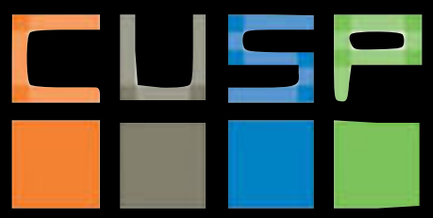
Urban Informatics

Fall 2018

dr. federica bianco fbianco@nyu.edu

 @fedhere 



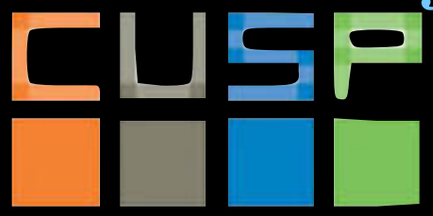
XI: Clustering

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.

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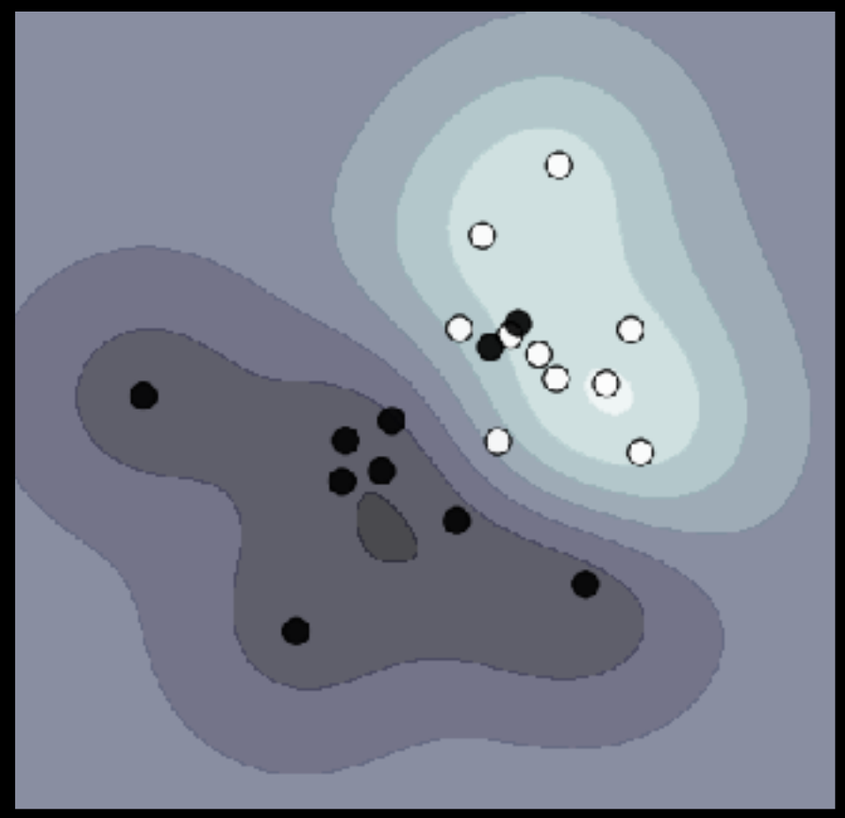
supervised learning

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



XI: Clustering

machine learning

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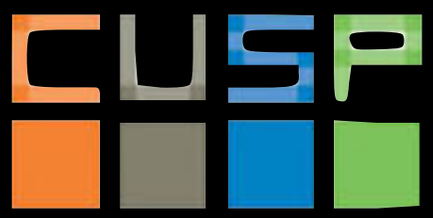
supervised learning

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

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

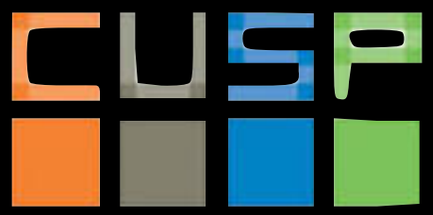
prediction

unsupervised methods

understanding structure

organizing + compressing data

(classification, feature learing)



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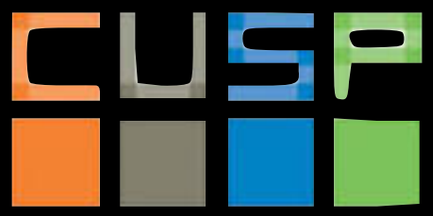
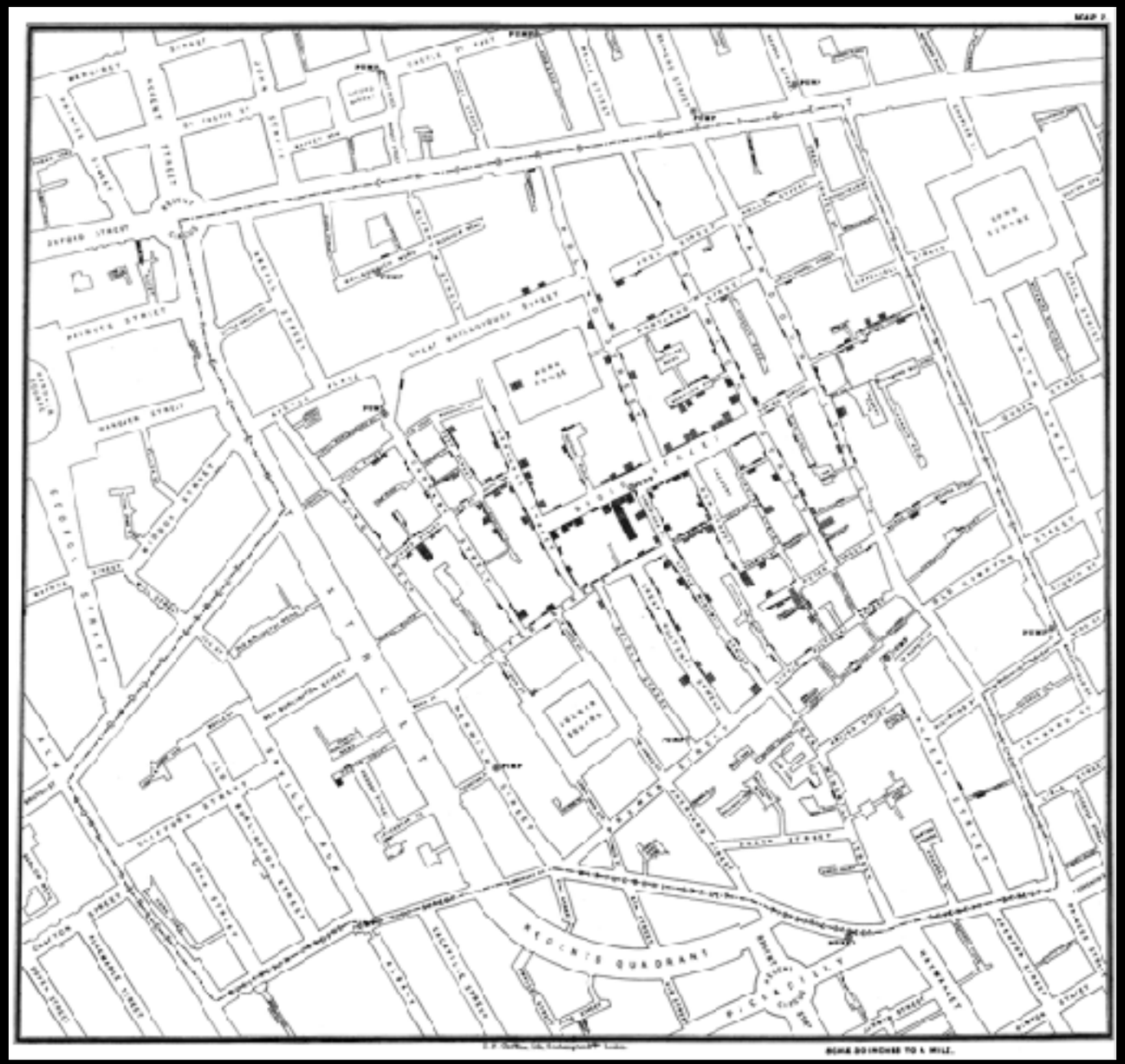


What is clustering?

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*.

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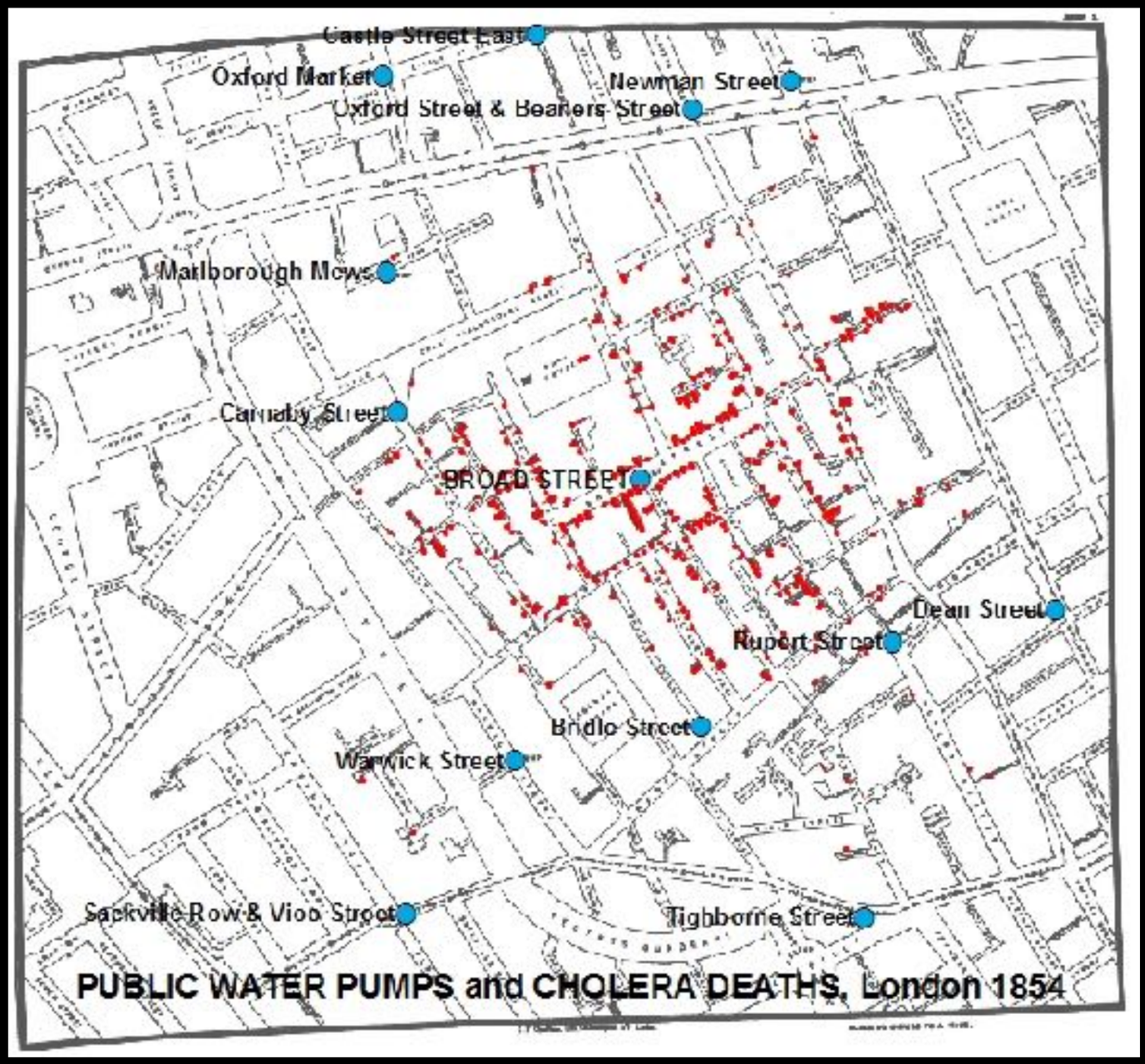

digitization by John Mackenzie, University of Delaware

https://www1.udel.edu/johnmack/frec682/cholera/cholera2.html

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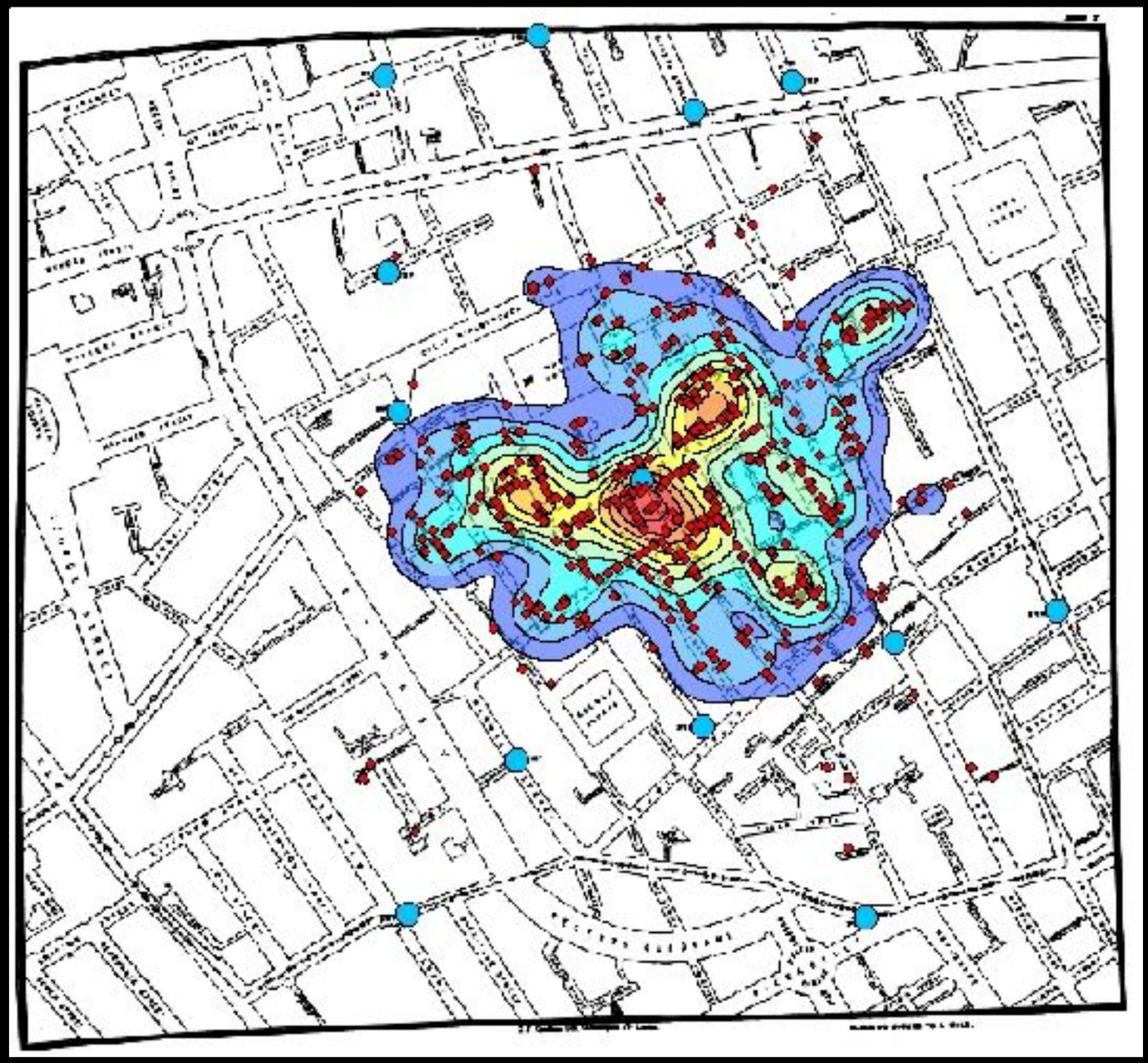

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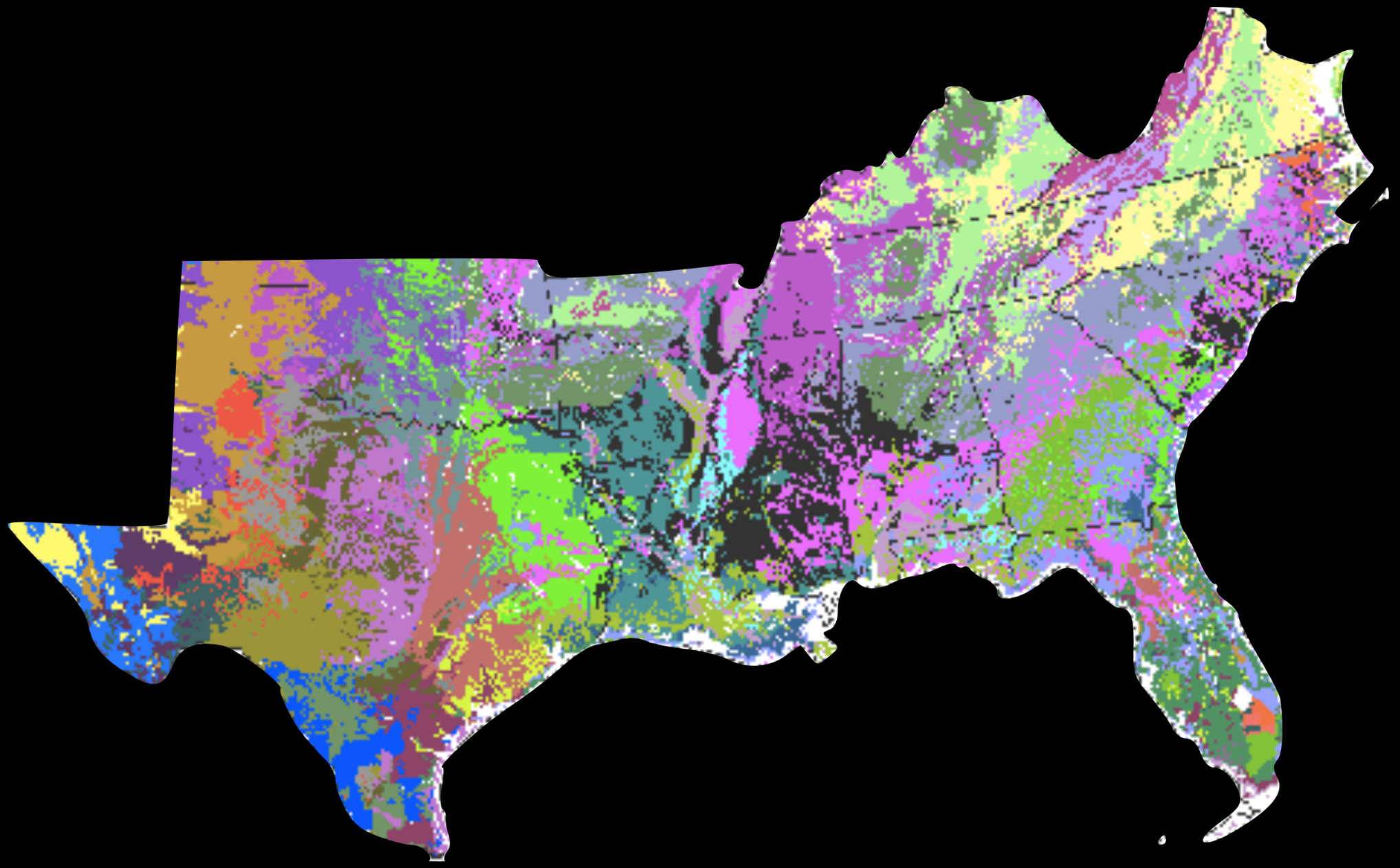


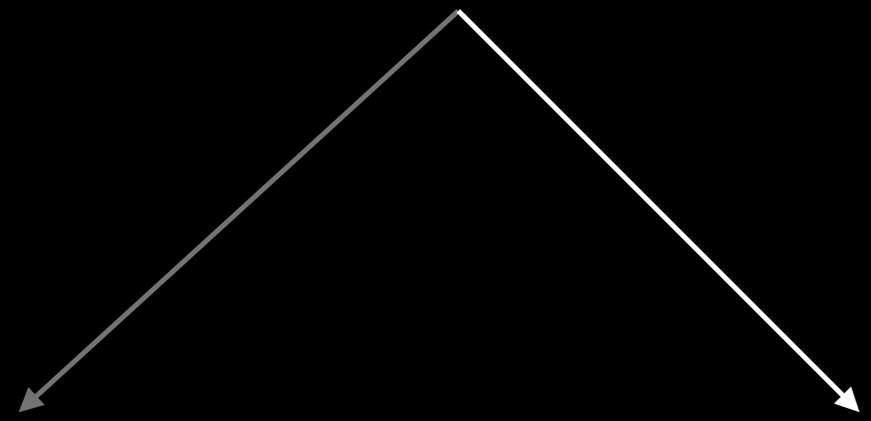
A Spatial Clustering Technique for the Identification of Customizable Ecoregions

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

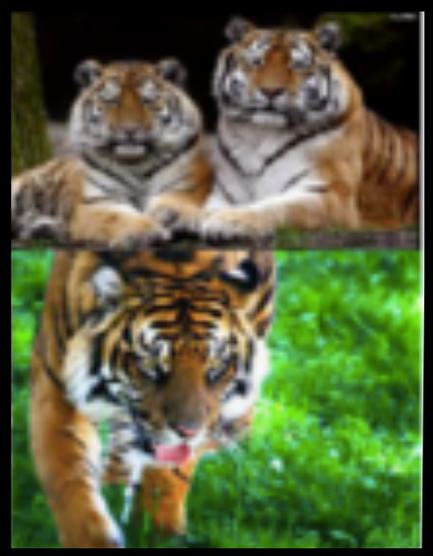
GOAL:
partitioning data in *maximally homogeneous*, *maximally distinguished* subsets.

machine learning

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

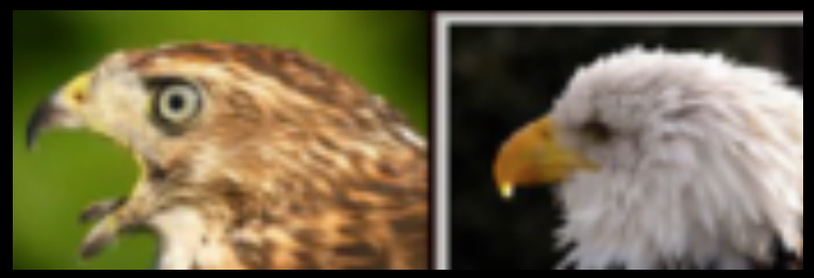
what is a cluster?

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



tigers

whales

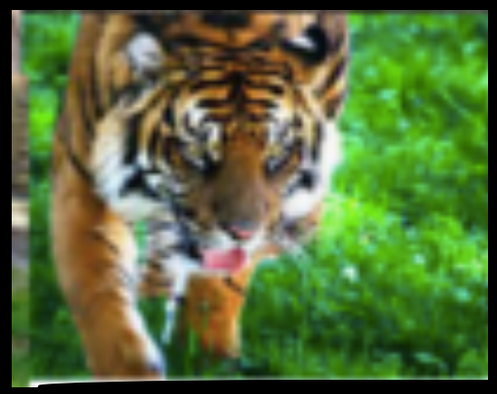


eagles

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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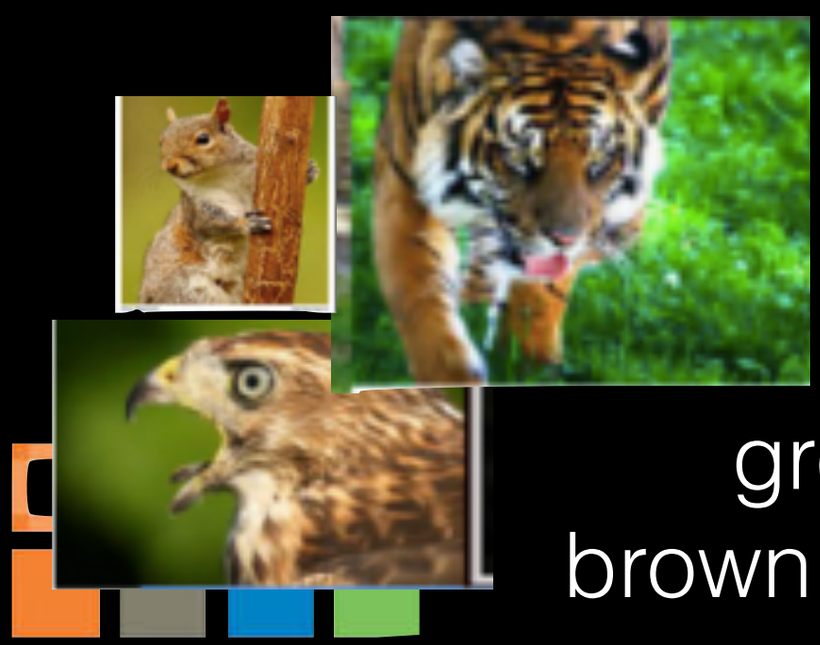
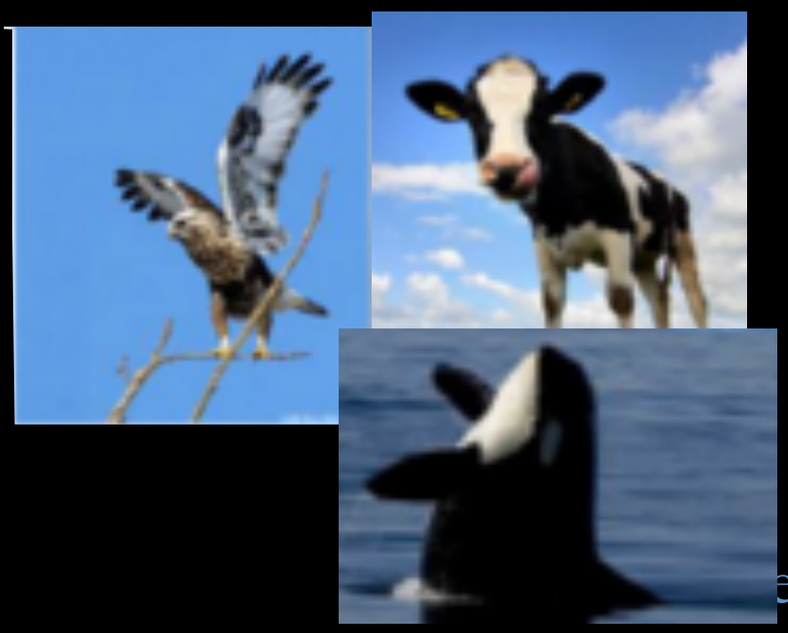


green
brown & white

blue
black
&
white



ering

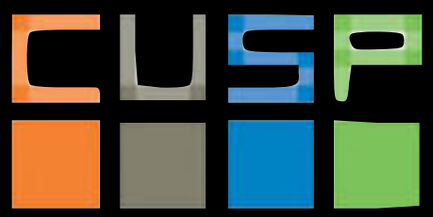
https://github.com/fedhere/UInotebooks/blob/master/cluster/imageProcessingKmeans.ipynb

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

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

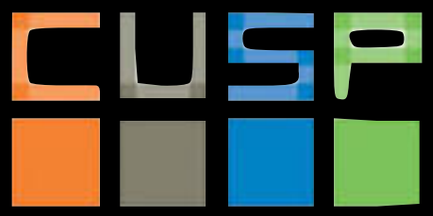
The ideal clustering algorithm:

- 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



CUSP

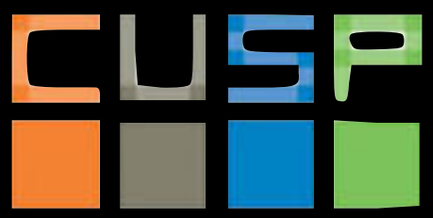
Defining the distance



Distance Metrics Continuous variables

Minkowski family of distances

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



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

N features (dimensions)

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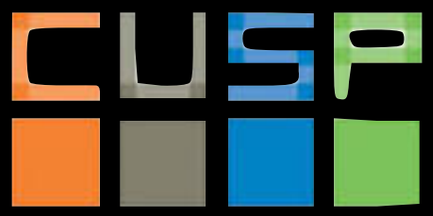
$$D(i,j) > 0$$

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

$$D(i,j) \equiv D(j,i)$$

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



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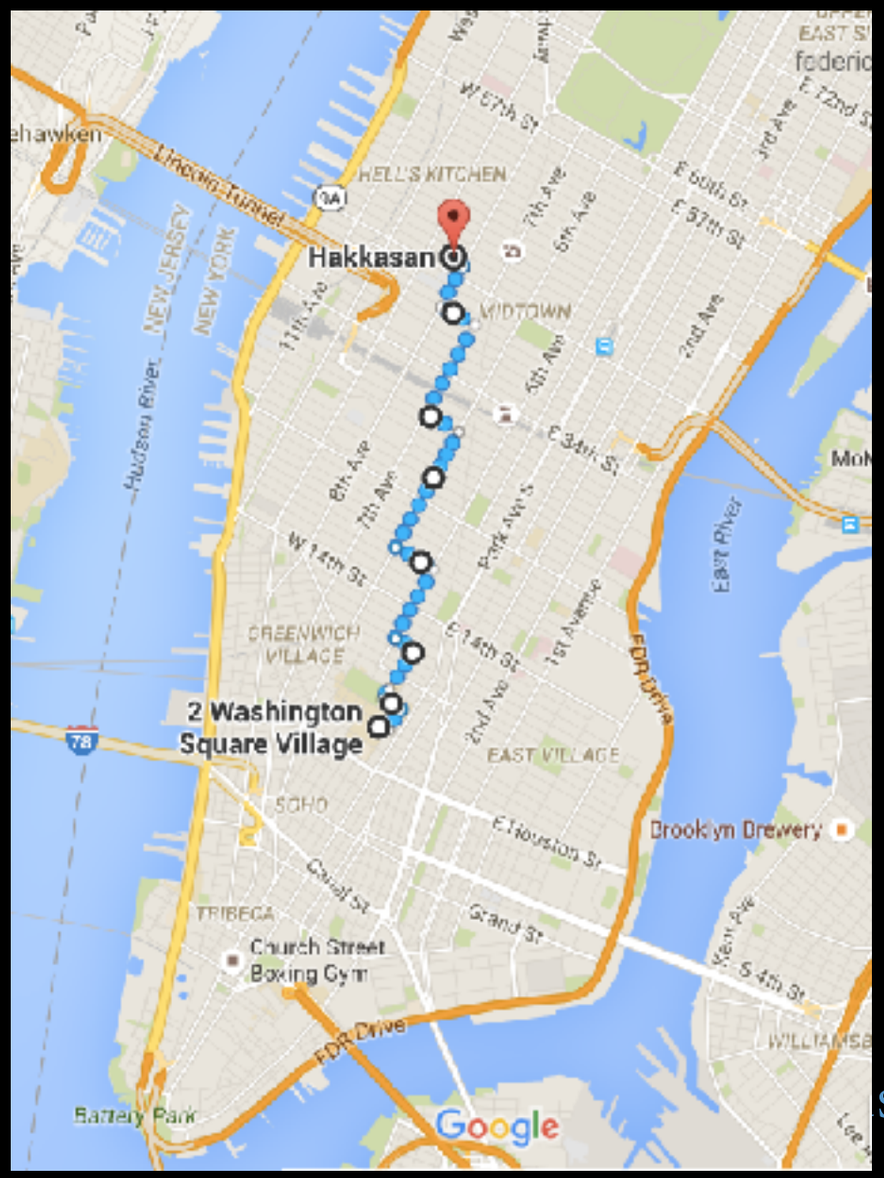
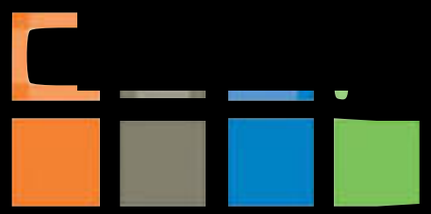


Manhattan: p = 1

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



stering

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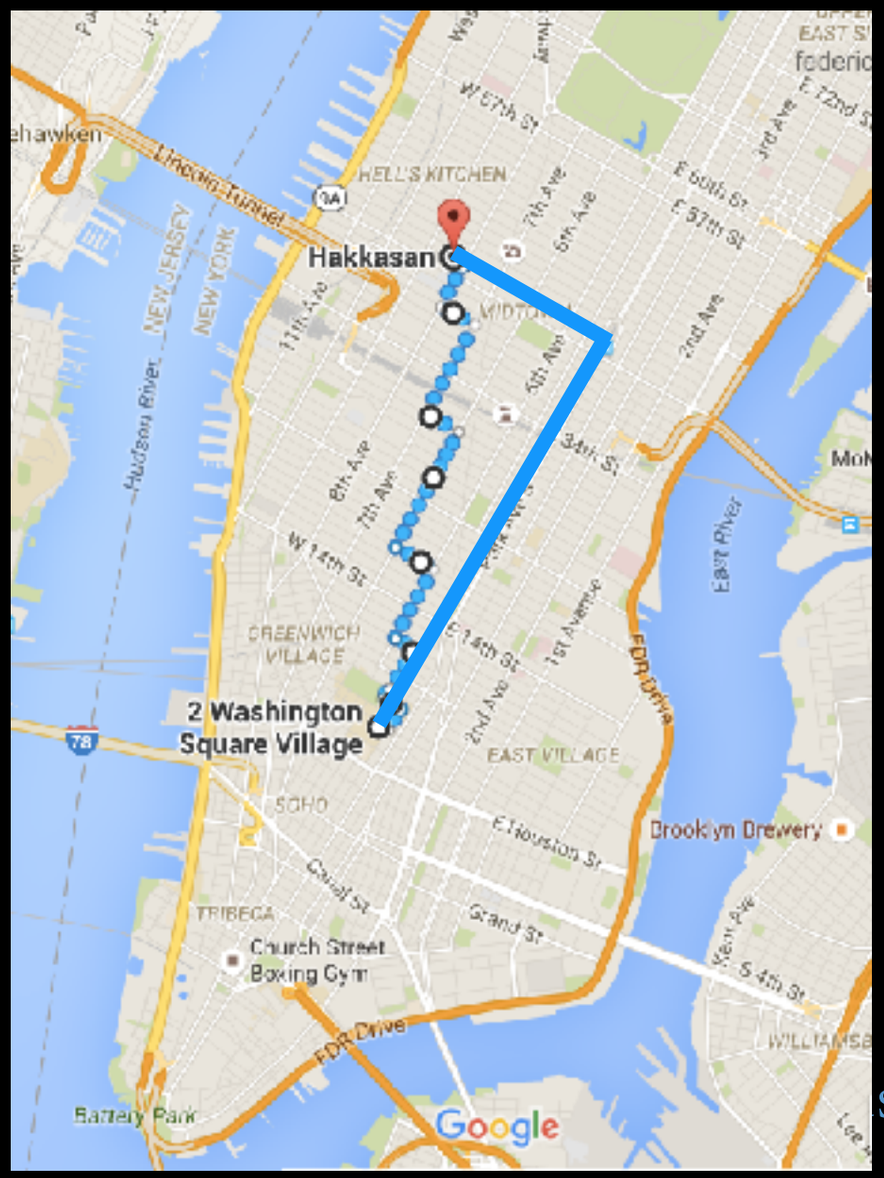

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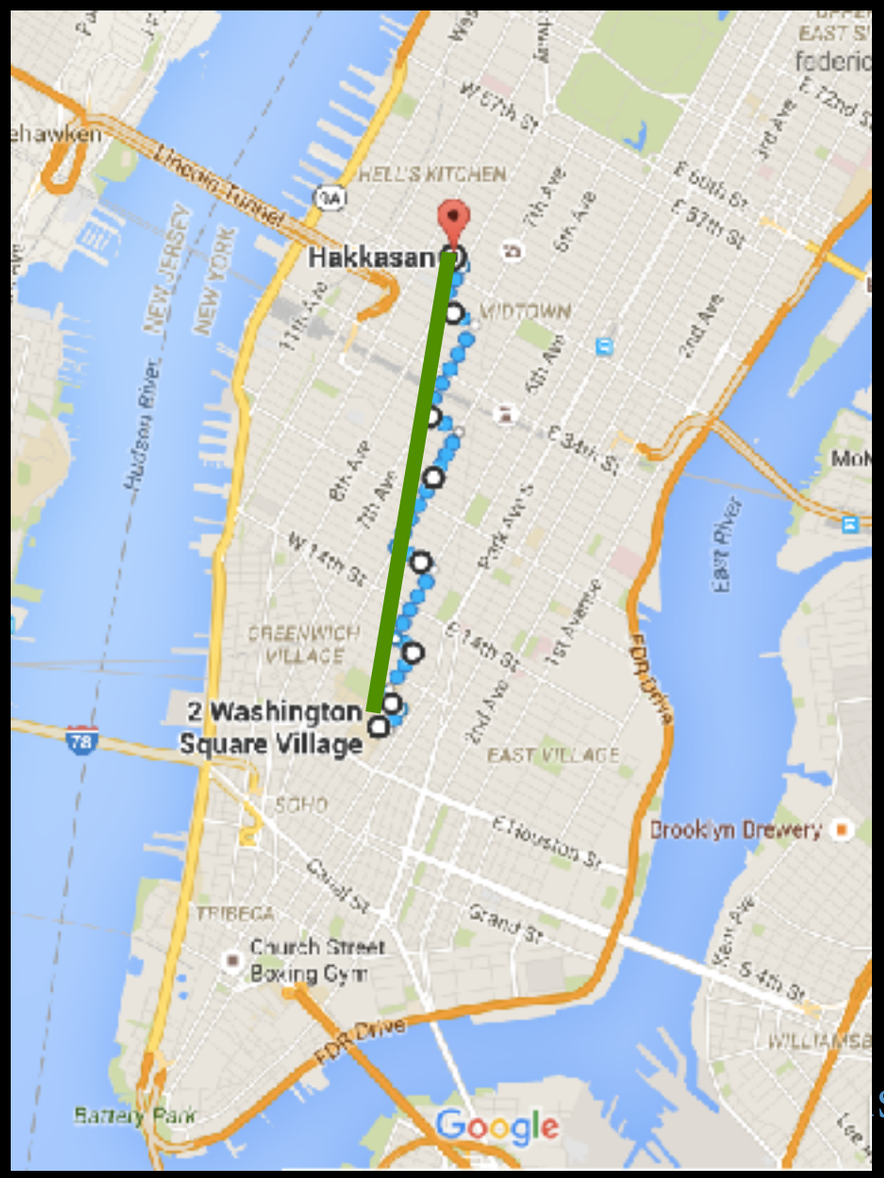
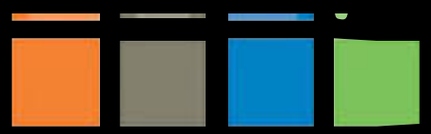


Euclidean: p = 2

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



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Distance Metrics Continuous variables

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

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

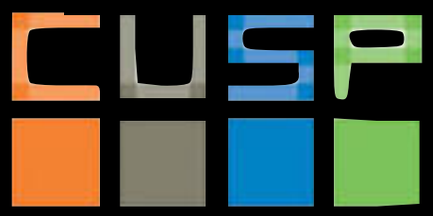
Minkowski family of distances

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

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

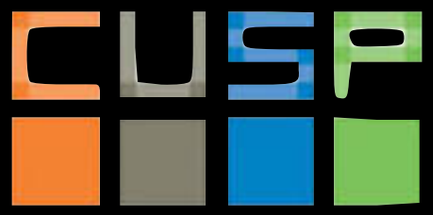
	1	0	*sum*
1	a	b	$a+b$
0	c	d	$c+d$
sum	$a+c$	$b+d$	p

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

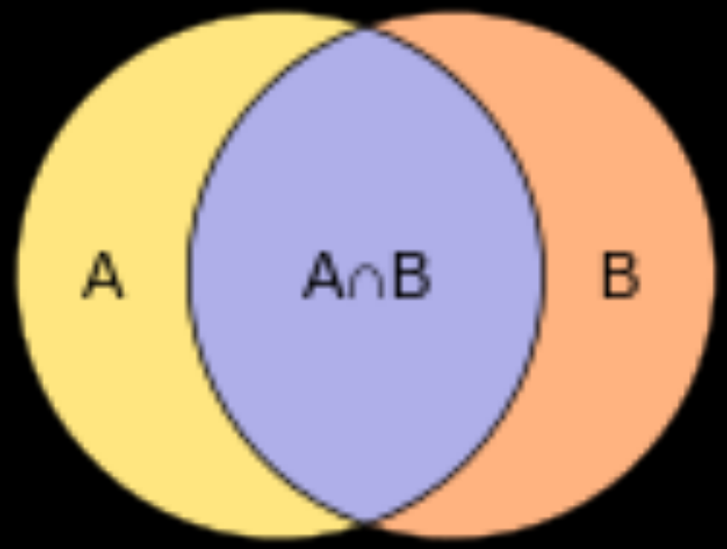


Distance Metrics Sets variables

Uses presence/absence data

Jaccard similarity coefficient S_j

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



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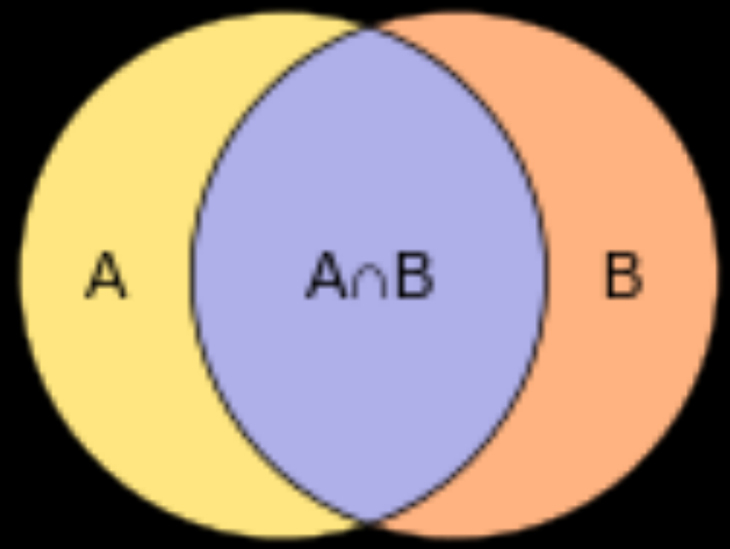

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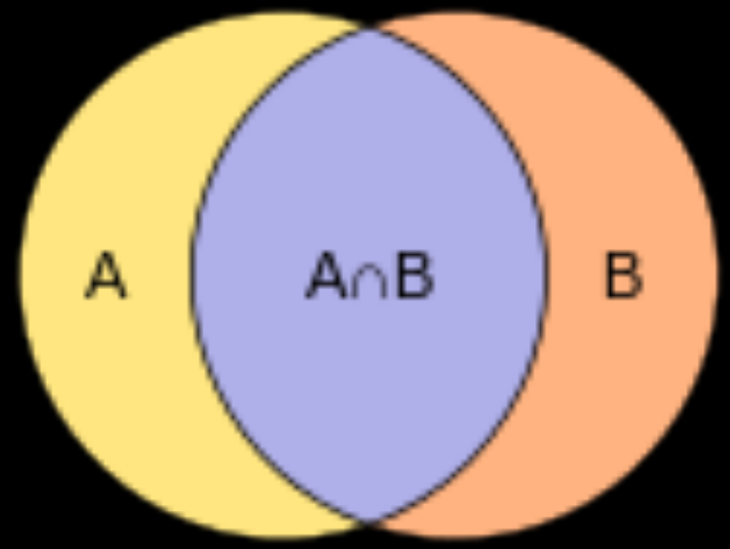
Distance Metrics Sets variables

Uses presence/absence data

Jaccard distance $D_j = 1 - S_j$

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



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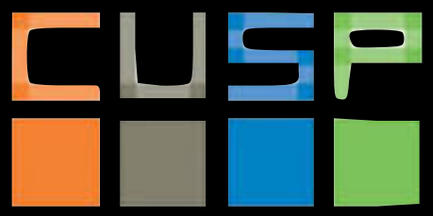
https://github.com/fedhere/UInotebooks/blob/master/cluster/categoricalDistances.ipynb

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)

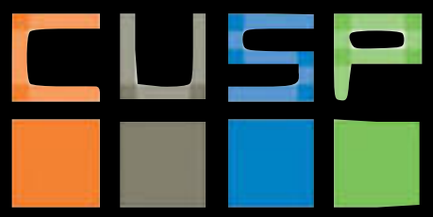
  Soft Clustering
  Expectation Maximization (Dempster,Laird,Rubin ’77)

- **Hirarchical**
  agglomerative

  devisive

- **Density based :**

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



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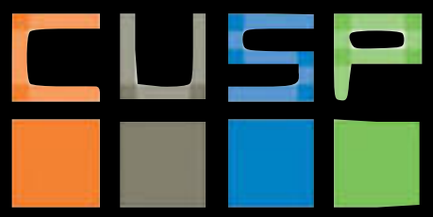


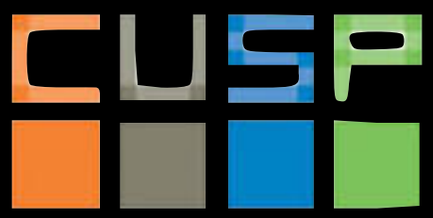
K-means:

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:

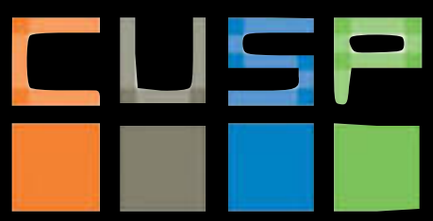
Minimizes the intra cluster variance

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

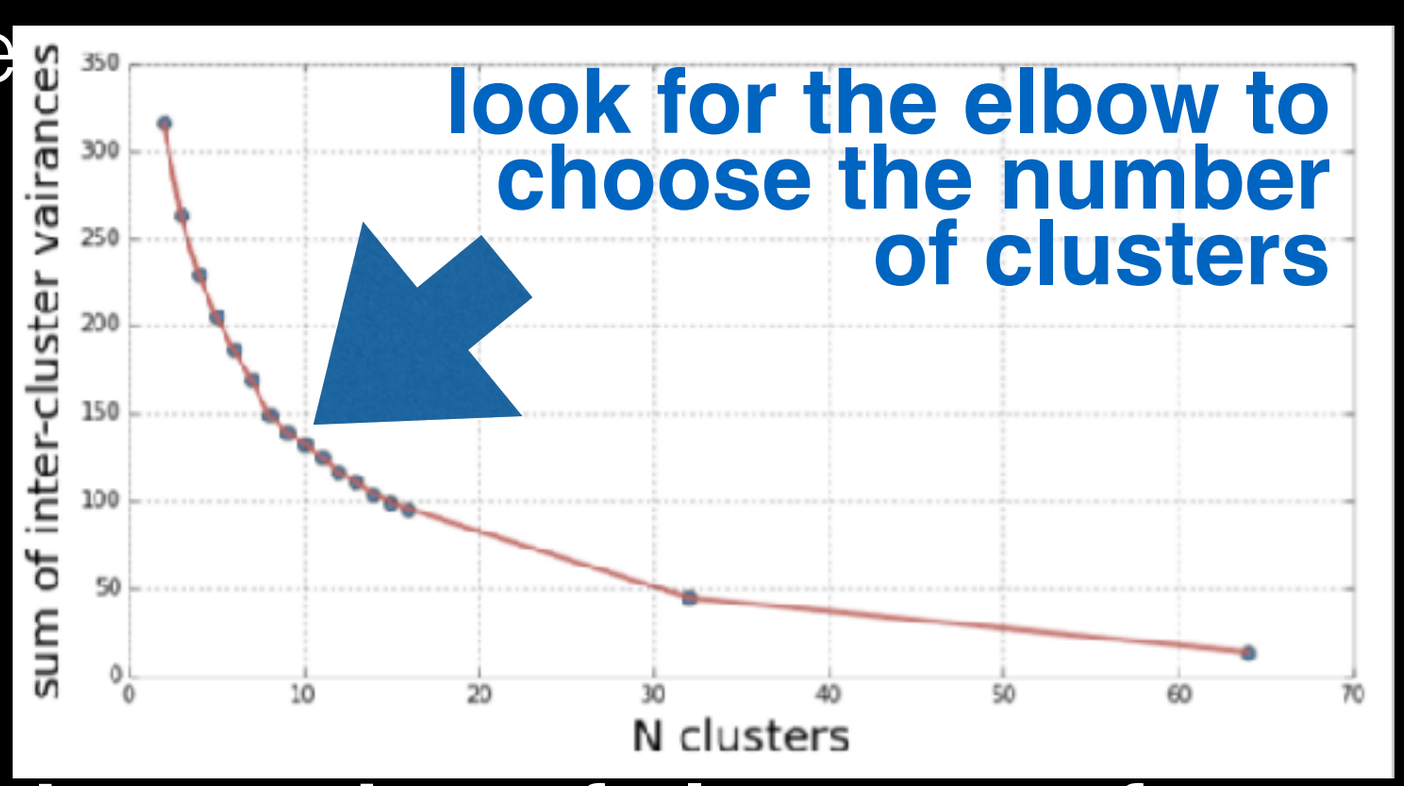
https://github.com/fedhere/UInotebooks/blob/master/cluster/kmeans.ipynb

K-means:

Minimizes the intra cluster variance

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



Must declare the number of clusters upfront

Clustering methods

- **Partitioning**

  Hard clustering

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

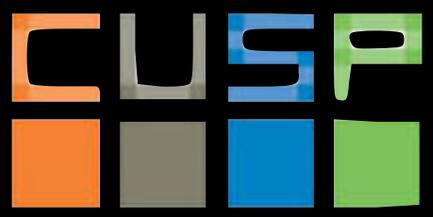
  Soft Clustering
  Expectation Maximization (Dempster,Laird,Rubin ’77)

- **Hirarchical**
  agglomerative

  devisive

- **Density based :**

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



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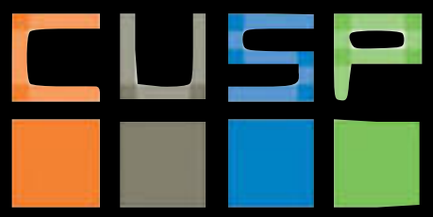
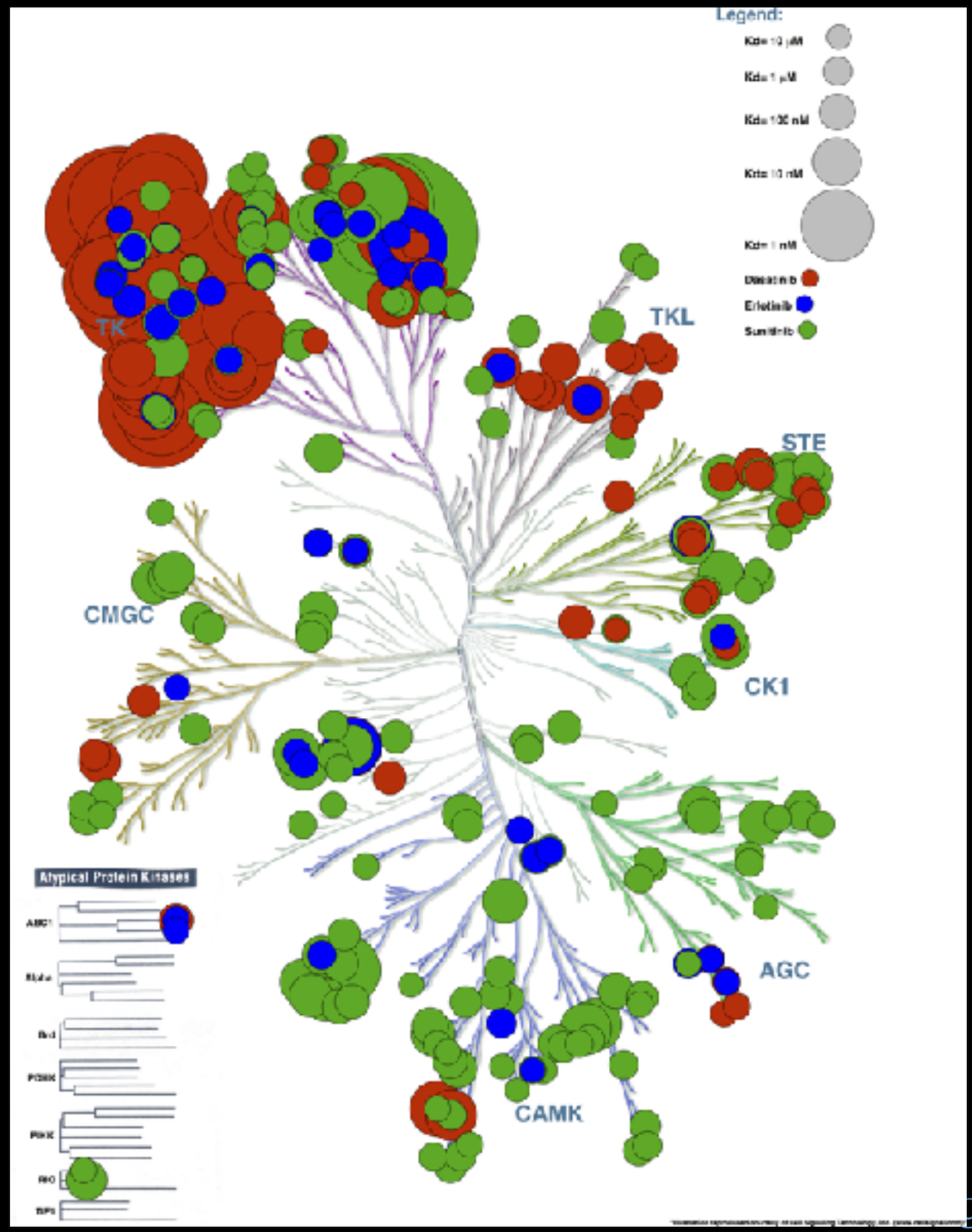
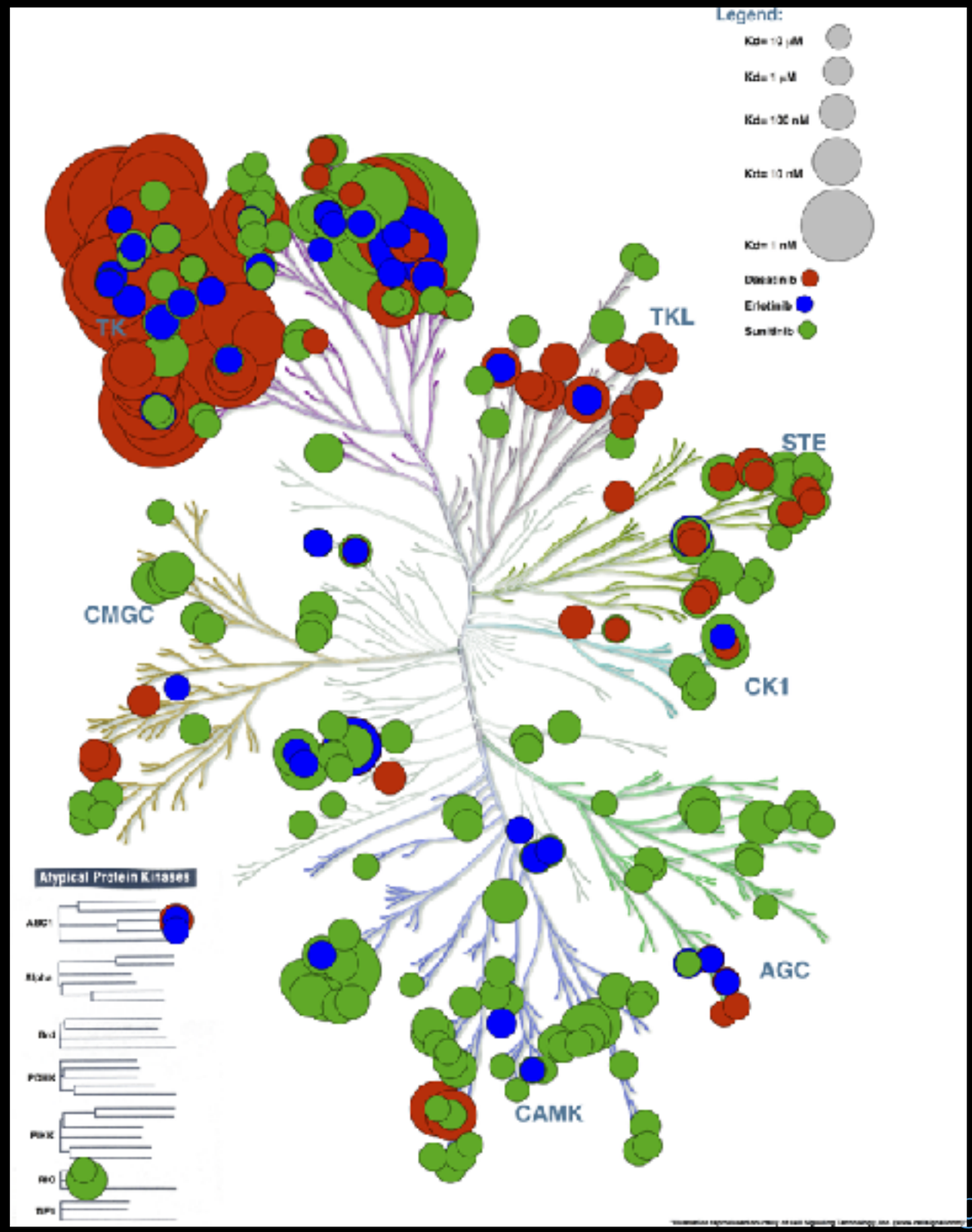


hierarchical clustering



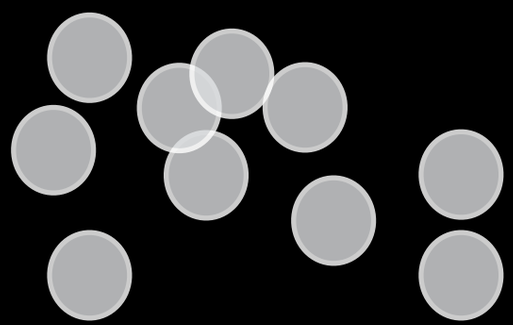
hierarchical clustering

removes the issue of deciding K (number of clusters)



hierarchical clustering

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



hierarchical clustering

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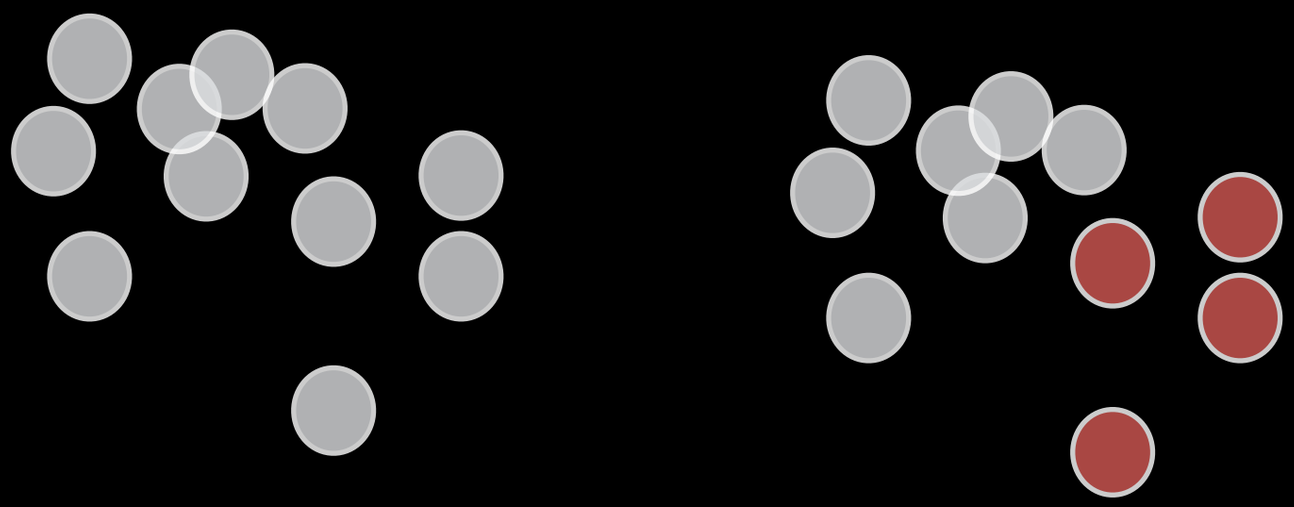

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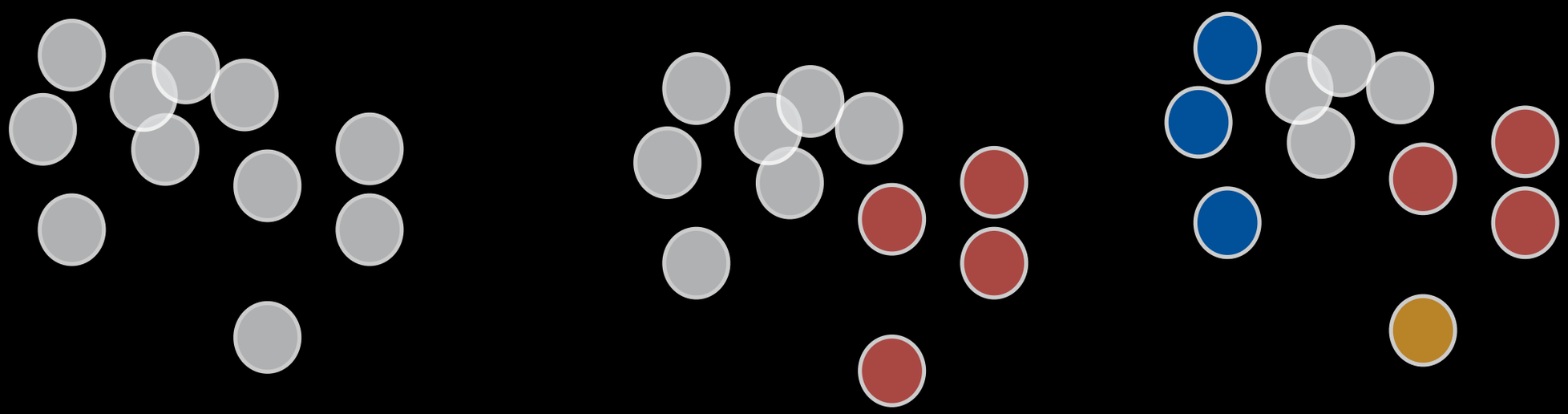

hierarchical clustering

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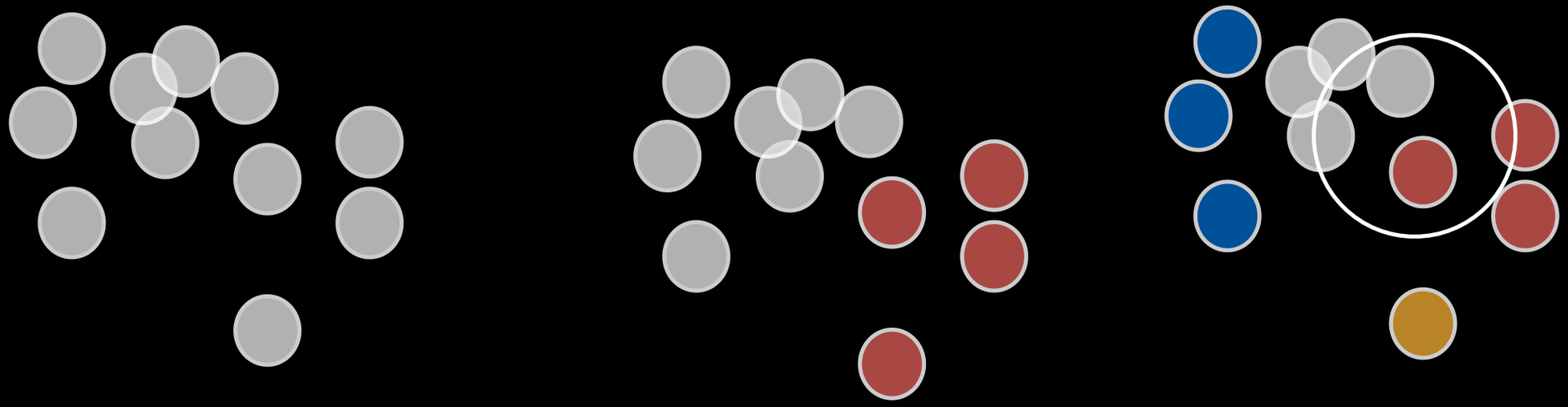
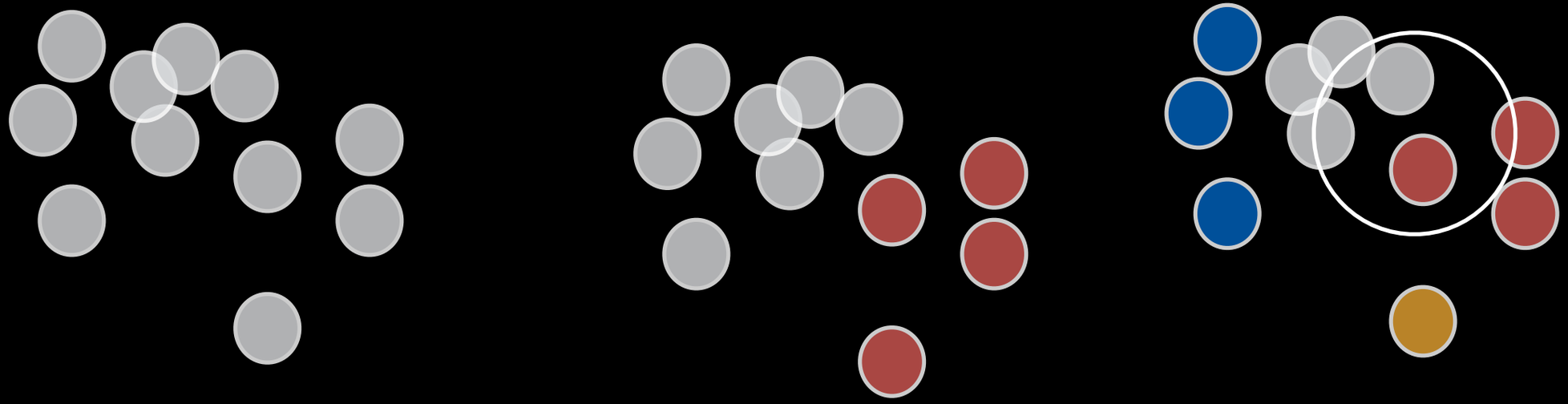


it is
non-deterministic

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



it is
non-deterministic

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

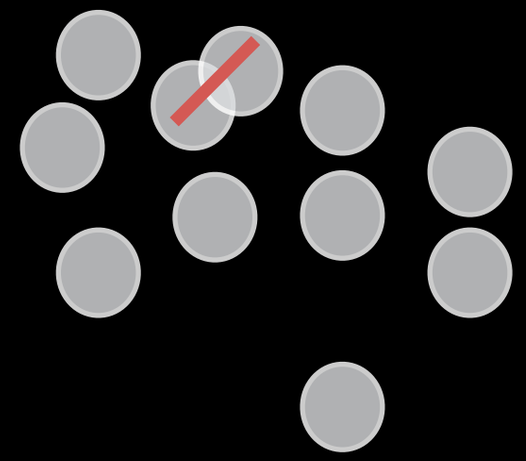
it is simple and
fast:
complexity

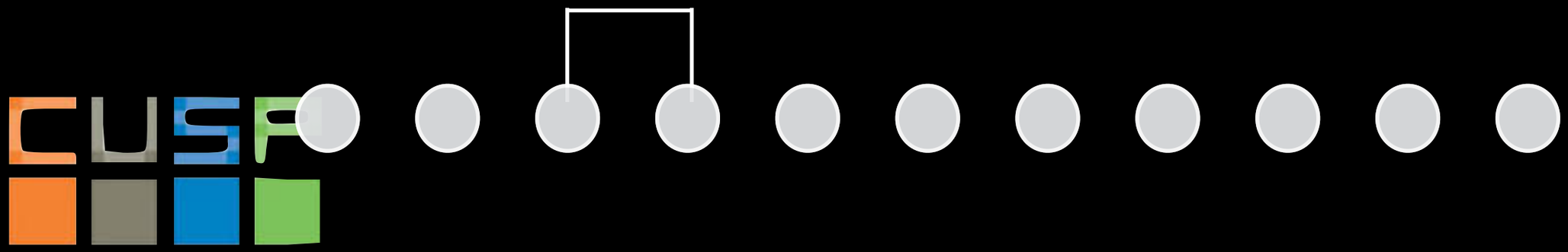
O(NdK $\log_k$N)

hierarchical clustering

agglomerative

bottom-up





hierarchical clustering

agglomerative

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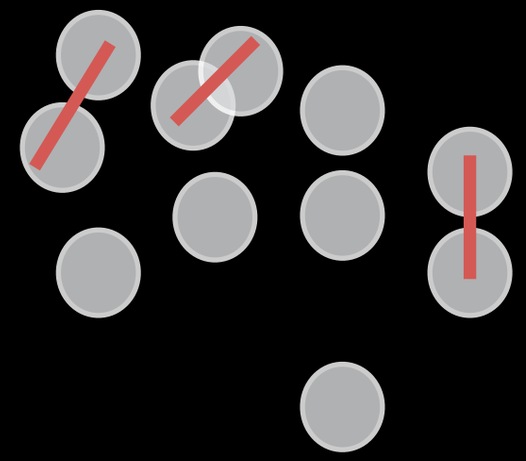
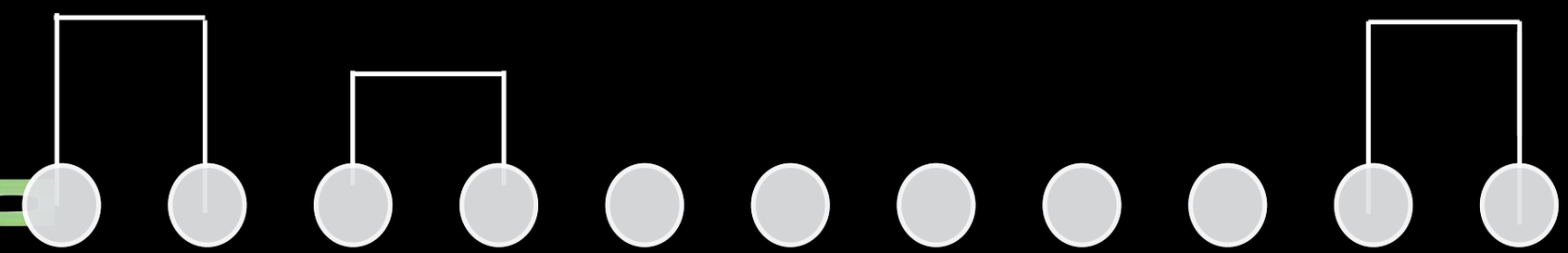
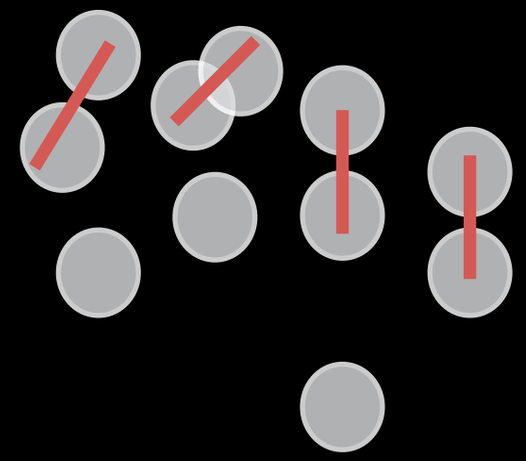


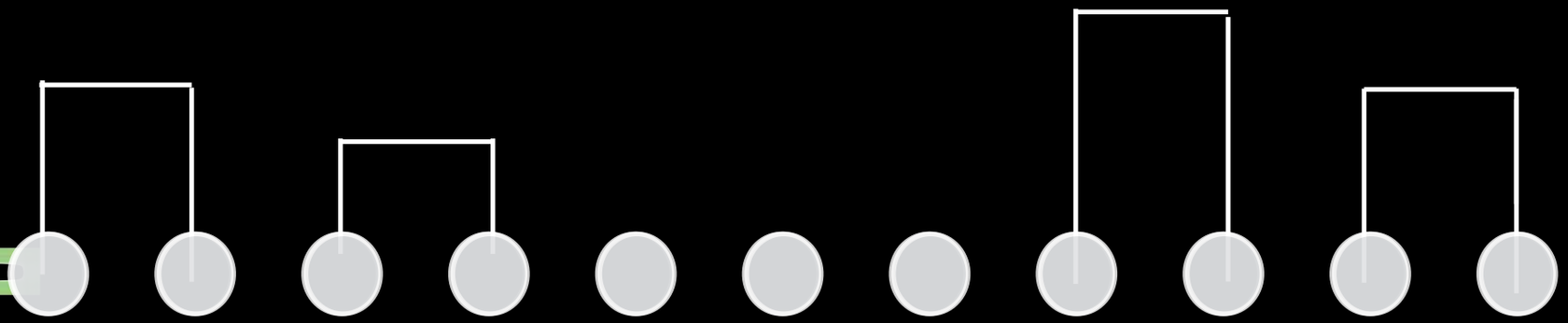


hierarchical clustering

agglomerative

bottom-up





hierarchical clustering

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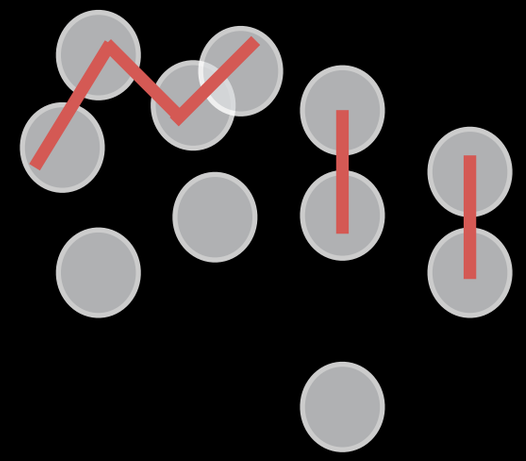

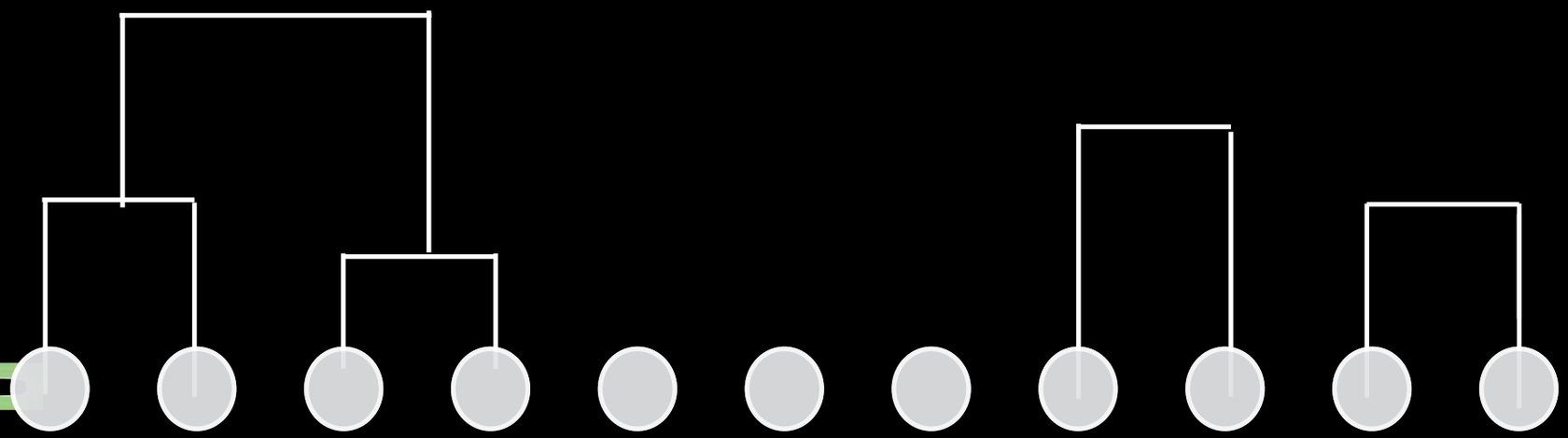

hierarchical clustering

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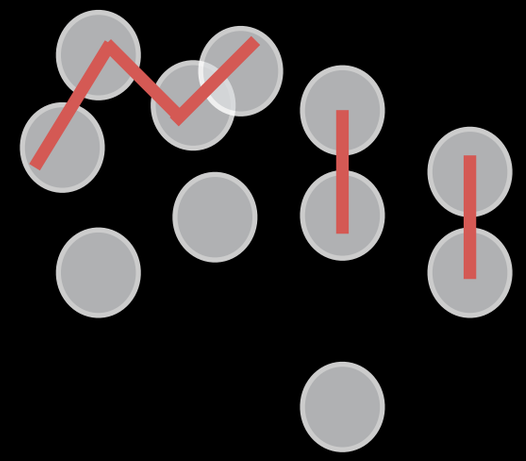
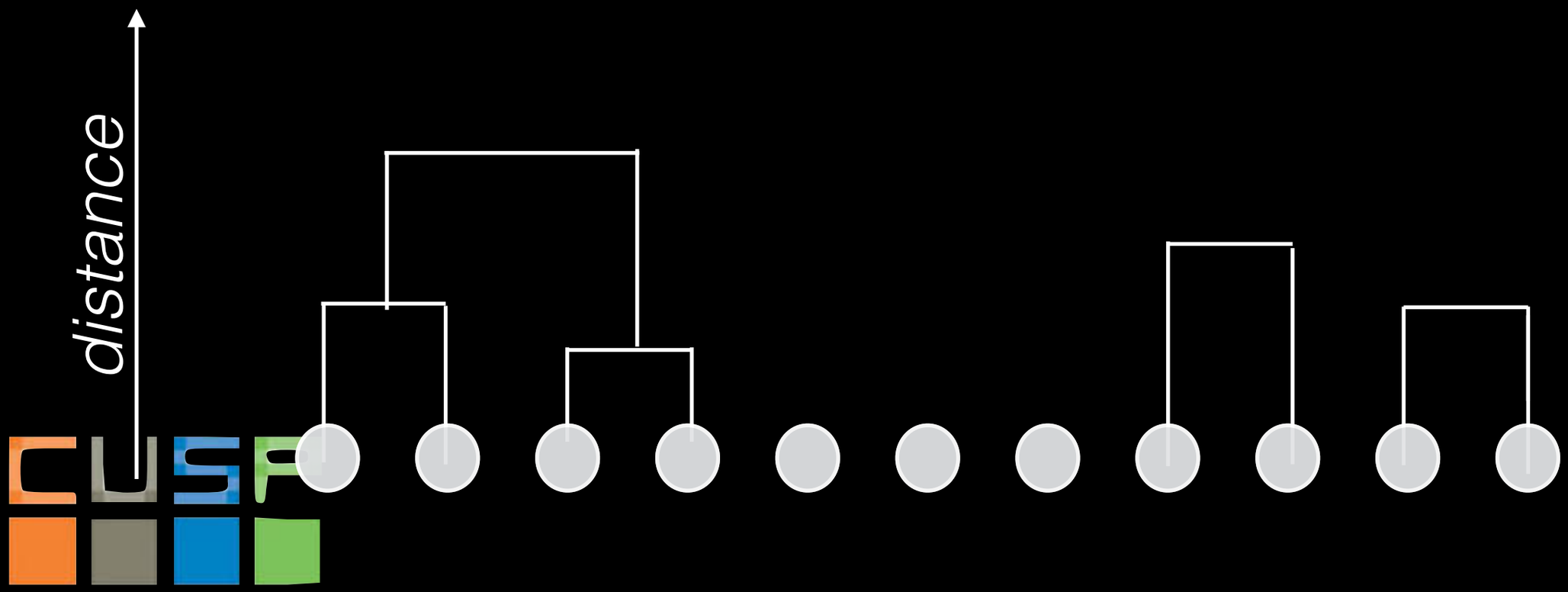
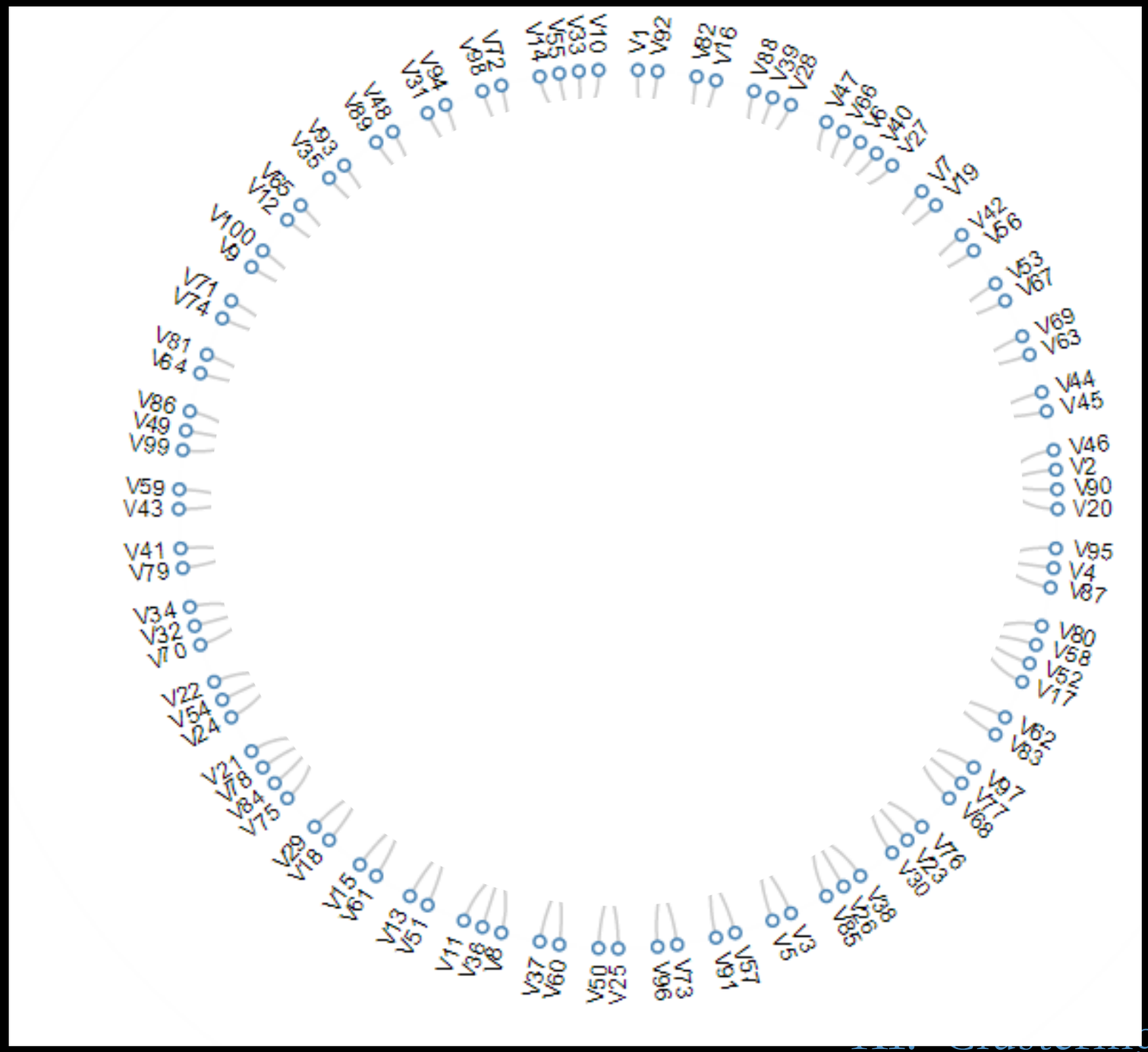




hierarchical clustering

agglomerative
bottom-up

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



hierarchical clustering

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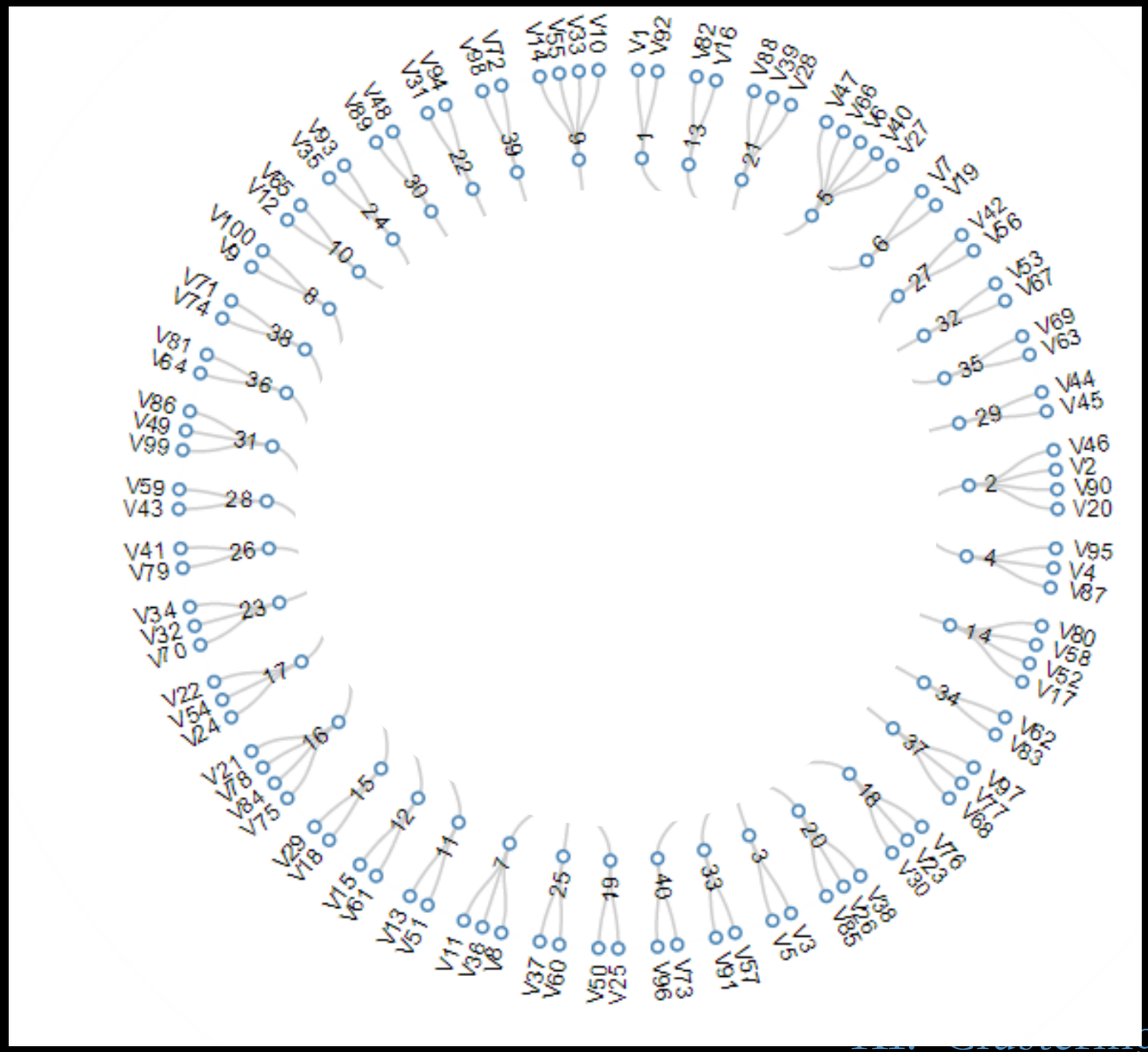

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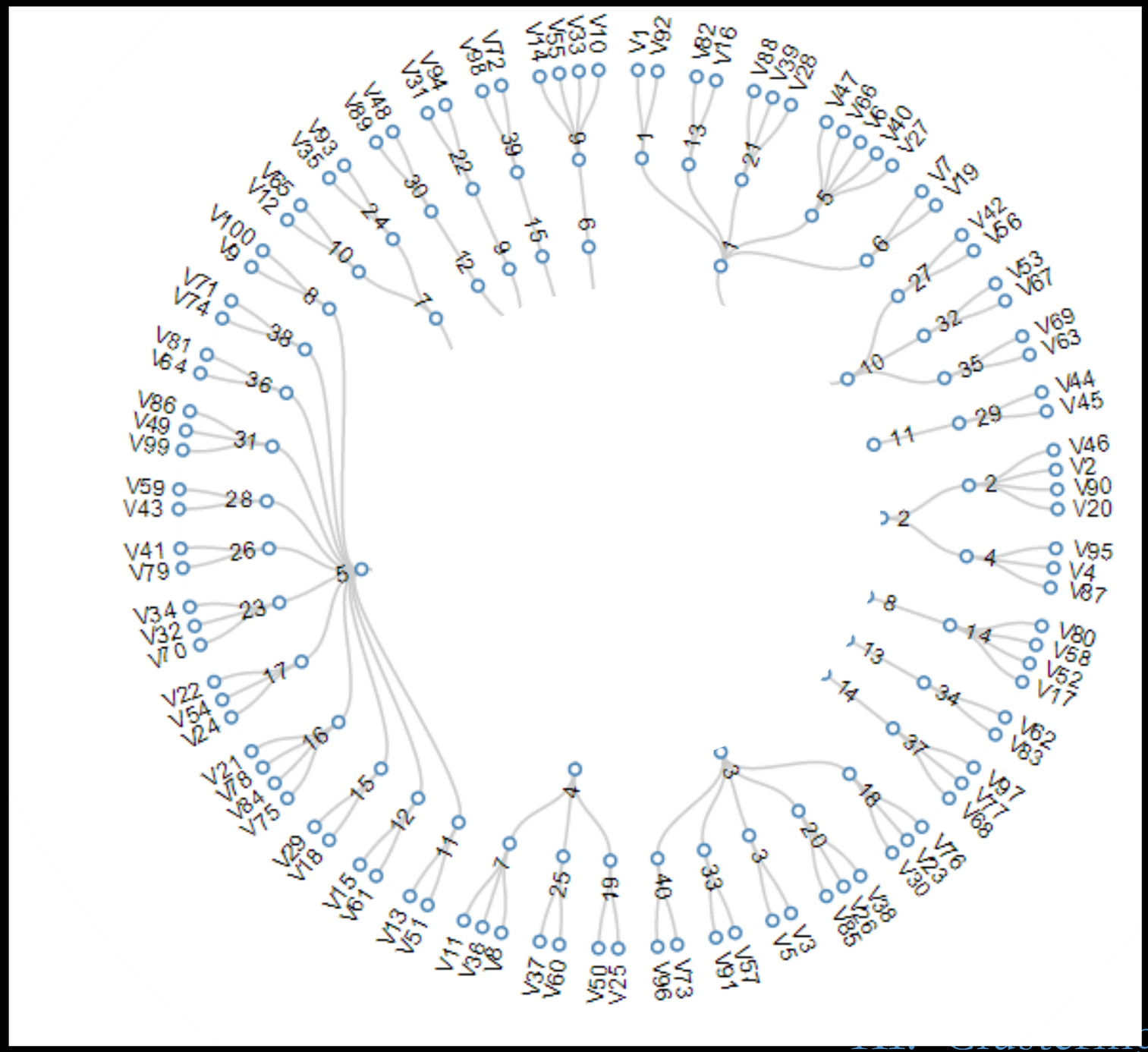

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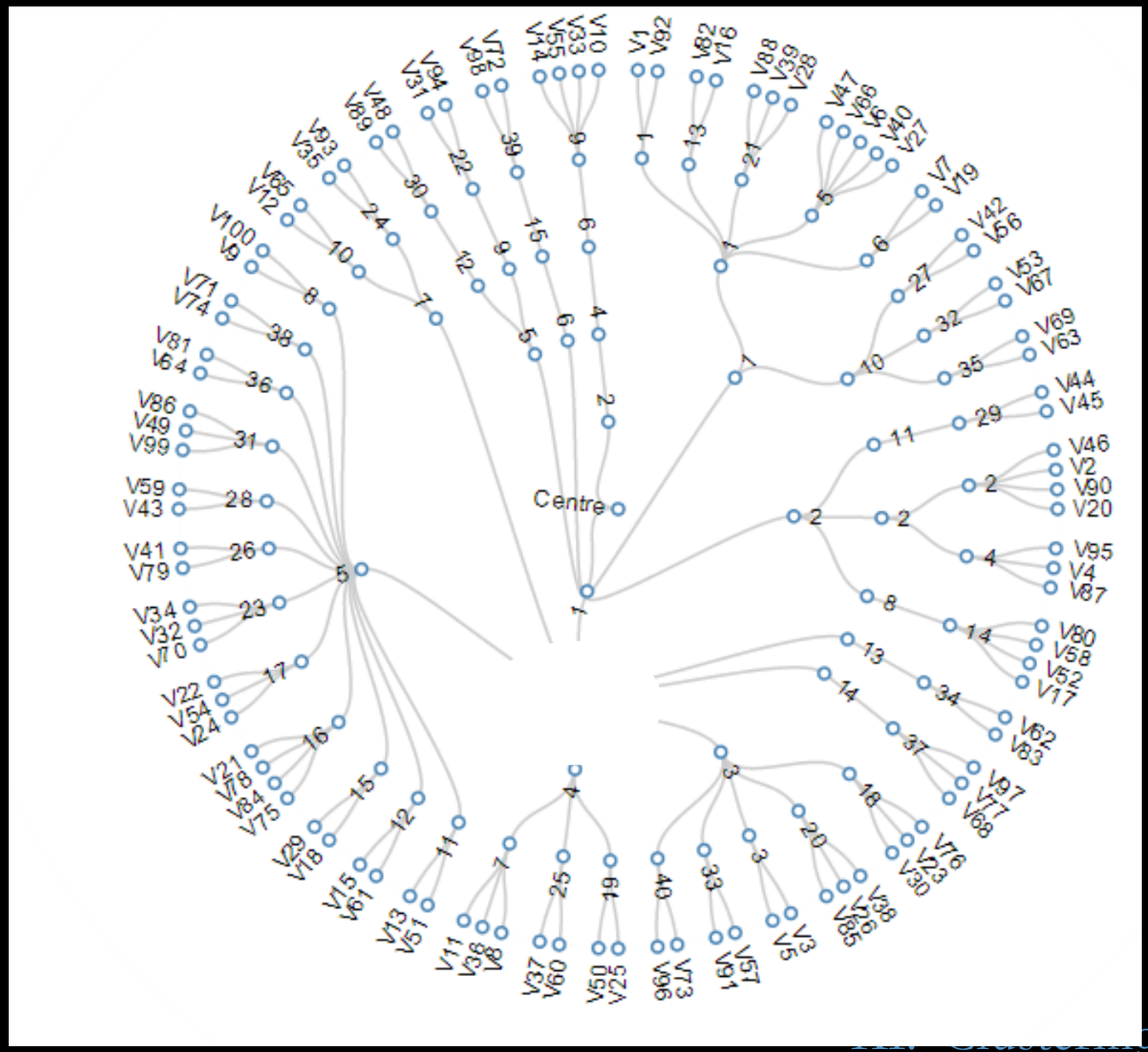
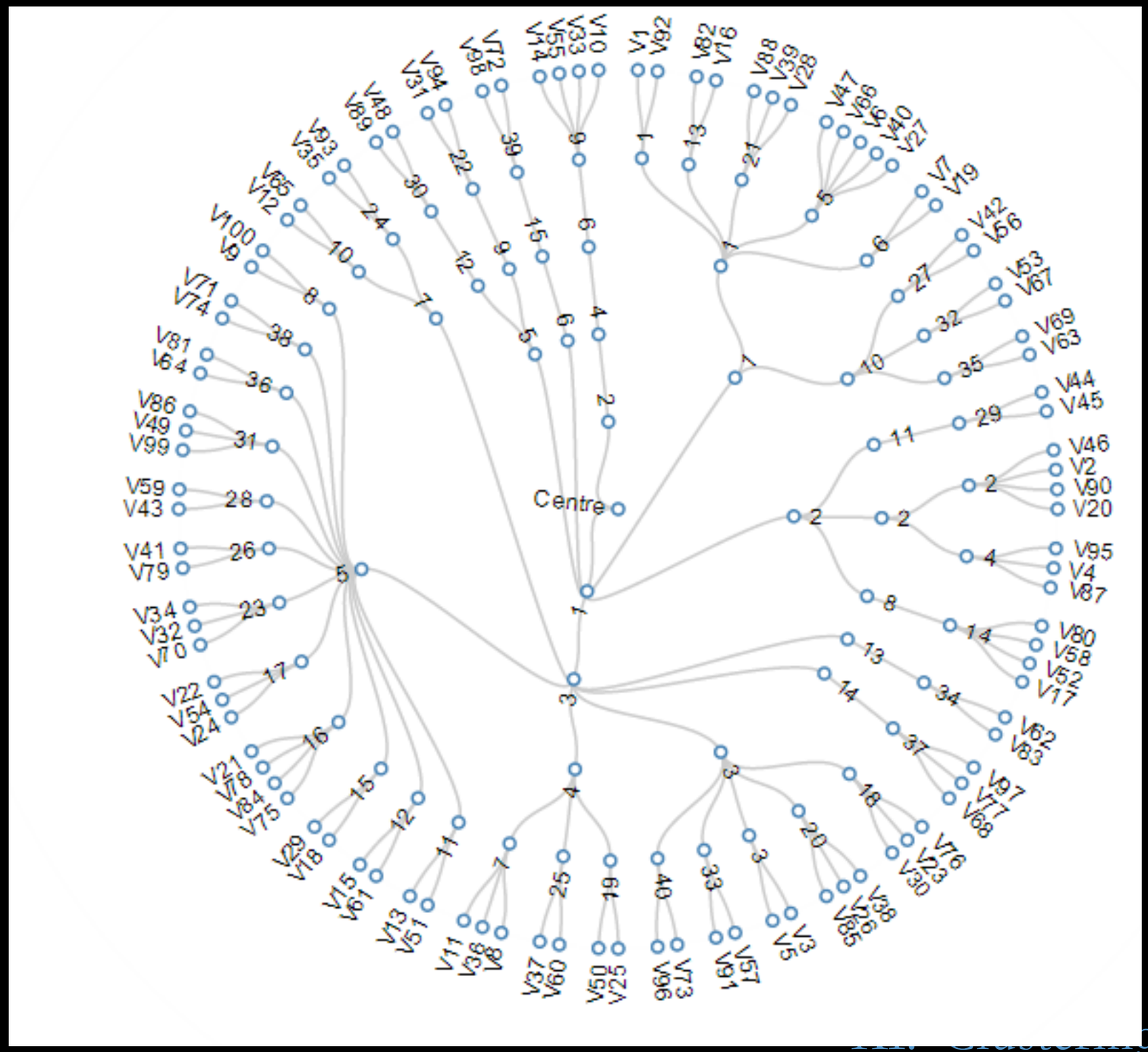


CUSP

hierarchical clustering

agglomerative
bottom-up

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



CUSP

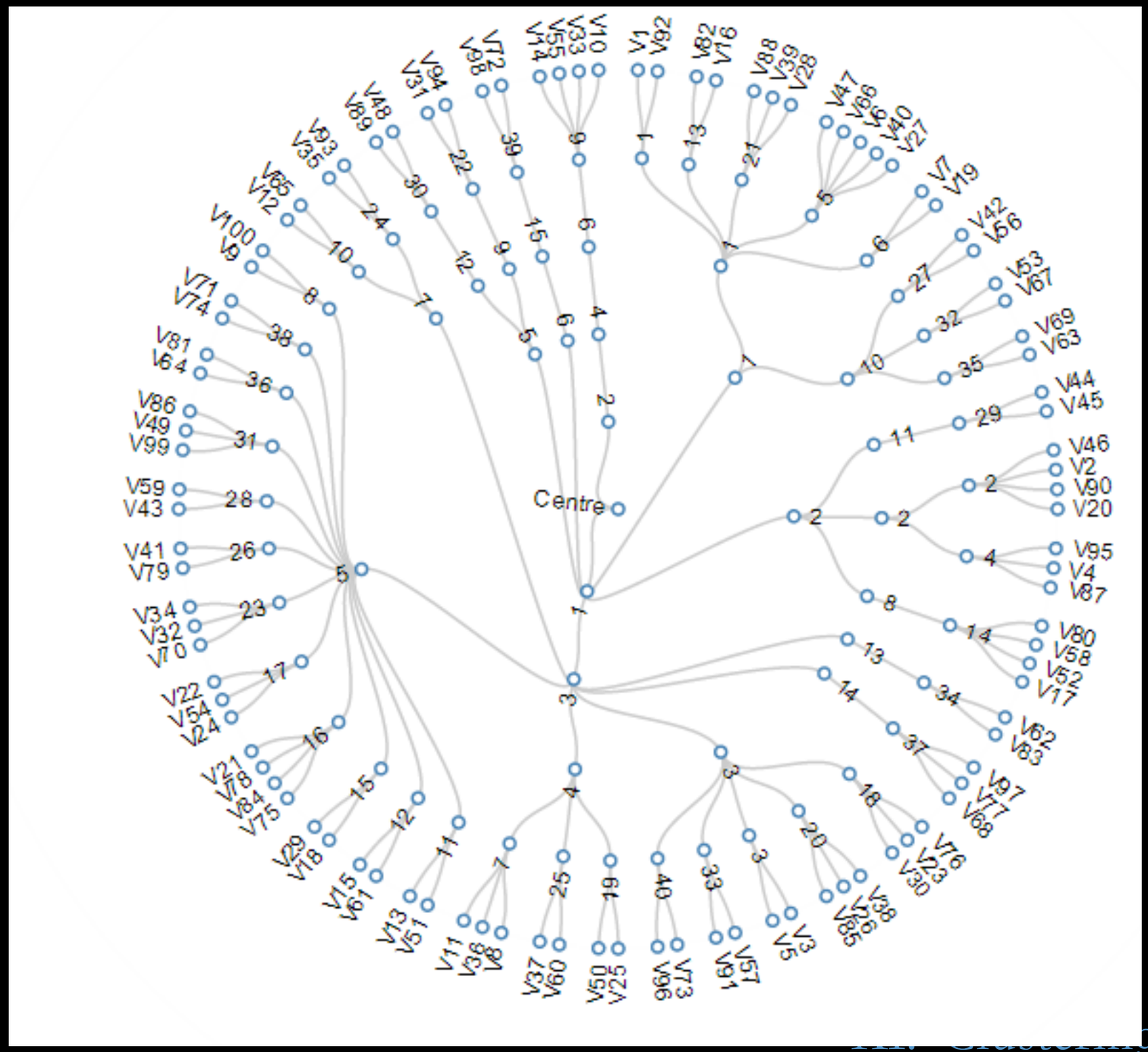
hierarchical clustering

agglomerative
bottom-up

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

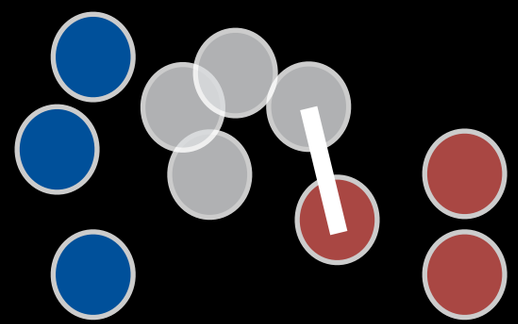
it is slow, though it can be optimize: complexity

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

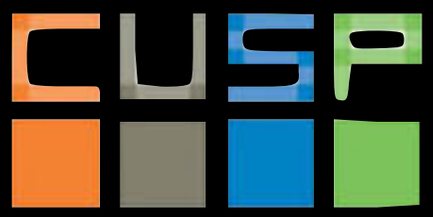


hierarchical clustering

agglomerative
bottom-up



Requires to define
- a distance &
- a “linkage”



hierarchical clustering

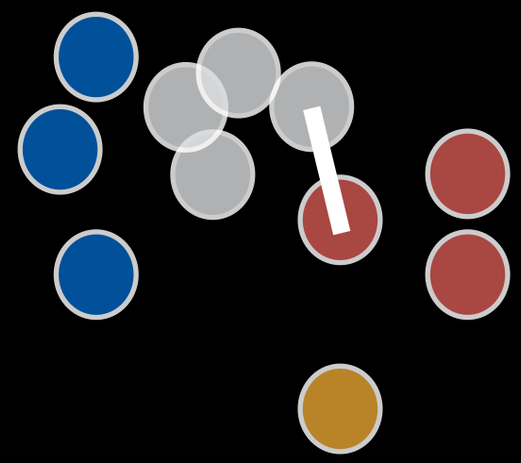
agglomerative
bottom-up

single link distance

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

complete link distance

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



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hierarchical clustering

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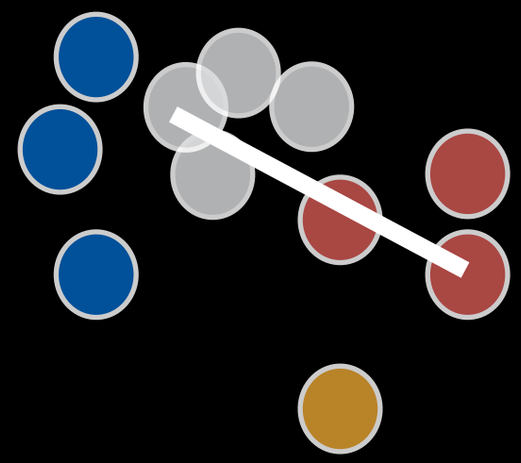

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hierarchical clustering

agglomerative
bottom-up

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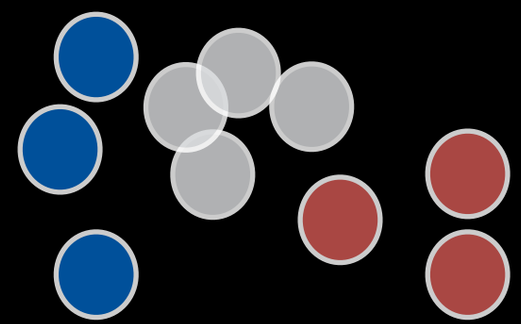
$D(c1,c2) = \min(D(x_{c1}, x_{c2}))$

complete link distance

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

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



a common distance:

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:

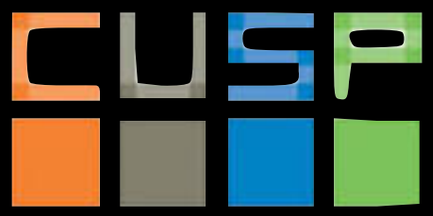
- Eucledian and other Minchowski metrics
- geospacial distances
- metrics for non continuous data

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

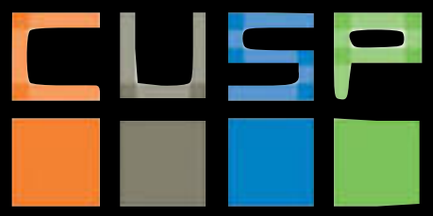


RESOURCES:

a comprehensive review of clustering methods

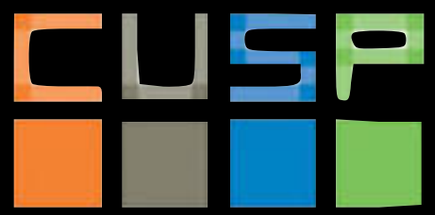
Data Clustering: A Review, Jain, Mutry, Flynn 1999
https://www.cs.rutgers.edu/~mlittman/courses/lightai03/jain99data.pdf

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/



Fourier

$$F(\omega) = \frac{1}{2\pi} \int f(t) e^{-i\omega t} \, dt$$



Fourier

$$F(\omega) = \frac{1}{2\pi} \int f(t) e^{-i\omega t} \, dt$$

takes a function in time domain

Fourier

$$F(\omega) = \frac{1}{2\pi} \int f(t) e^{-i\omega t} \, dt$$

takes a function in time domain

to a function in frequency domain

Fourier

$$F(\omega) = \frac{1}{2\pi} \int f(t) e^{-i\omega t} \, dt$$

takes a function in space domain

to a function in spatial frequency domain

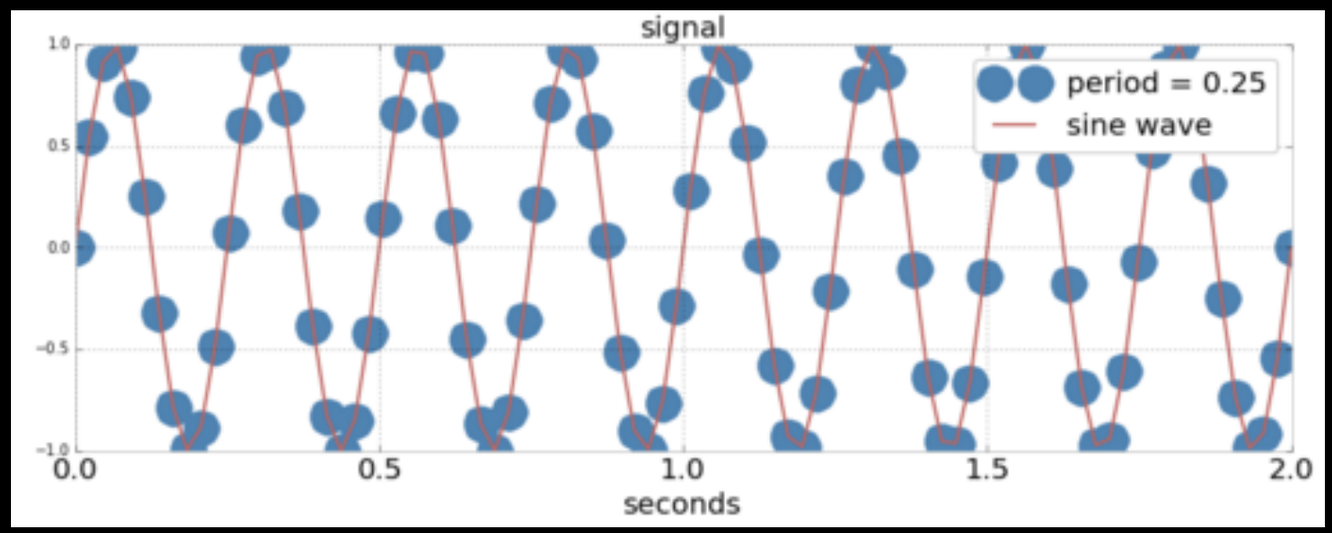
Fourier

$$F(\omega) = \frac{1}{2\pi} \int f(t) e^{-i\omega t} \, dt$$

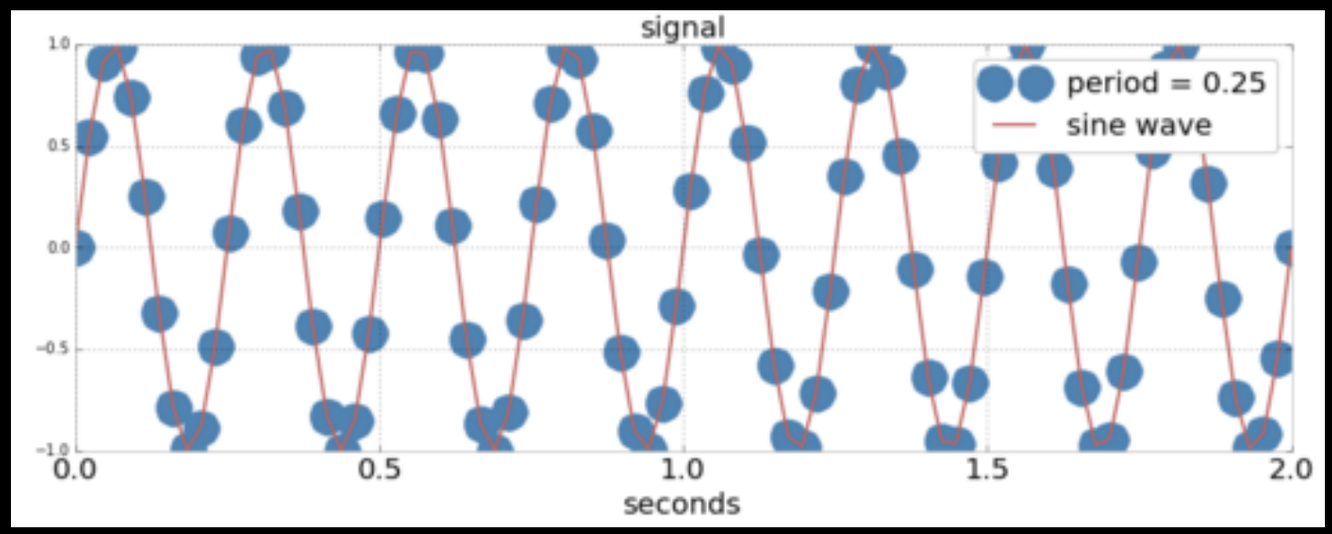
takes a function in space domain
f(t) is measured in seconds

to a function in spatial frequency domain
f(t) is measured in 1/seconds
or Hz

Fourier


signal
period = 0.25
sine wave
1.0
0.5
0.0
−0.5
−1.0
0.0
0.5
1.0
1.5
2.0
seconds

Fourier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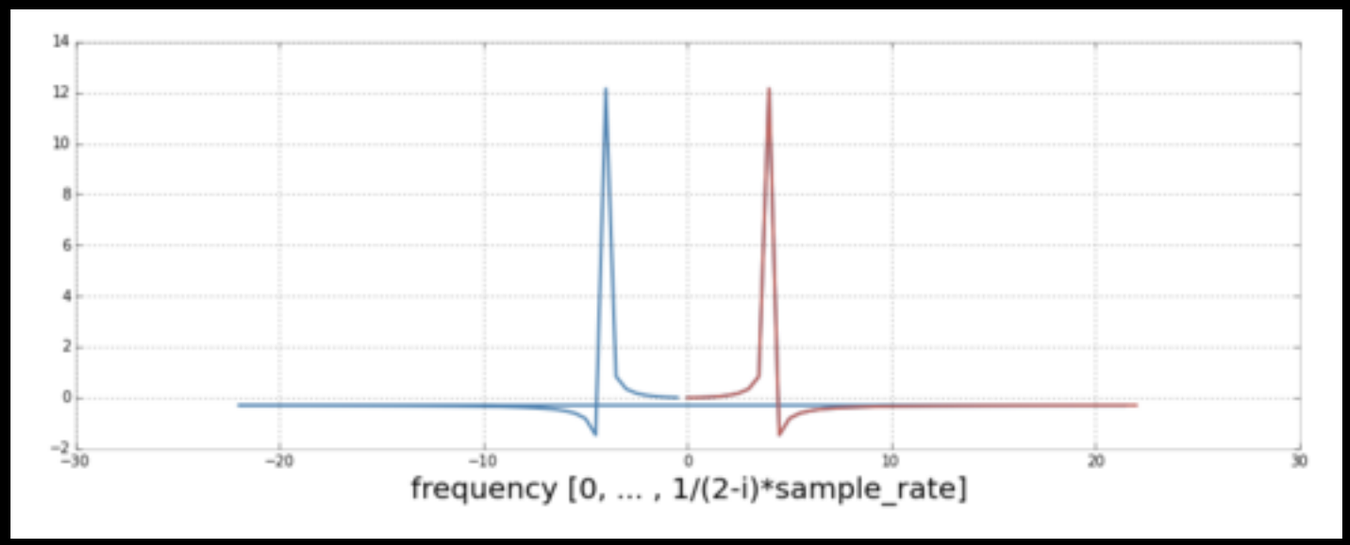
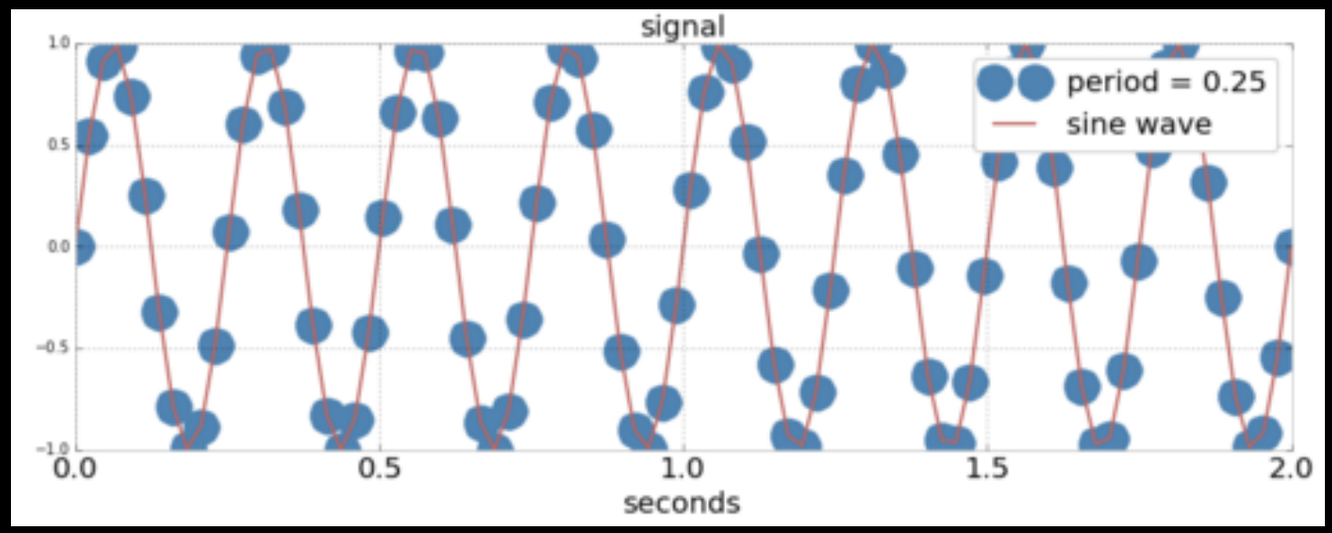
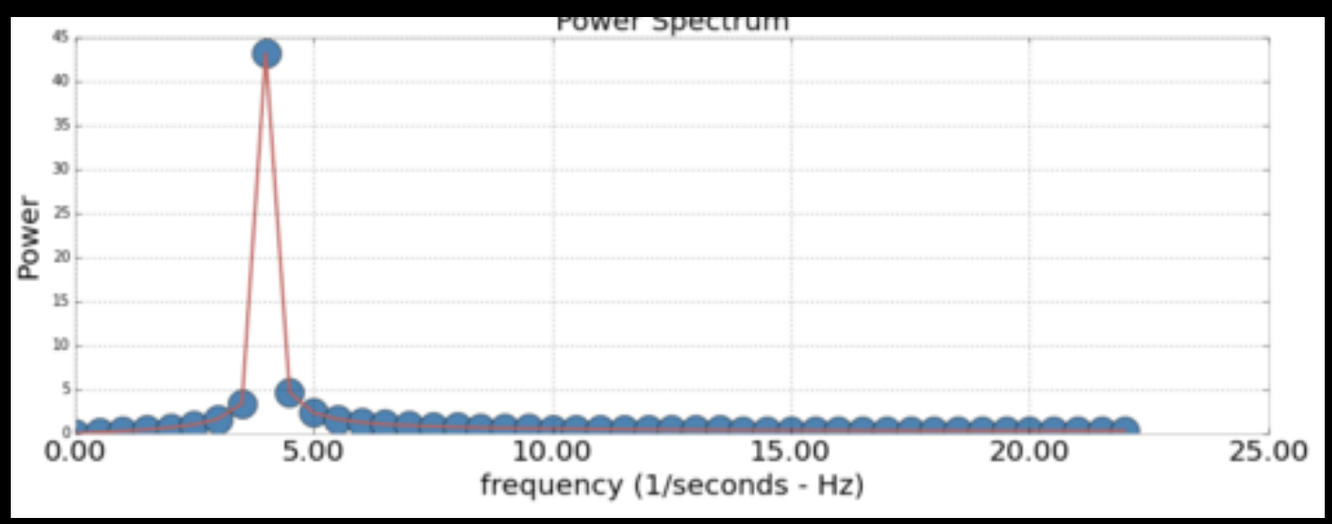

14
12
10
8
6
4
2
0
−2
−30
−20
−10
0
10
20
30
frequency [0, ... , 1/(2-i)*sample_rate]

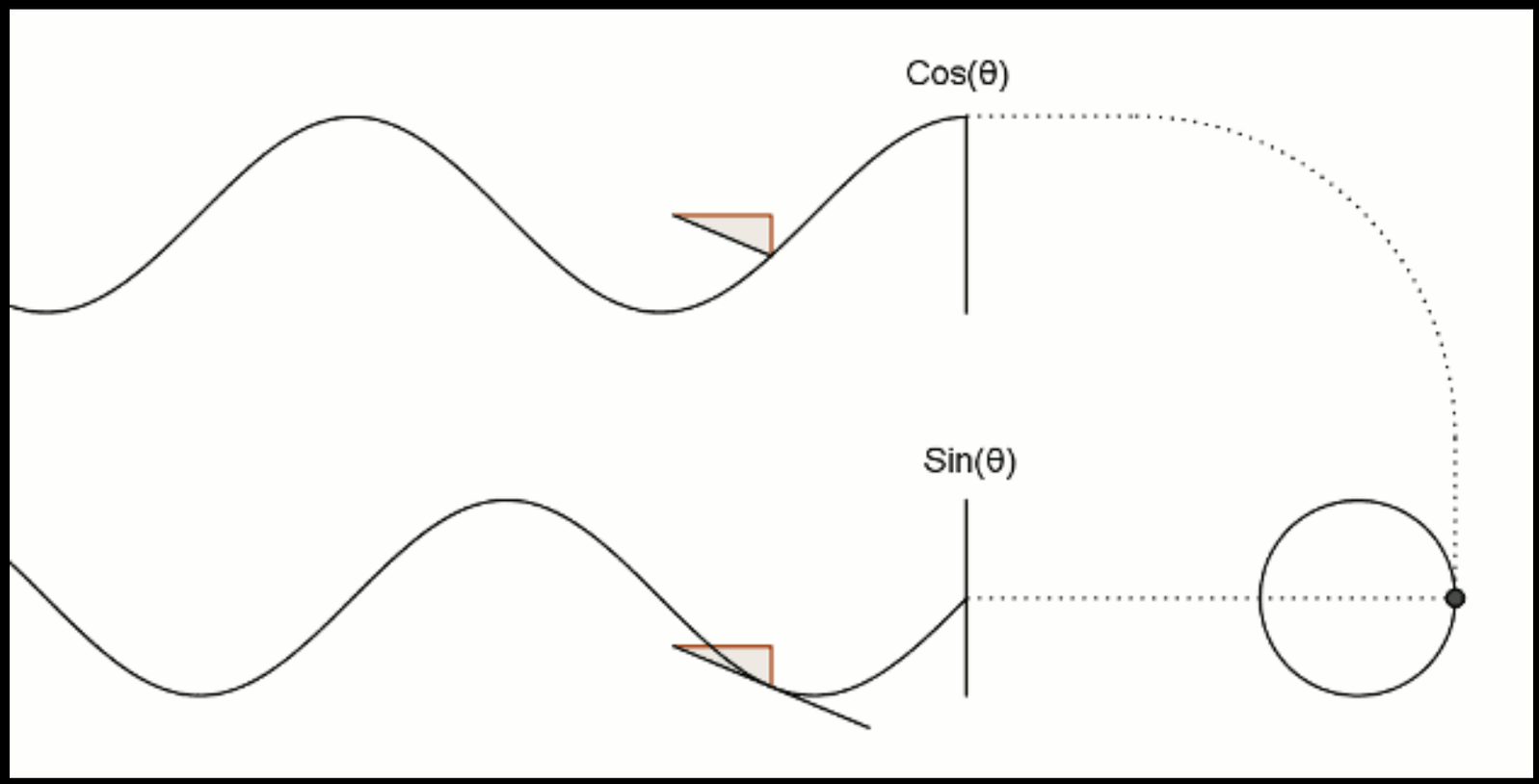
The absolute value of the square of the Fourier transform this is called a Power spectrum.
High value of the power spectrum indicate periodicity at the corresponding frequency

Fourier





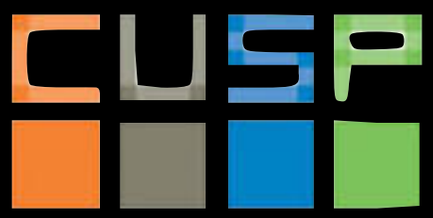
Cosine and Sine… just in case



http://www.businessinsider.com/7-gifs-trigonometry-sine-cosine-2013-5

Fourier

https://github.com/fedhere/UInotebooks/blob/master/fourier.ipynb



Homework:

Reading: an excellent analysis of time series
by Jake Vander Plas
(UW e-science center)

https://jakevdp.github.io/blog/2014/06/10/is-seattle-really-seeing-an-uptick-in-cycling/

READING:

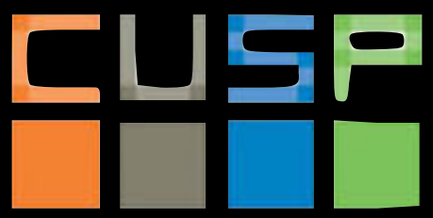
your data aint that big…
https://www.chrisstucchio.com/blog/2013/hadoop_hatred.html

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
```