{\sum_i P(g_j|x_i)(x_i - \mu_j)^2}{\sum_i P(g_j|x_i)}$$



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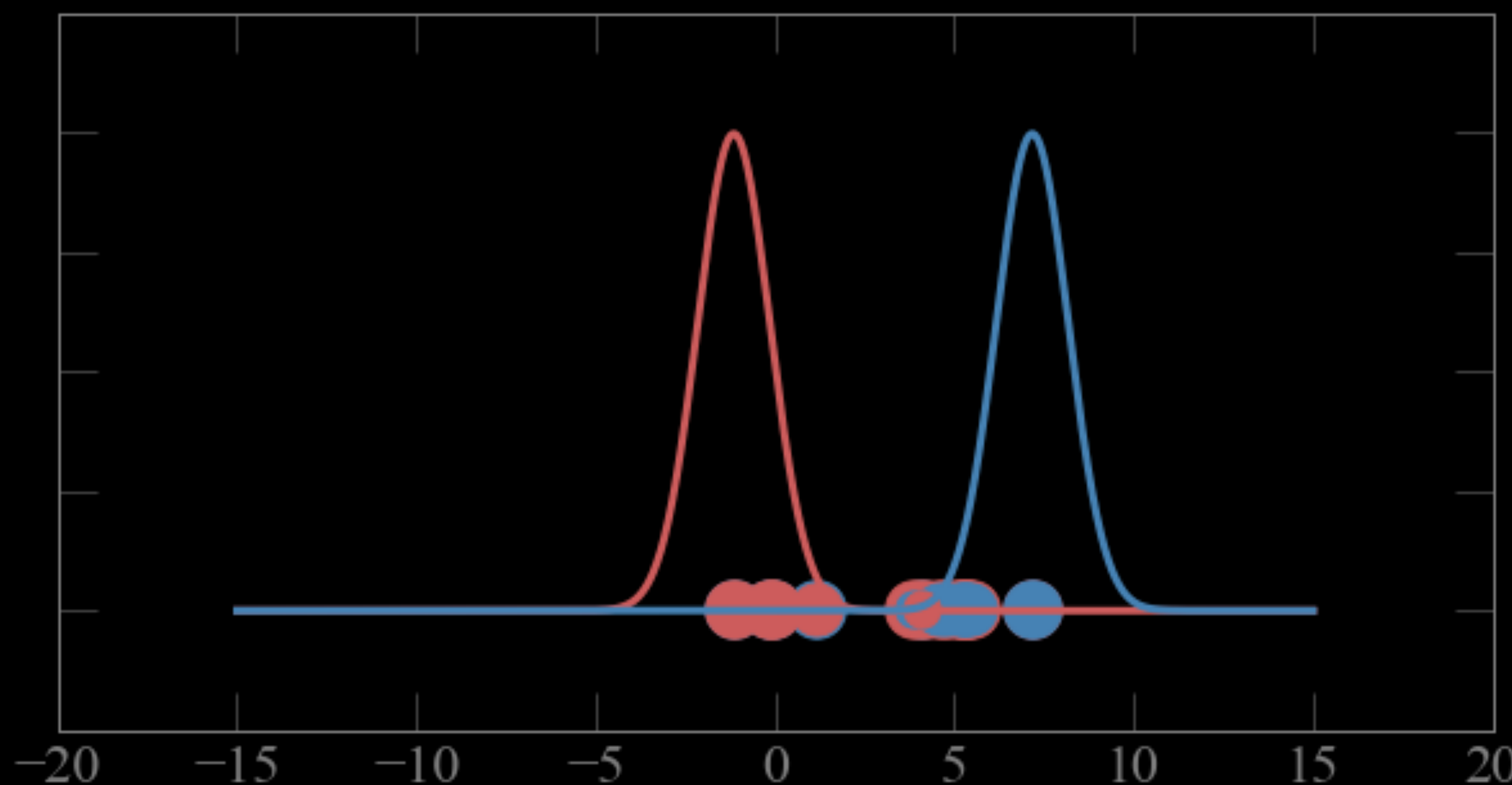
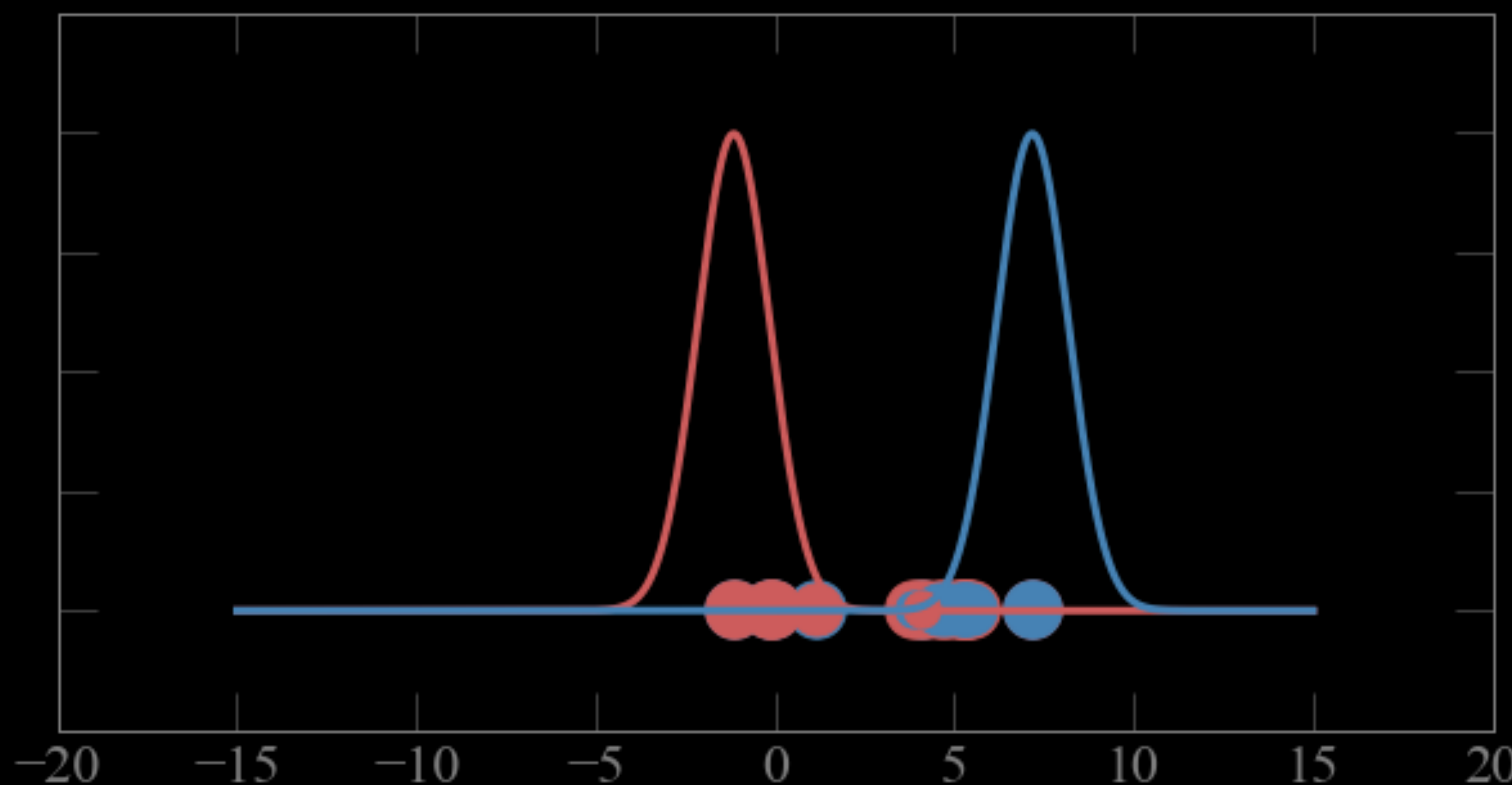


$$P(g_1|x_i) = \frac{P(x_i|g_1)P(g_1)}{P(x_i|g_1)P(g_1)+P(x_i|g_2)P(g_2)}$$

calculate the new p_ji … rinse, repeat

EM

$$\mu_i = \frac{\sum_j P(g_i|x_j)x_j}{\sum_j P(g_i|x_j)} \qquad \sigma\_j = \frac{\sum_i P(g_j|x_i)(x_i - \mu_j)^2}{\sum_i P(g_j|x_i)}$$



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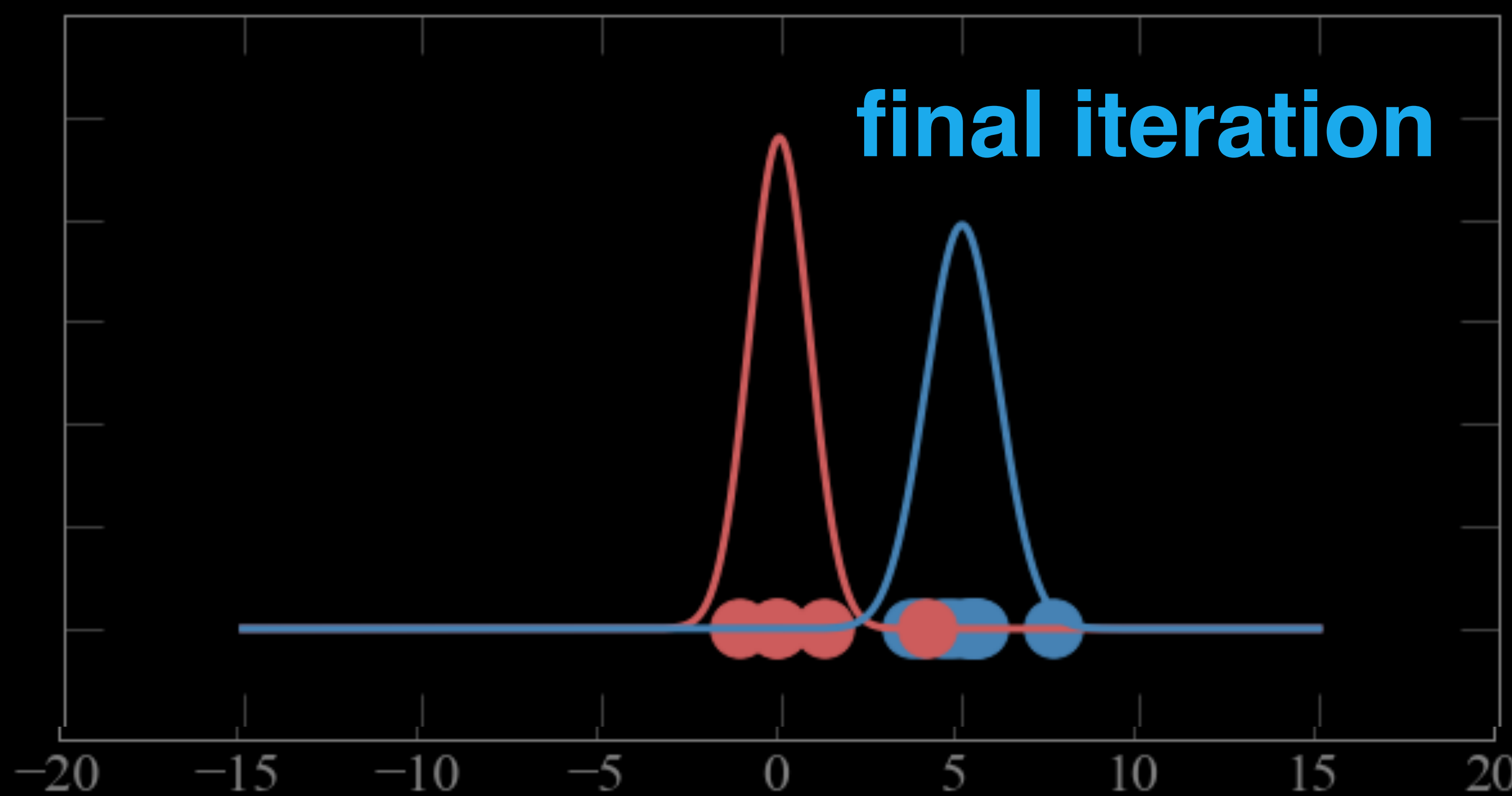

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… till it converges

Expectation Maximization:

1. **Choose N "centers" guesses:** like in K-means

2. **Calculate the probability of each distribution given the point (Expectation step)**

3. **Calculate the new centers and variances as weighted averages of the datapoints, weighted by the probabilities**

4. **Iterate 2&3 till convergence**: when gaussian parameters no longer change

Expectation Maximization:

Order: #clusters #dimensions #iterations #datapoints #parameter ***O(KdNp)***

based on Bayes theorem

Its non-deterministic: the result depends on the (random) starting point

It only works where a probability distribution for the data points can be defines (or equivalently a likelihood)

Must declare the number of clusters and the shape of the pdf upfront

Clustering methods

- **Partitioning**

  Hard clustering

  K-means (McQueen '67)
  K-medoids (Kaufman & Rausseeuw '87)

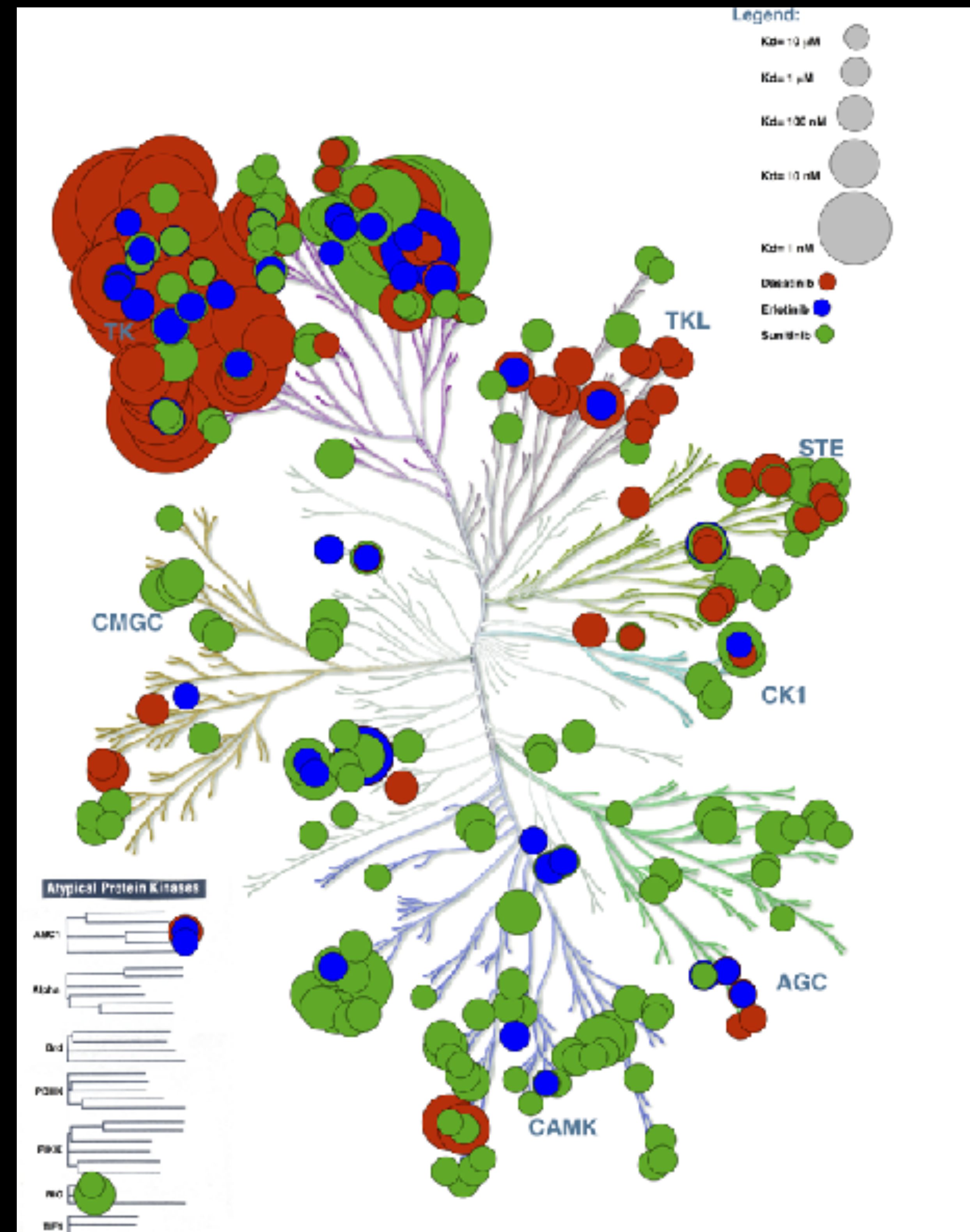
  Soft Clustering
  Expectation Maximization (Dempster,Laird,Rubin '77)

- **Hirarchical**
  agglomerative

  devisive

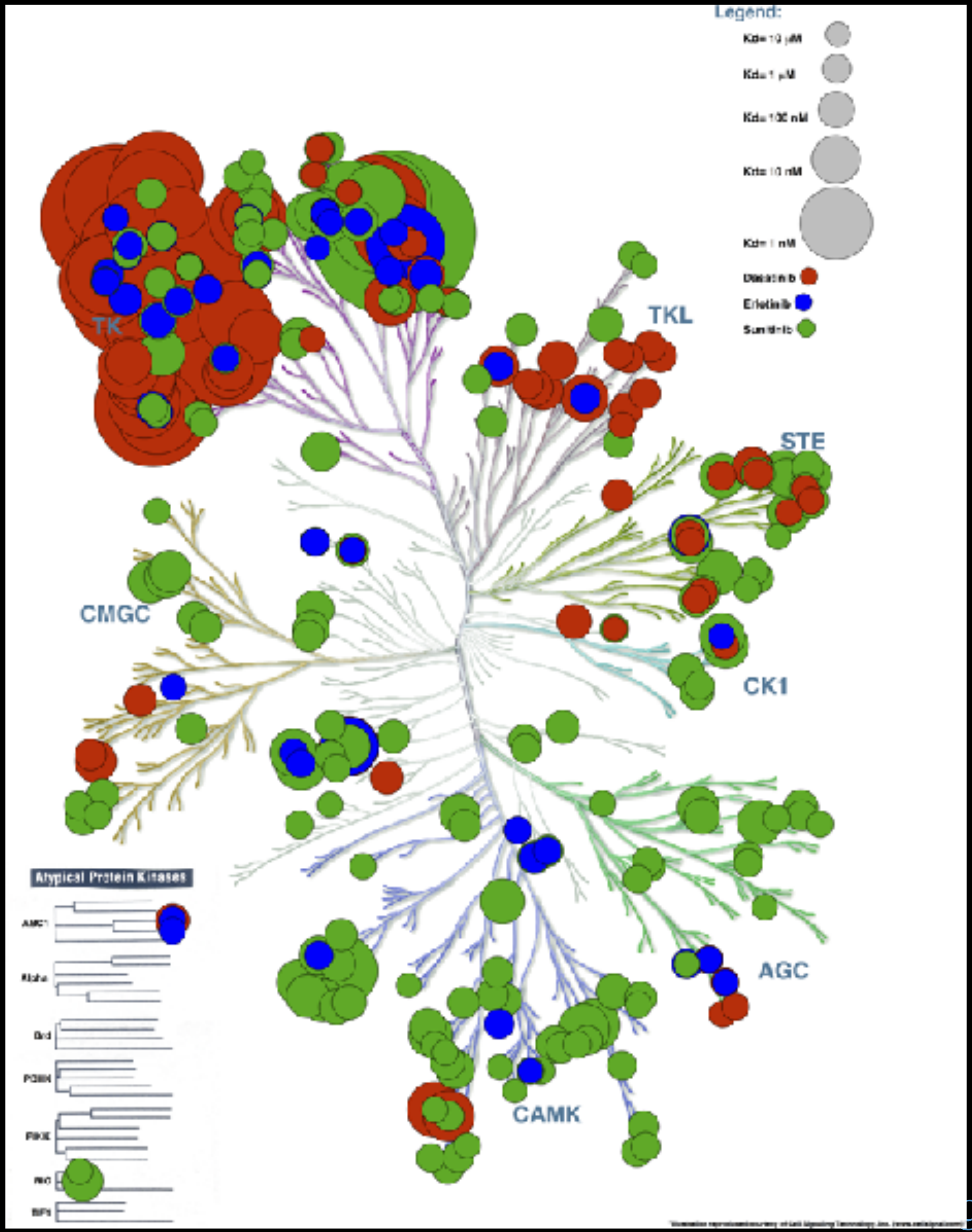
- **also:**
  - **Density based**
  - **Grid based**
  - **Model based**

hierarchical clustering



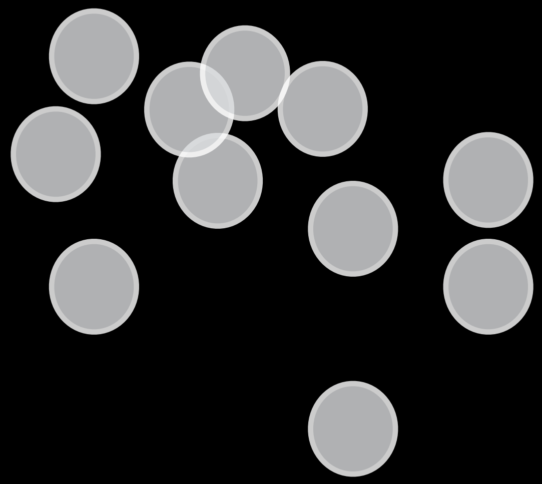
hierarchical clustering

removes the issue of deciding K (number of clusters)



hierarchical clustering

devisive *(top-down)*: e.g. hierarchical k-mean



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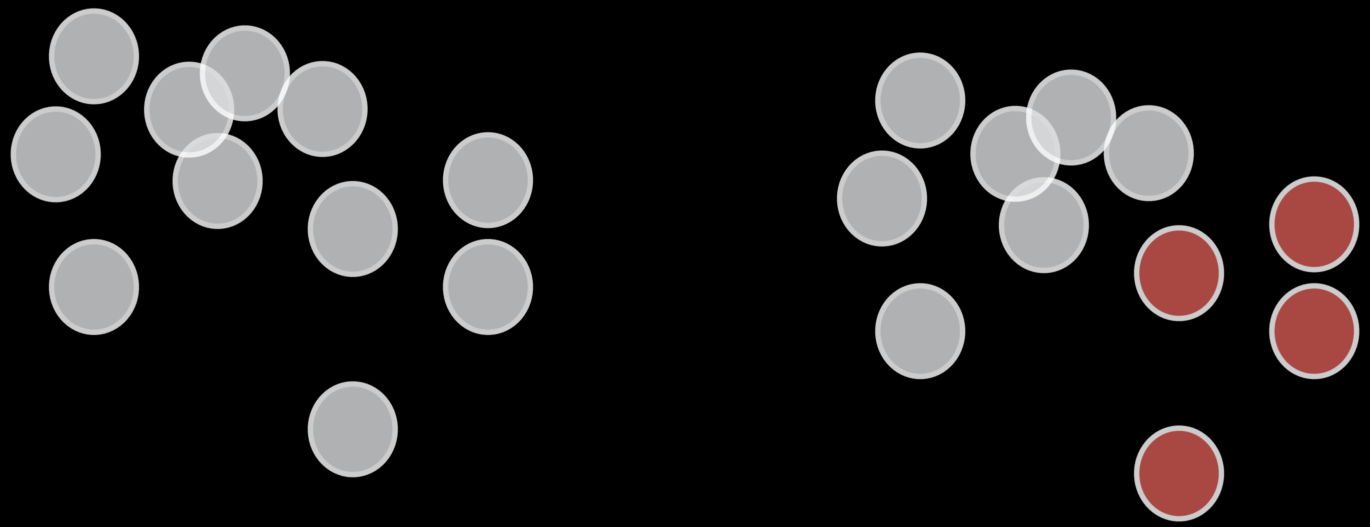

hierarchical clustering

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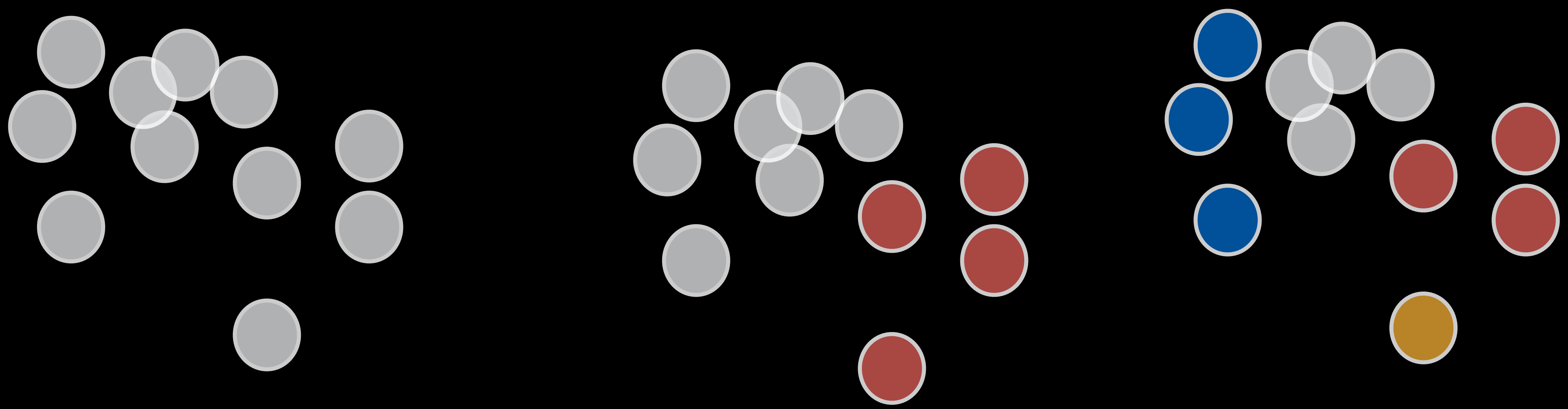

hierarchical clustering

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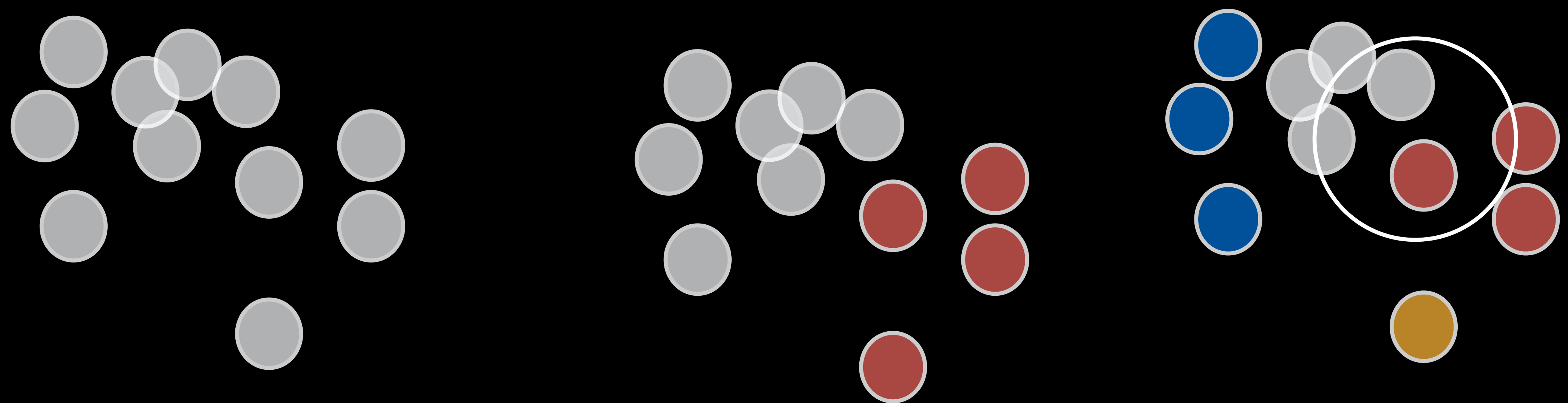
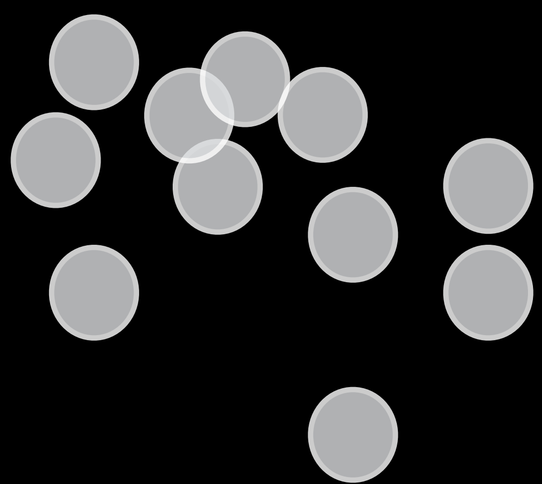


it is non-deterministic

it is *greedy* - just as k-means two nearby points may end up in separate clusters

hierarchical clustering

devisive *(top-down)*: e.g. hierarchical k-mean



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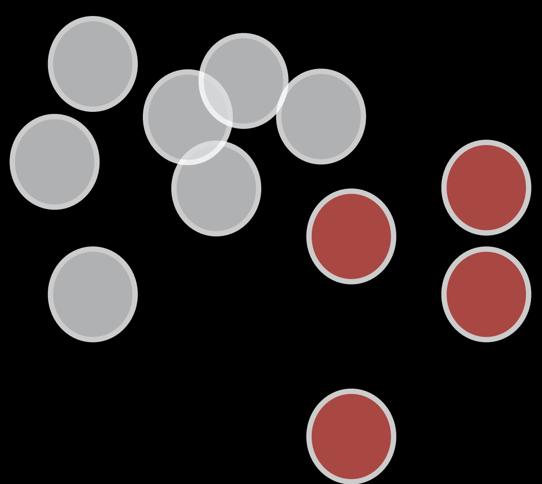

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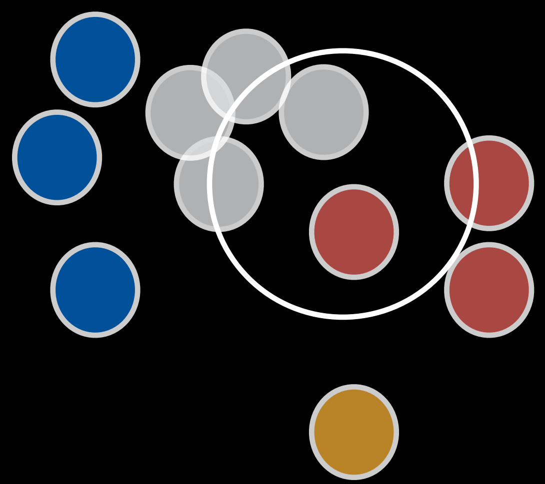
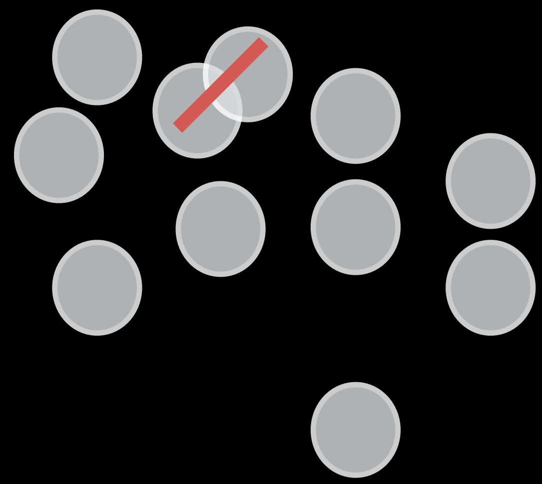


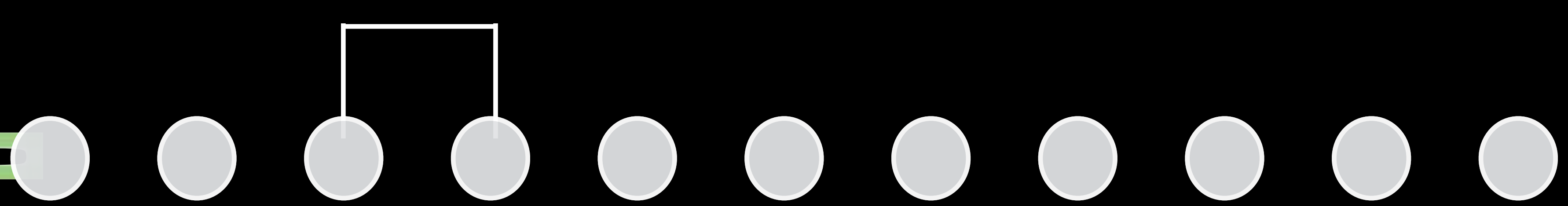
it is simple and fast: complexity

$\mathbf{O(NdK \log_K N)}$

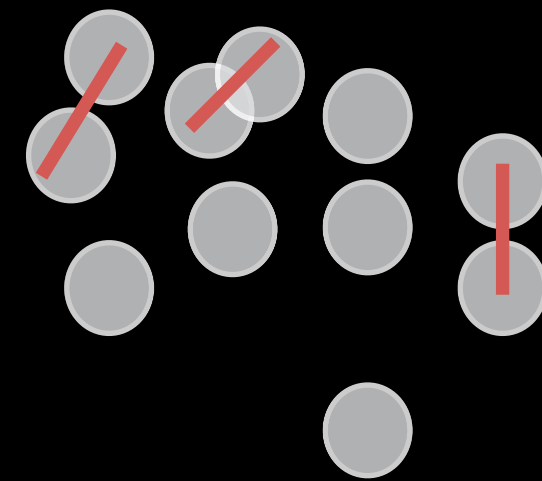
hierarchical clustering



agglomerative
bottom-up



hierarchical clustering



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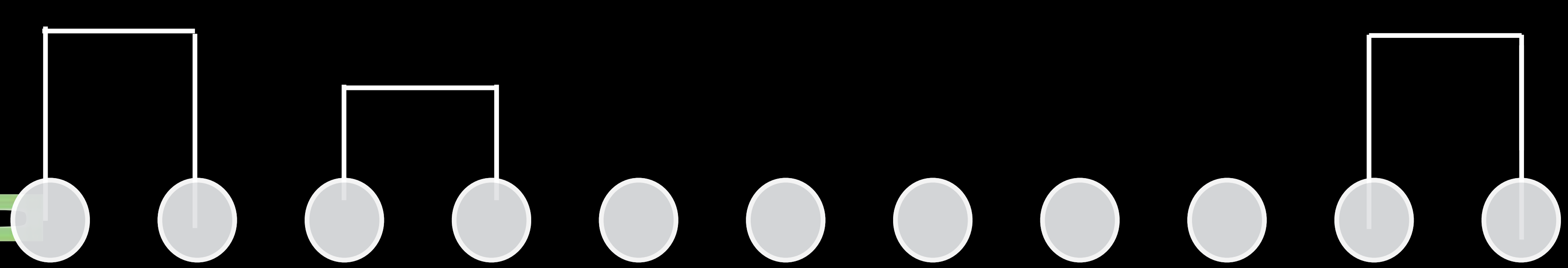
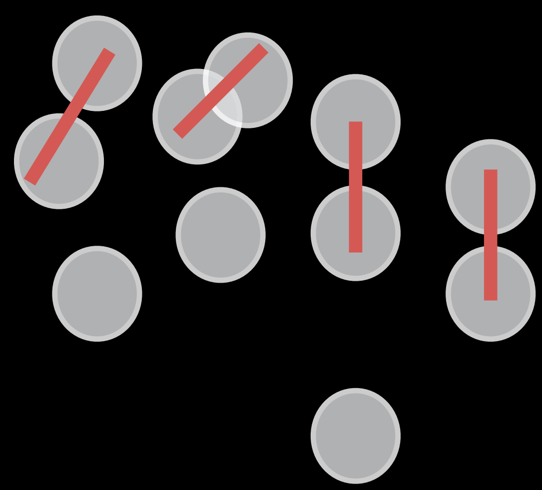
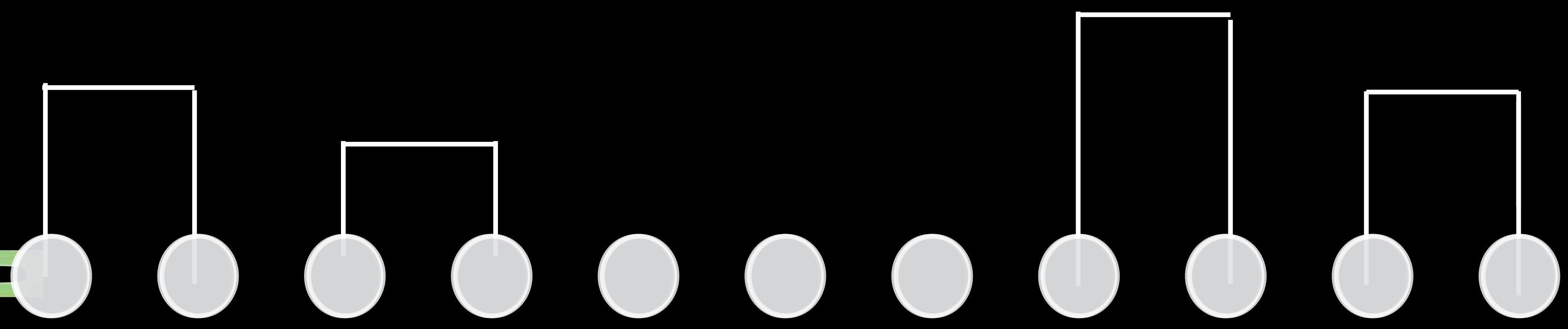


hierarchical clustering

agglomerative
bottom-up





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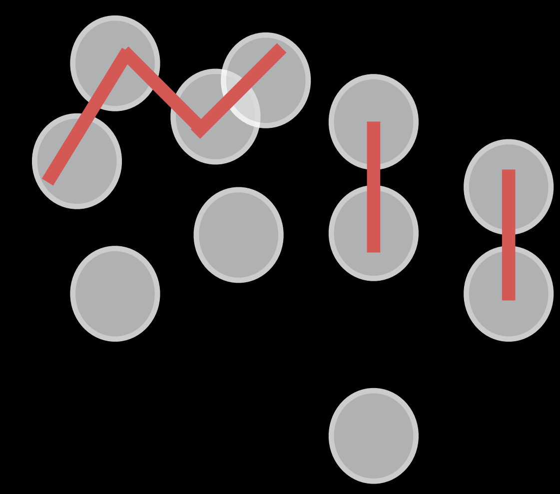

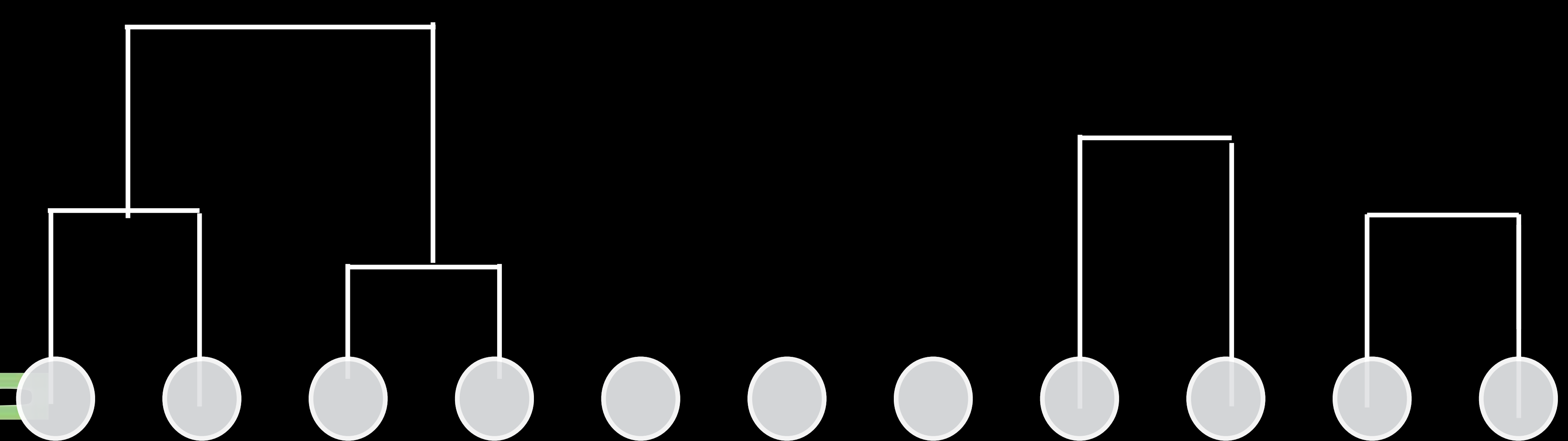

hierarchical clustering

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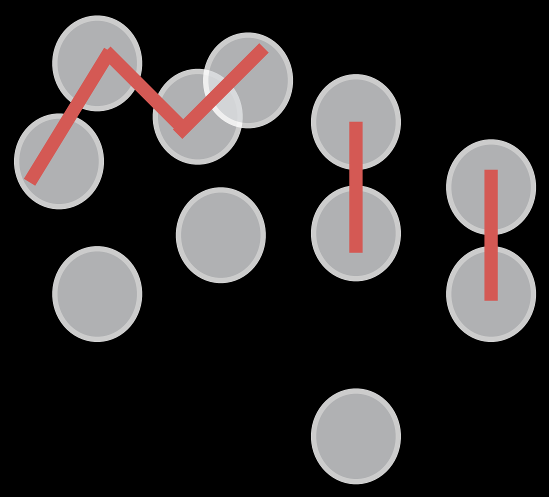
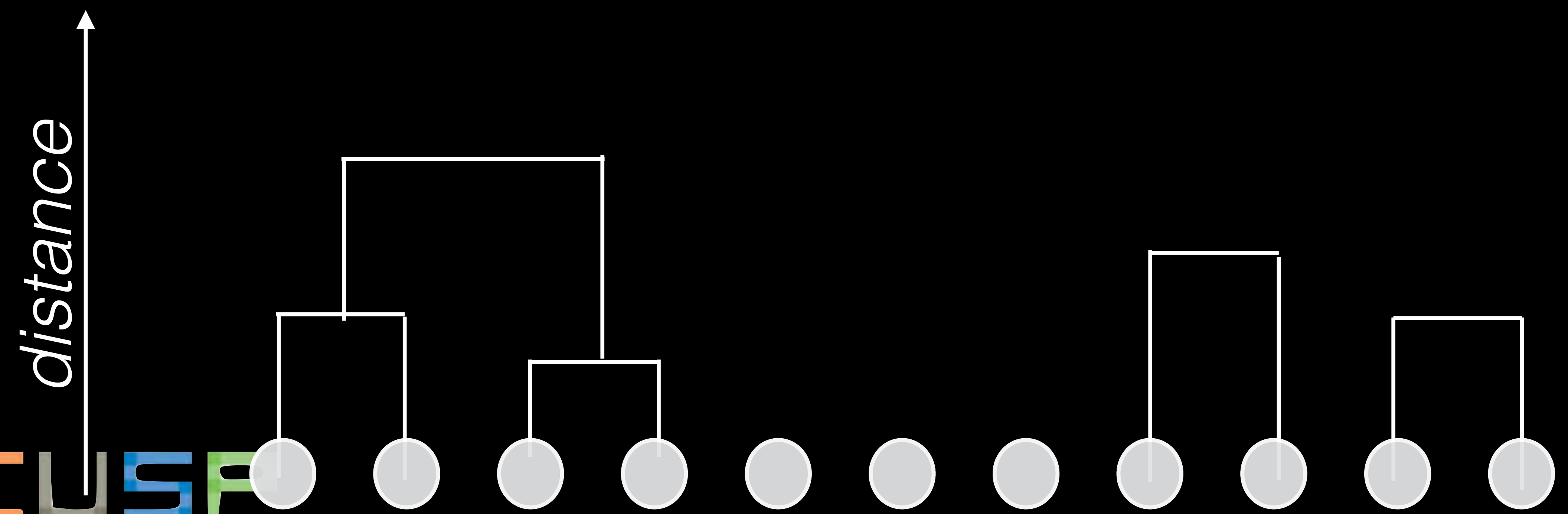
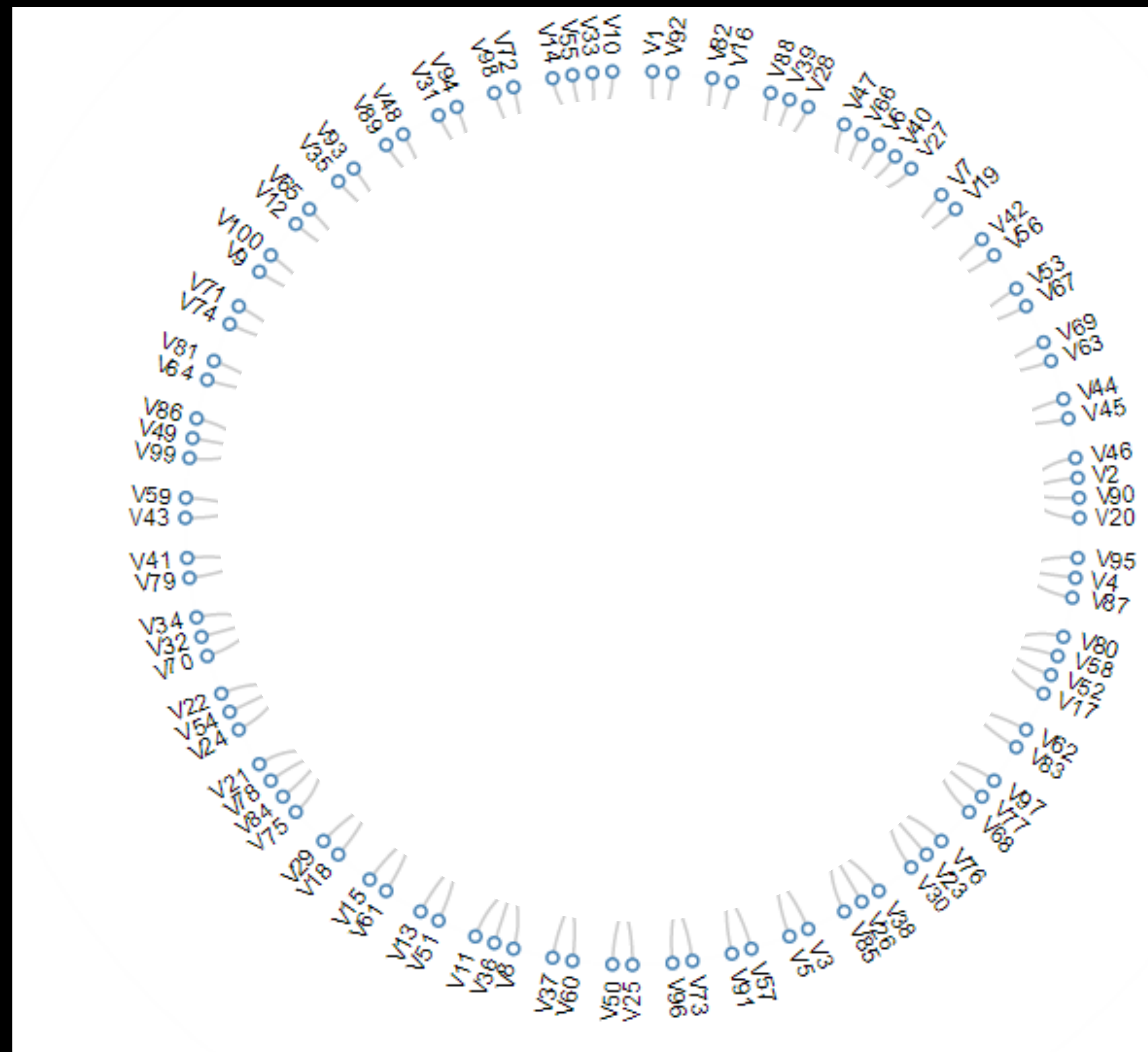




hierarchical clustering

agglomerative
bottom-up

computationally intense because every ***cluster pair*** distance has to be calculate



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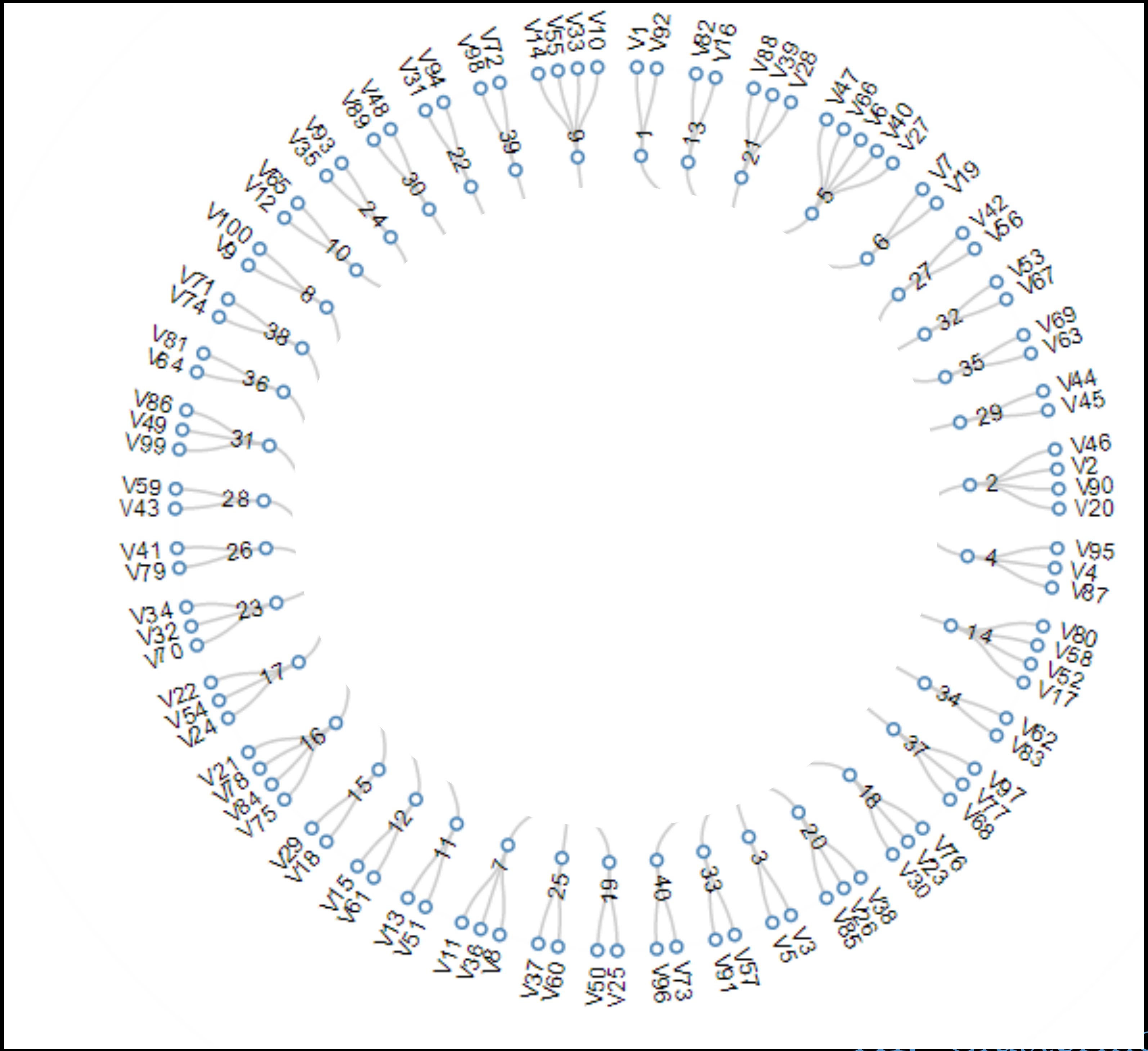

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agglomerative
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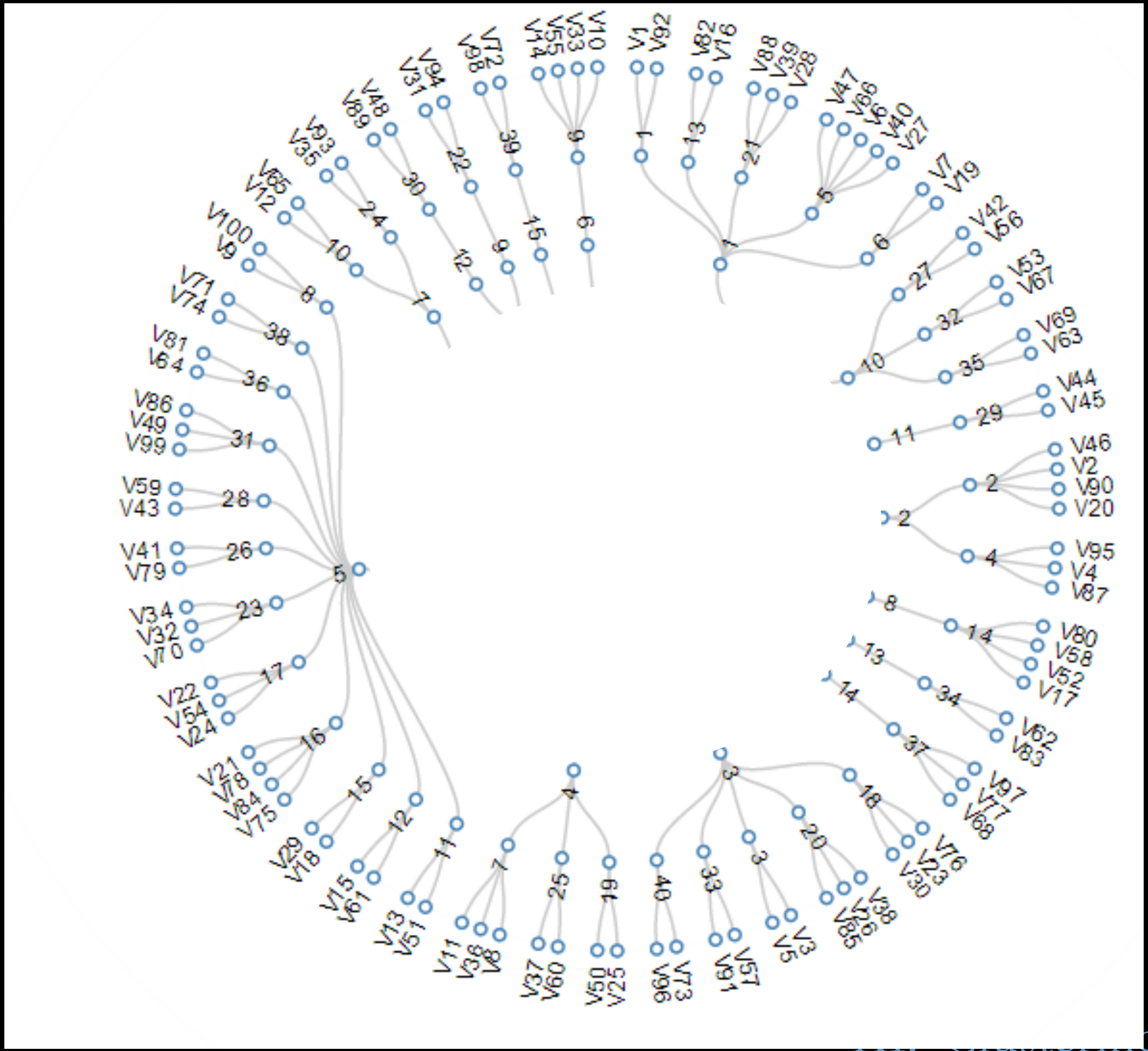

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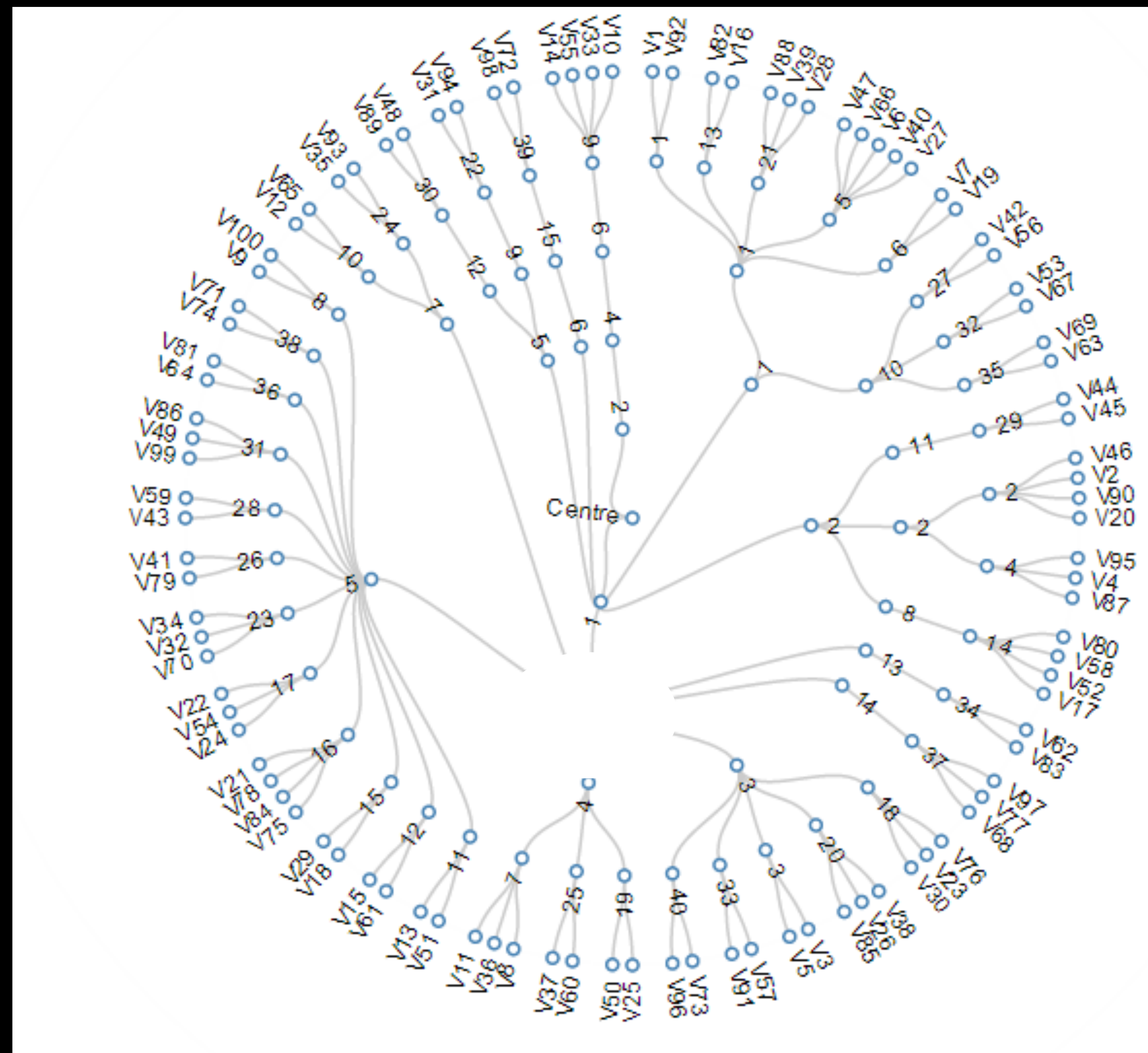

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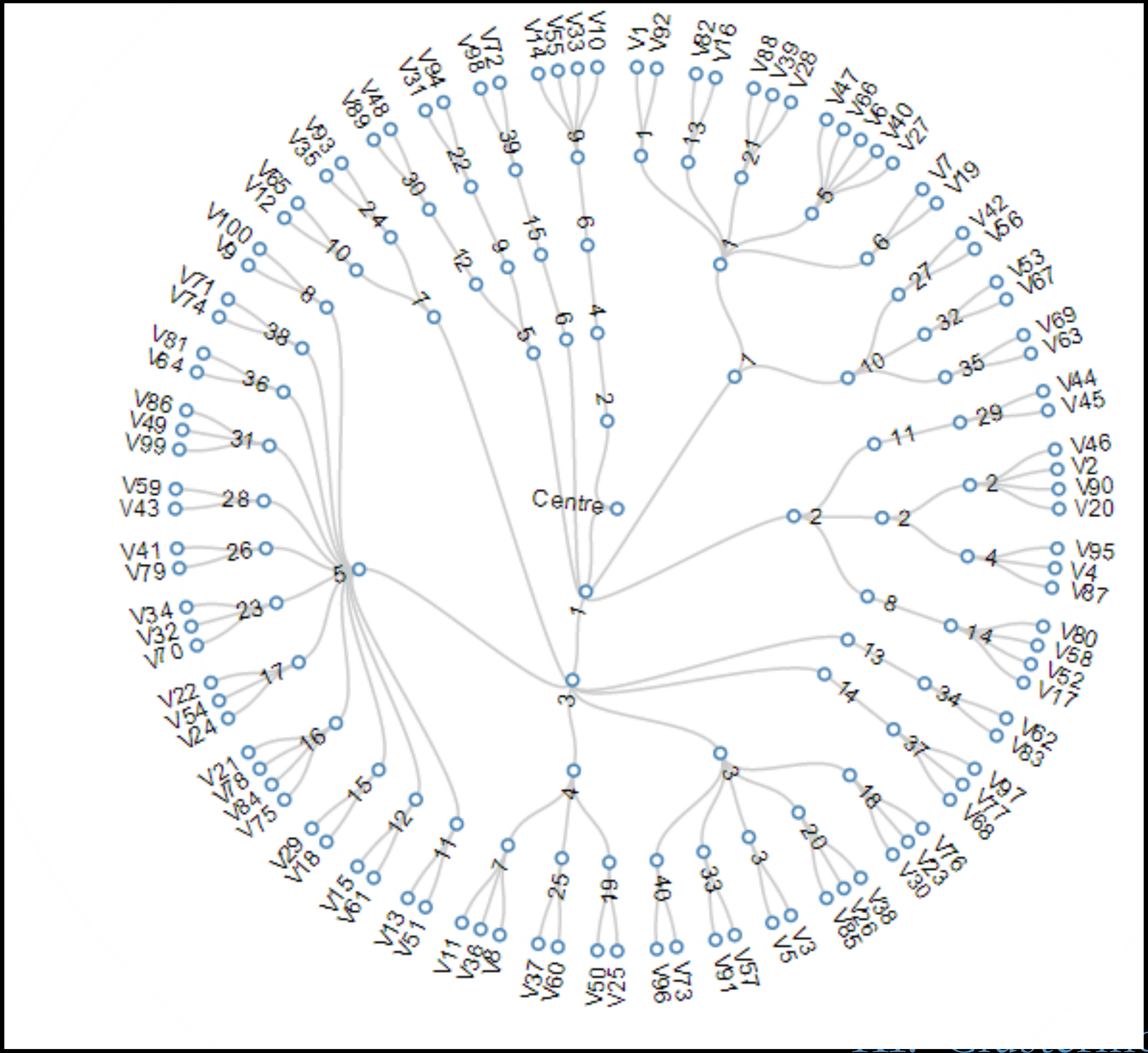


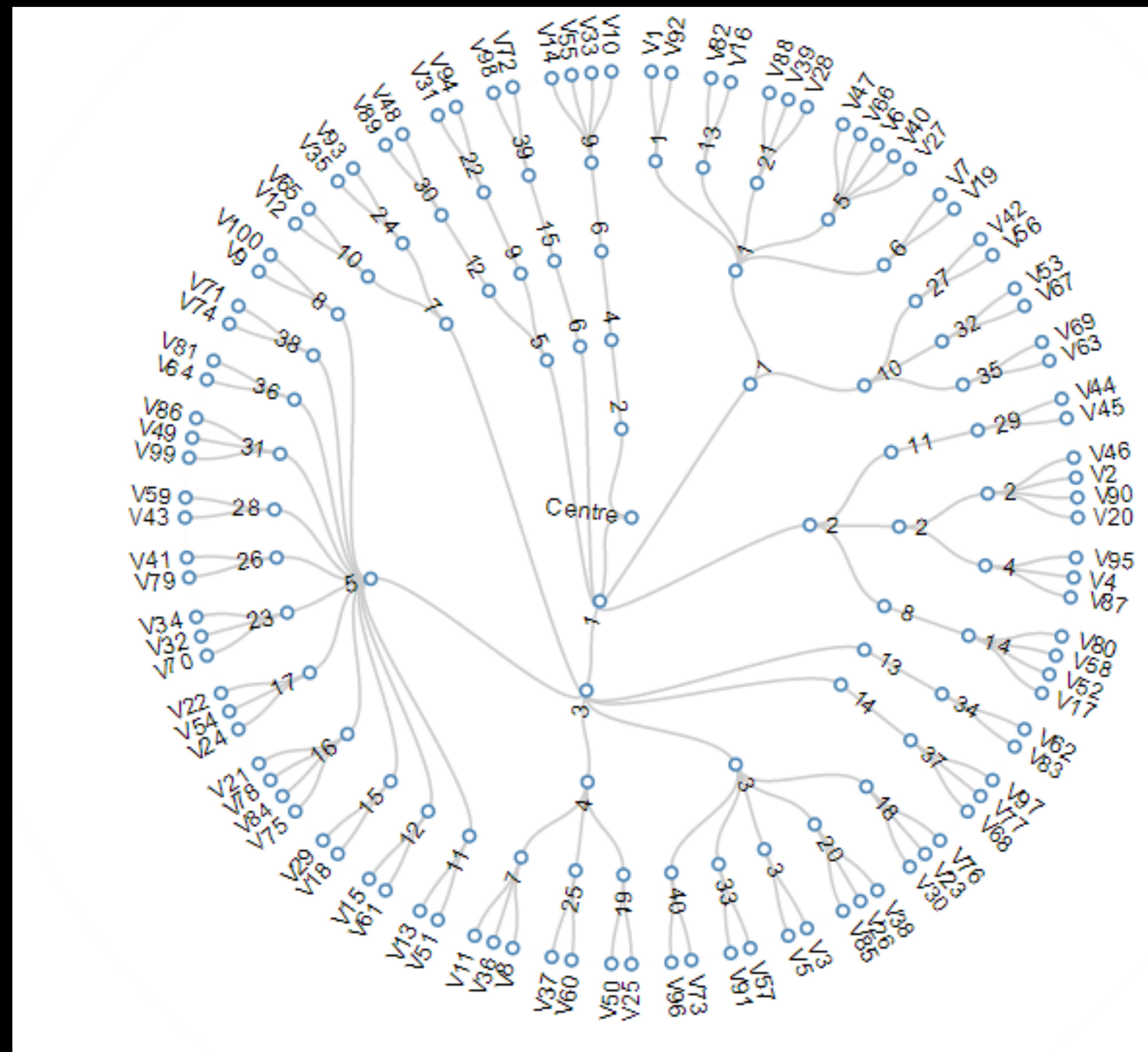
hierarchical clustering

agglomerative
bottom-up

computationally intense because every ***cluster pair*** distance has to be calculate

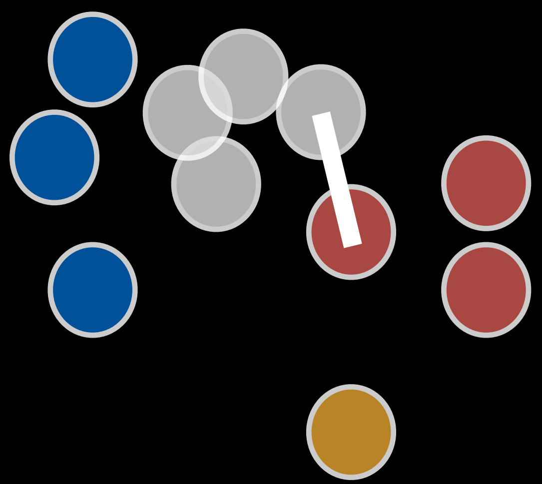
it is slow, though it can be optimize: complexity

$O(N^2d+ N^3)$



hierarchical clustering

agglomerative
bottom-up



single link distance

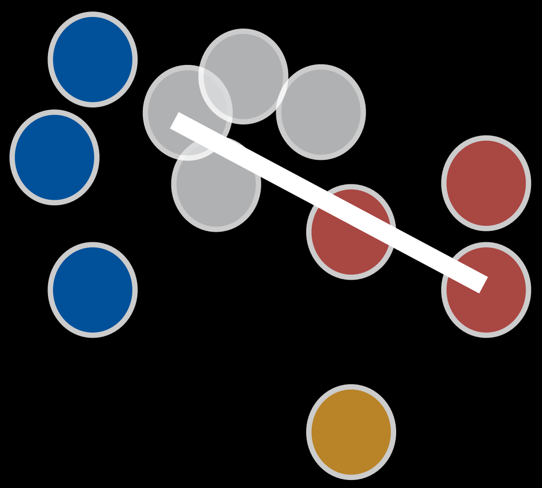
$$D(c1,c2) = \min(D(x_{c1}, x_{c2}))$$

complete link distance

$$D(c1,c2) = \max(D(x_{c1}, x_{c2}))$$

hierarchical clustering

agglomerative
bottom-up



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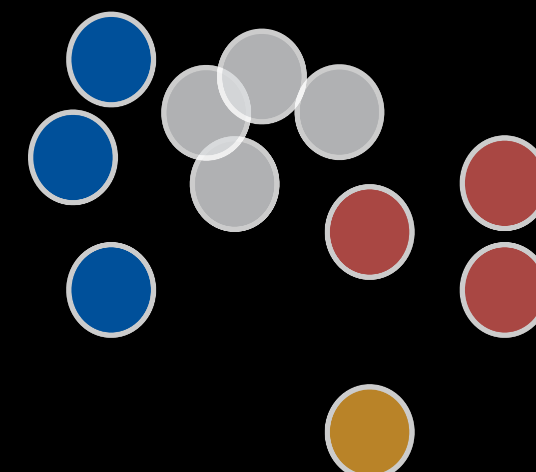

single link distance

$D(c1,c2) = \min(D(x_{c1}, x_{c2}))$

complete link distance

$D(c1,c2) = \max(D(x_{c1}, x_{c2}))$

centroid distance

$D(c1,c2) = \mathrm{mean}(D(x_{c1}, x_{c2}))$

ward distance

minimizes variance

$$D_{tot} = \sum_{j} \sum_{i, x_i \in C_j} (x_i - \mu_j)^2$$

ering

https://github.com/fedhere/UInotebooks/blob/master/cluster/thanksgivingClustering.ipynb

Summary and Key concepts

clustering is easy, but interpreting results is tricky

Distane metrics:

- Eucledian and other Minchowski metrics
- geospacial distances
- metrics for non continuous data

Partitioning methods: inexpensive, typically non deterministic

- Hard methods: *K-means, K-medoids*
- Soft (or fuzzy) methods: (i.e. probabilistic approach)
  - *Expectation Maximization Mixture models*

Hierarchical methods:

- divisive vs agglomerative, dendrograms

RESOURCES:

a comprehensive review of clustering methods

Data Clustering: A Review, Jain, Mutry, Flynn 1999
https://www.cs.rutgers.edu/~mlittman/courses/lightai03/jain99data.pdf

a blog post on how to generate and interpret a scipy dendrogram by Jörn Hees
https://joernhees.de/blog/2015/08/26/scipy-hierarchical-clustering-and-dendrogram-tutorial/

READING:

your data aint that big…
https://www.chrisstucchio.com/blog/2013/hadoop_hatred.html

HW: cluster NYC business history

1. cluster the economic trends in NYC using 2 methods: use K-Means and another method of your choice (e.g. DBscan, agglomerative clustering): use the time behavior of the number of establishments per zip code as your feature space

2. see if the clusters based on the time behavior also form spatial clusters.
   map the time-based clusters
   (e.g. with geopanda as a heat map).
   attempt an interpretation.

HW: cluster NYC business history

Use census data for NYC businesse:
number of establishments per zip code for ~20 years since 1994

you can get the zip code info (list of NYC zip codes and shape files for plotting) here:
http://data.nycprepared.org/dataset/nyc-zip-code-tabulation-areas/resource/0c0e14e9-78e1-404e-97b0-c2fabceb3981

this is the link to the census business data
http://www.census.gov/econ/cbp/download/
you can download manually, which is labour intensive, or on the terminal via ftp, which requires some wrangling, but i did that for you! (see below)

```
for ((y=93; y<=99; y+=1)); do wget zbp$y\totals.zip; done
for ((y=0; y<=9; y+=1)); do wget ftp://ftp.census.gov/econ200$y\/CBP_CSV/zbp0$y\totals.zip; done
for ((y=10; y<=15; y+=1)); do wget ftp://ftp.census.gov/econ20$y\/CBP_CSV/zbp$y\totals.zip; done
```