CS109 – Data Science

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AWS Clusters

- New and updated instructions for Spark 1.5 are on Piazza:

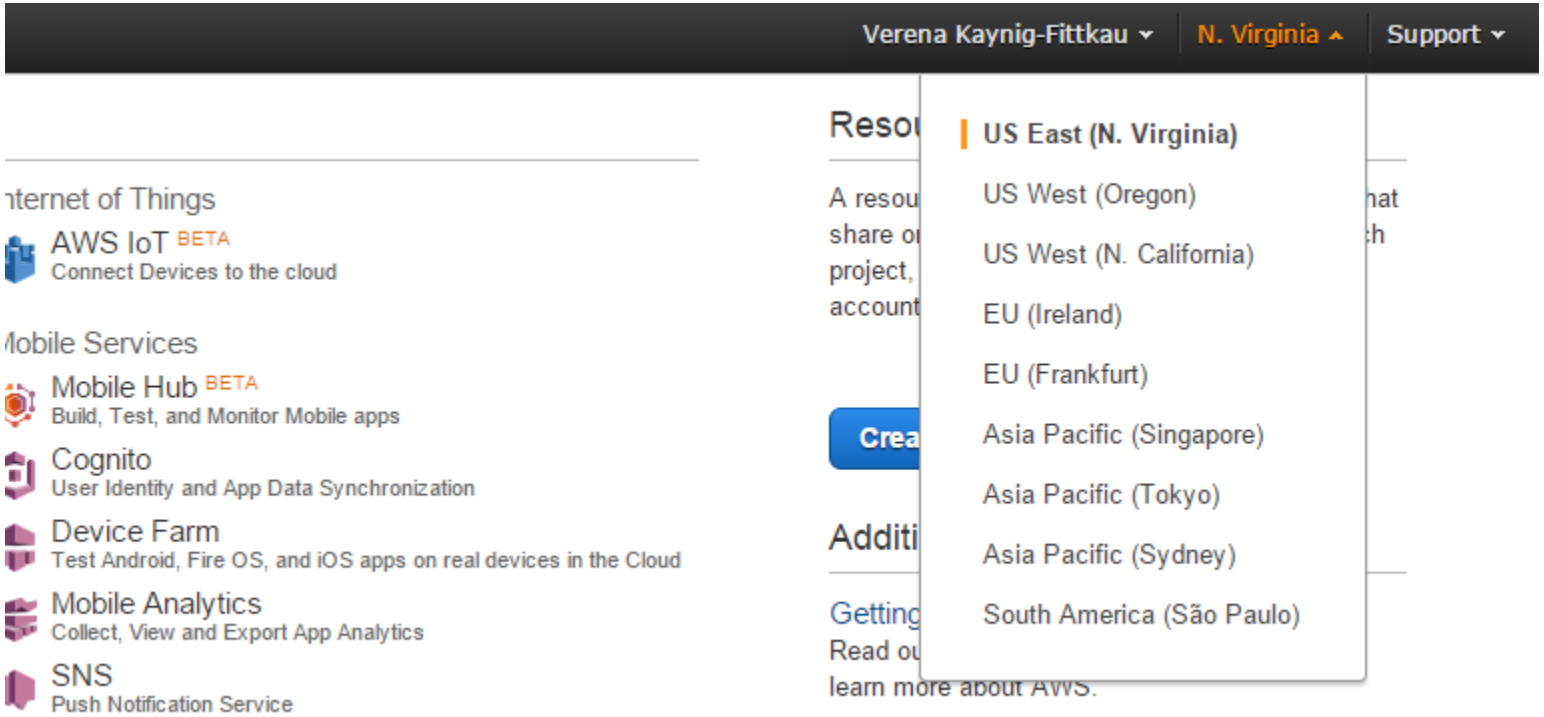
https://piazza.com/class/icf0cypdc3243c?cid=1369

Avoid Unnecessary Charges!

- Look at AWS console > Services > EMR
- There should be some terminated clusters there
- Check the region on the top right corner
- Make sure to change it to US East

https://piazza.com/class/icf0cypdc3243c?cid=1256

Region Setting in AWS



Announcements

- Final project
  - Team assignments have been posted to piazza
  - Make sure you are in a 3-4 person team
  - Try and date on the piazza thread
  - If you have problems write to staff@cs109.org

  - Project proposals are due on Thursday

  https://piazza.com/class/icf0cypdc3243c?cid=1317

Final Project Proposal

- Submit just **one form per team**.
- Do it as **early as possible**!
- No project approval until you meet your TF

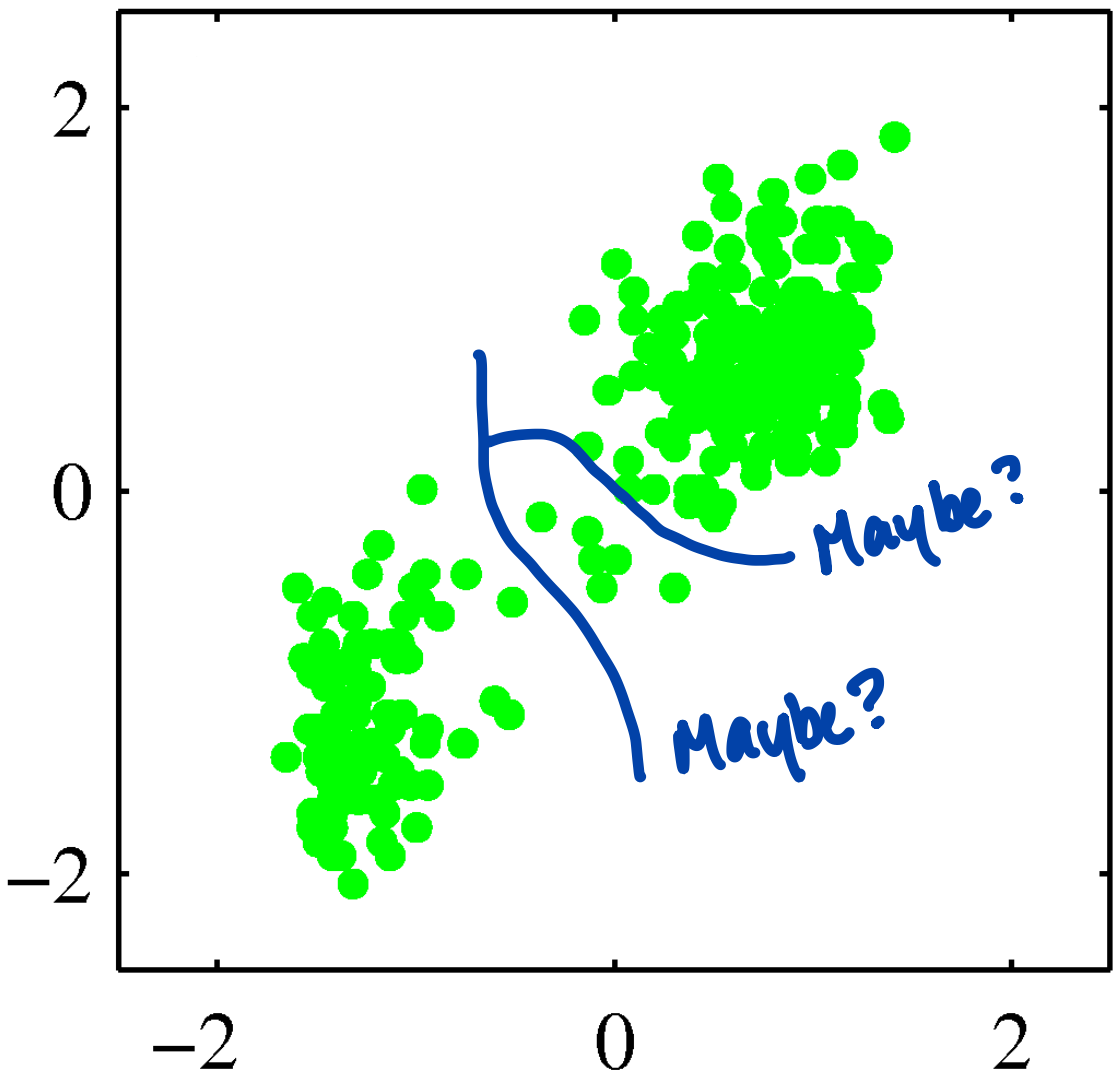
https://piazza.com/class/icf0cypdc3243c?cid=1317

Supervised vs. Unsupervised

- We mainly talked about supervised learning so far
- Joe already moved to unsupervised with LDA
- In these settings we have **no labels** in our training data.

Unsupervised Setting

No y value



Bishop, “Pattern Recognition and Machine Learning”, Springer, 2006

Unsupervised Learning

find existing and new patterns

- Find patterns in unlabeled data
- Sometimes used for a supervised setting in which labels are hard to get
- Can identify new patterns that you were not aware of.

Clustering Applications

- Google image search categories → above the general list of pictures
- Author Clustering: http://academic.research.microsoft.com/VisualExplorer#1048044
- Opening a new location for a hospital, police station, etc. → optimizing.
- Outlier detection

Can often use unsupervised then use supervised.

Unsupervised Learning

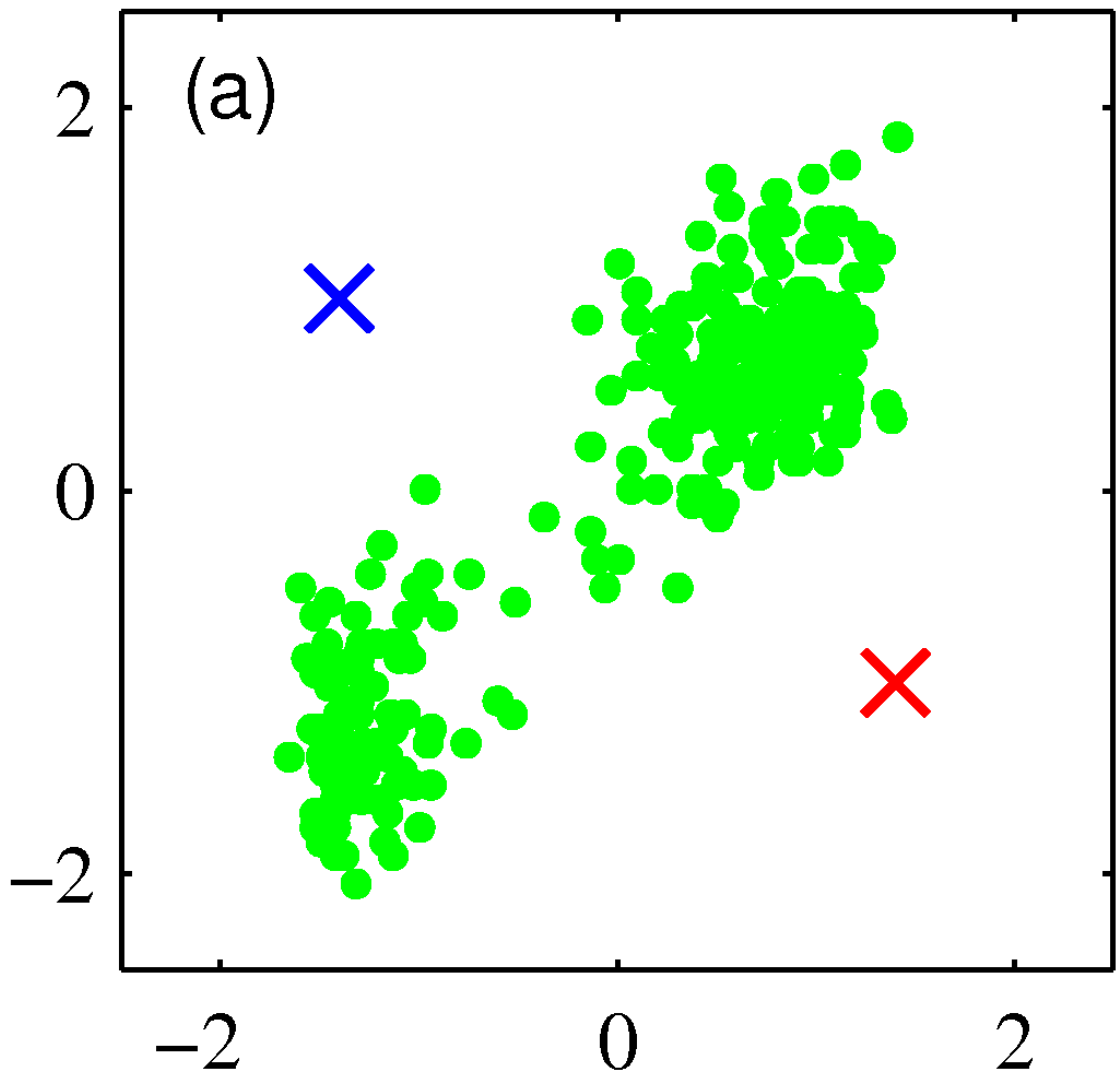
- K-means
- Mean-shift
- Hierarchical Clustering

- Rand index, stability

K-means – Algorithm

- Initialization:
  - choose k random positions
  - assign cluster centers $\mu^{(j)}$ to these positions

K-means



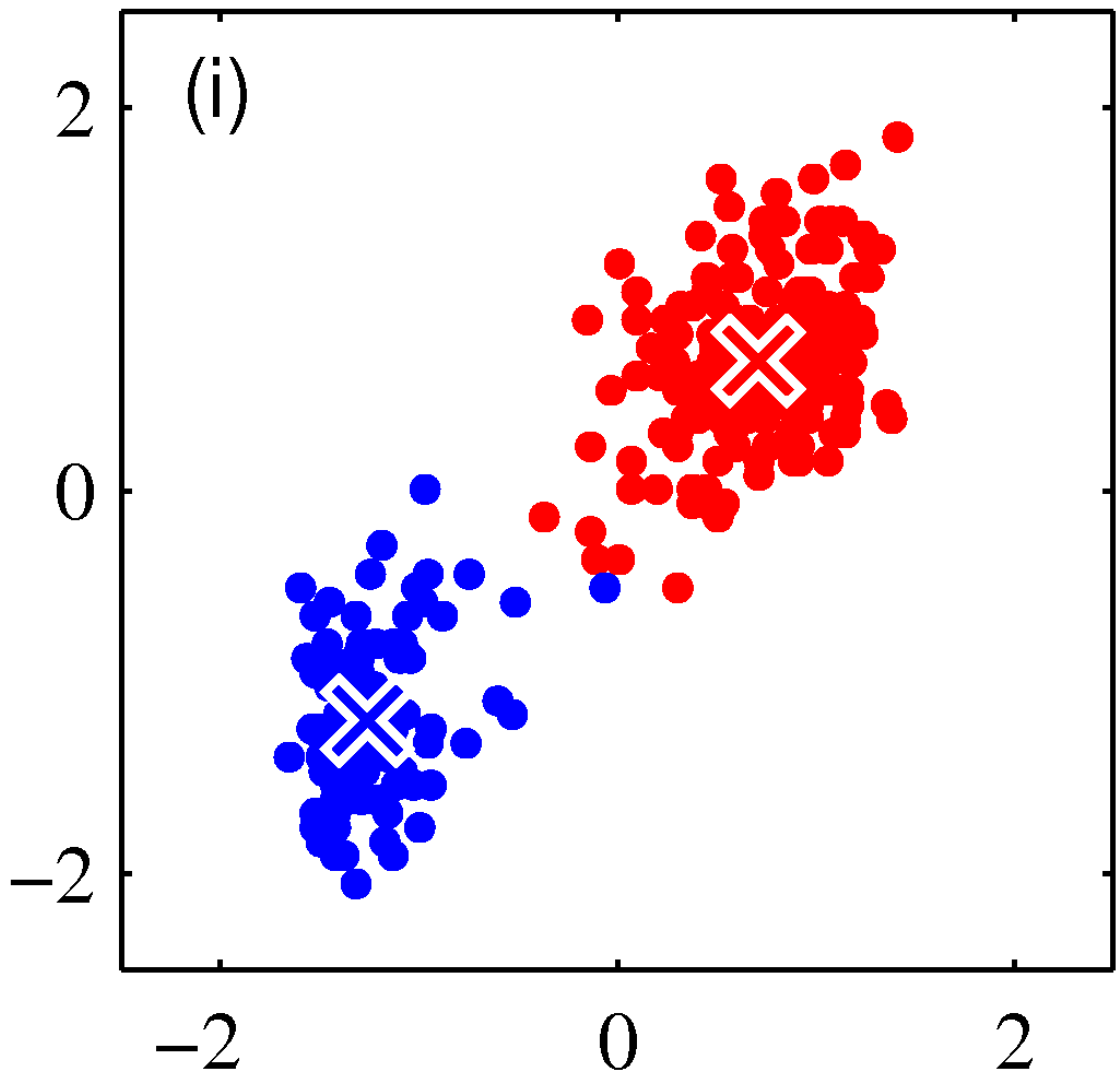
Bishop, “Pattern Recognition and Machine Learning”, Springer, 2006

K-means

- Until Convergence:
  - Compute distances $||x^{(i)} - \mu^{(j)}||$
  - Assign points to nearest cluster center
  - Update Cluster centers:

$$\mu^{(j)} = \frac{1}{N_j} \sum_{x_i \in C_j} x_i$$

K-means



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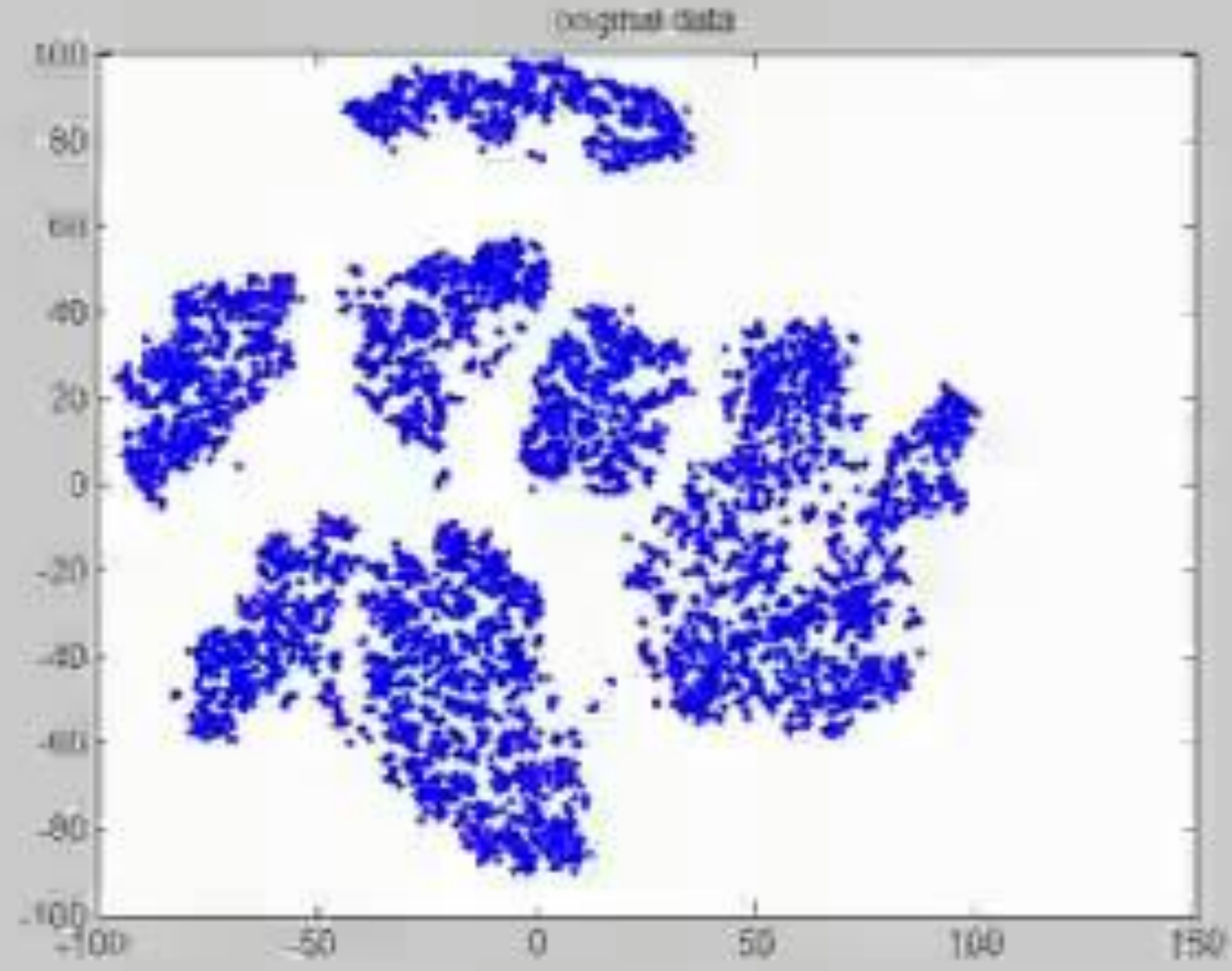

original data
100
80
60
40
20
0
-20
-40
-60
-80
-100
-100
-50
0
50
100
150

K-means Example

R

G

B

K-means Example

K-means Example

K-means Summary

- Guaranteed to converge
- Result depends on initialization

- Number of clusters is important

- Sensitive to outliers
  - Use median instead of mean for updates

Initialization Methods

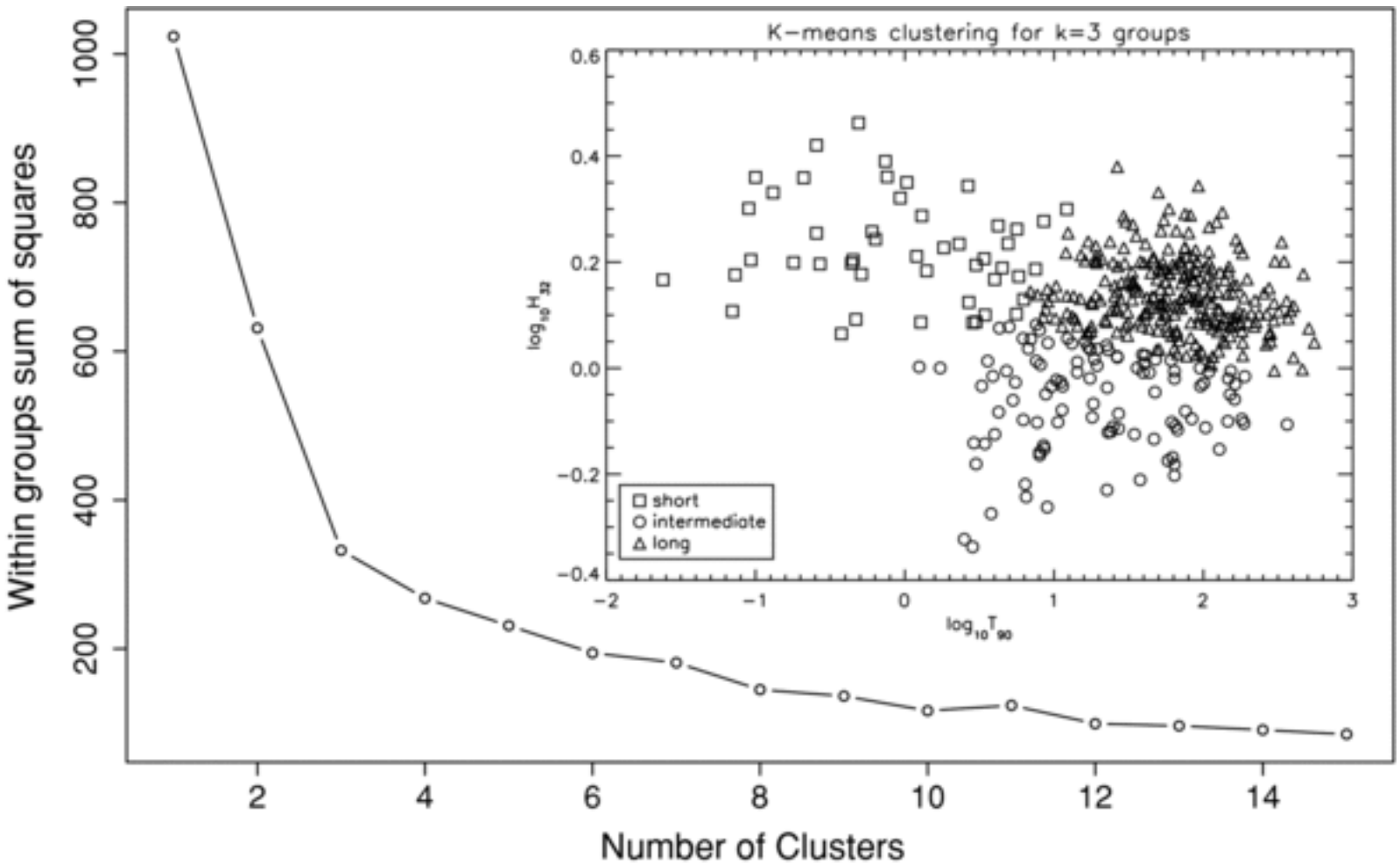
- Random Positions
- Random data points as Centers
- Random Cluster assignment to data points

- Start several times

How to find K

- Extreme cases:
  - K=1
  - K=N
- Choose K such that increasing it does not model the data much better.

“Knee” or “Elbow” method



http://m.iopscience.iop.org/article/10.1088/0004-637X/725/2/1955;jsessionid=9B96FCAF94036AA723BA5F9C78FB33D6.c1.iopscience.cld.iop.org

Cross Validation

- Use this if you want to apply your clustering solution to new unseen data

- Partition data into n folds
- Cluster on n-1 folds
- Compute sum of squared distances to centroids for validation set

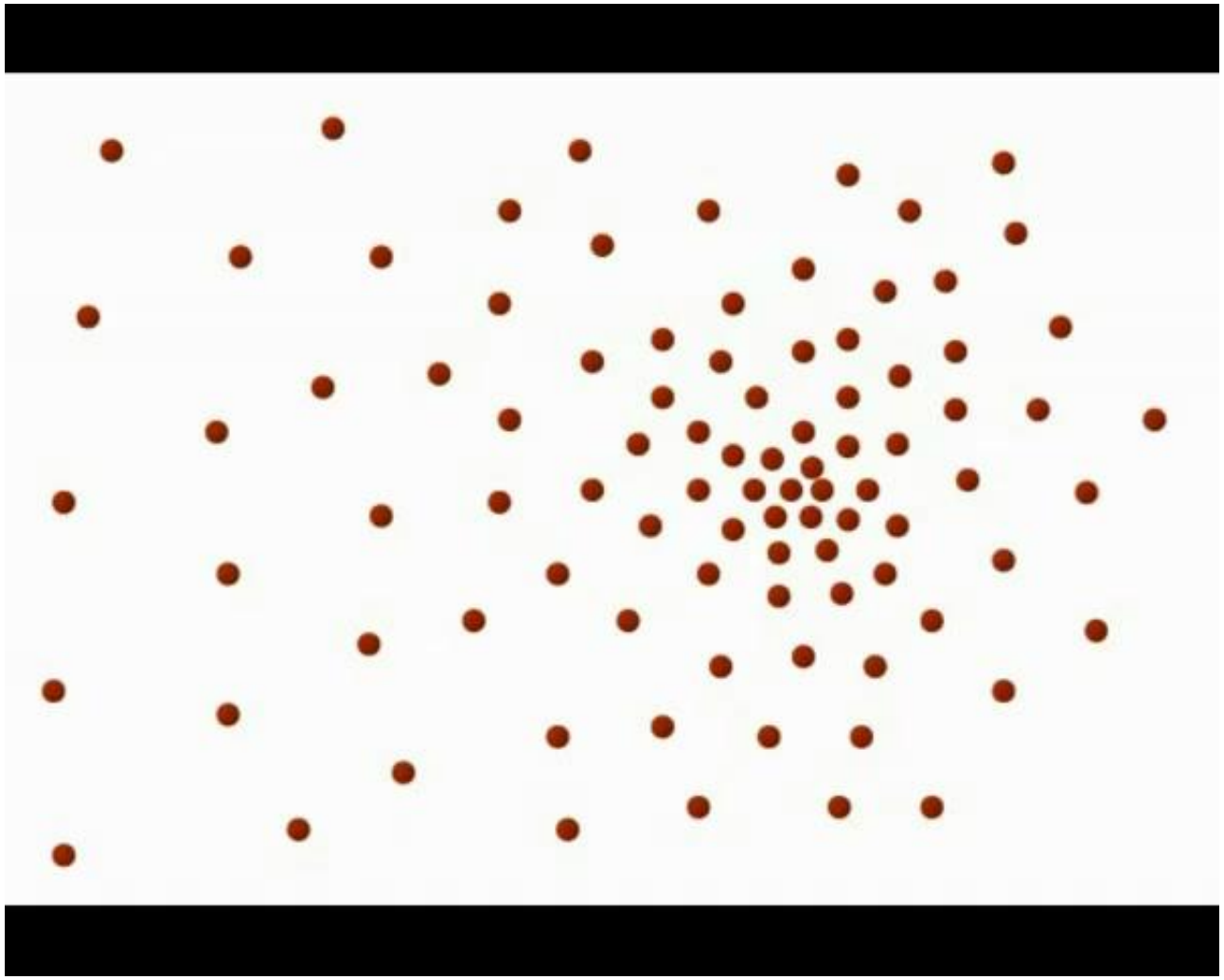
Getting Rid of K

- Having to specify K is annoying
- Can we do without?

Mean Shift

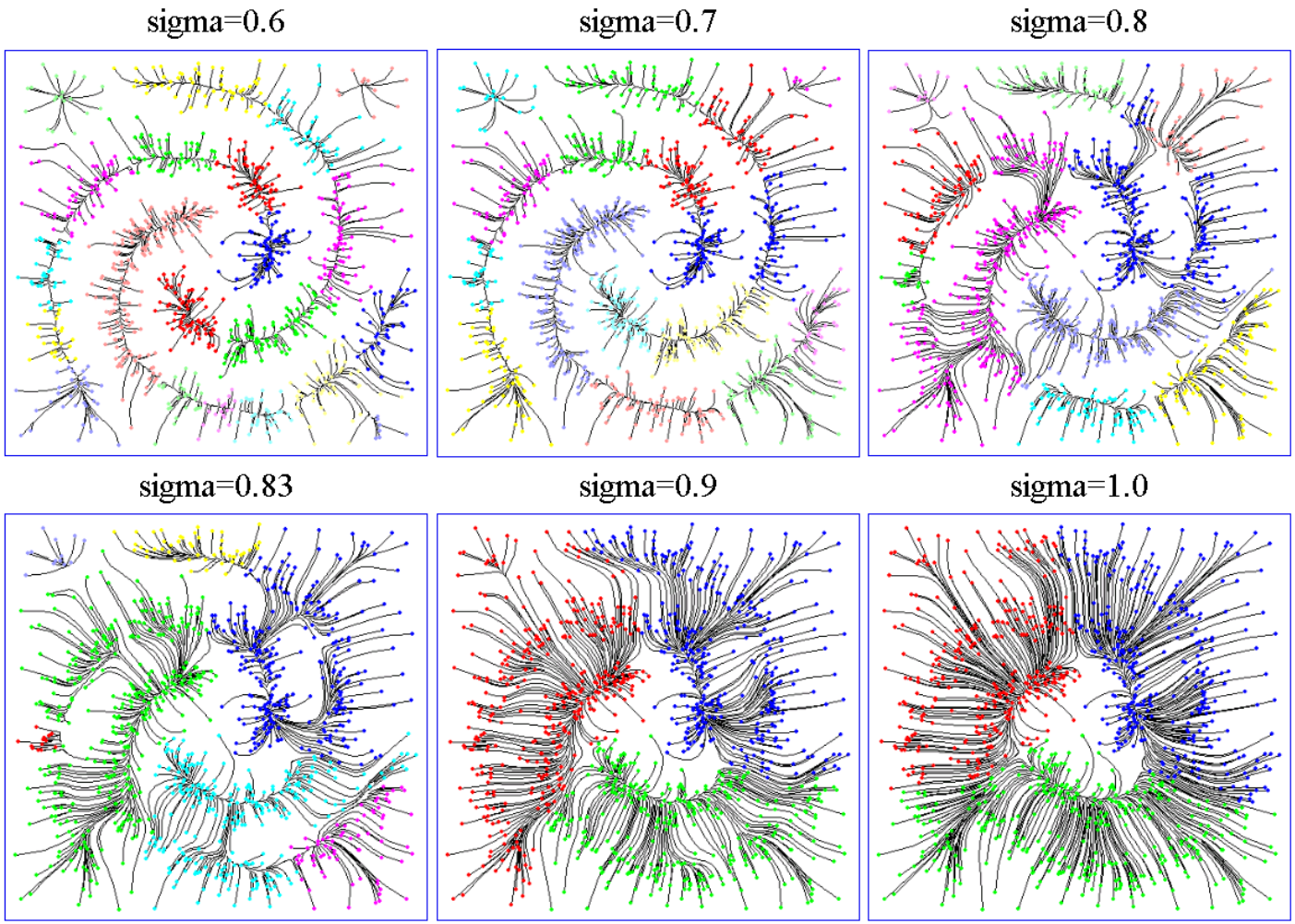
1. Put a window around each point
2. Compute mean of points in the frame.
3. Shift the window to the mean
4. Repeat until convergence

Mean Shift



http://www.youtube.com/watch?v=kmaQAsottT9s

Mean Shift



Fischer et al., “Clustering with the Connectivity Kernel“, NIPS (2003)

Mean Shift Summary

- Does not need to know number of clusters
- Can handle arbitrary shaped clusters
- Robust to initialization
- Needs bandwidth parameter (window size)
- Computationally expensive

- Very good article:

http://saravananthirumuruganathan.wordpress.com/2010/04/01/introduction-to-mean-shift-algorithm/

Multi-feature object trajectory clustering for video analysis

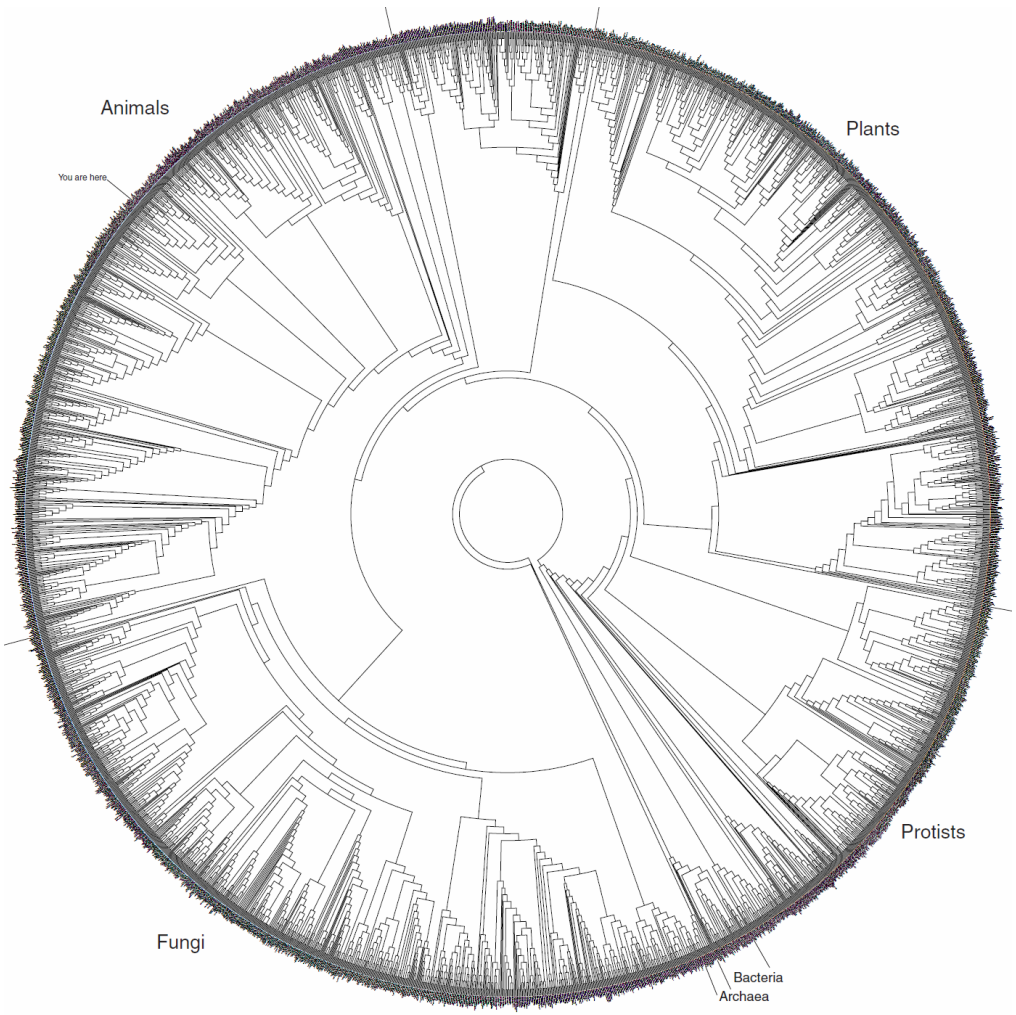
Nadeem Anjum Andrea Cavallaro

Parameters parameters

- For K means we need K and result depends on initialization
- For mean shift we need the window size and a lot of computation

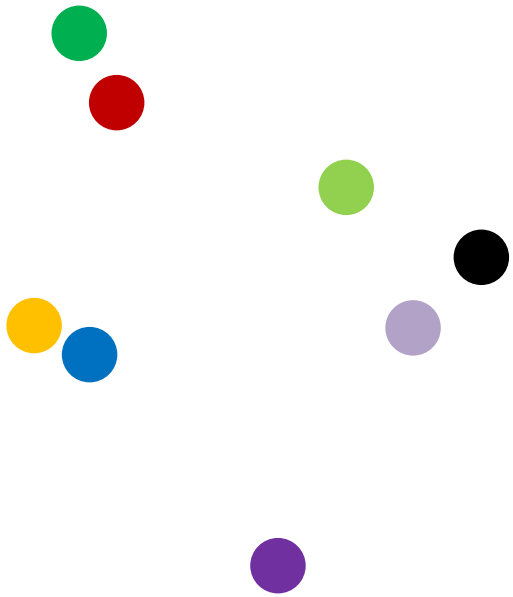
- Hierarchical Clustering keeps a history of all possible cluster assignments

Tree of Life



http://www.zo.utexas.edu/faculty/antisense/DownloadfilesToL.html

Hierarchical Clustering



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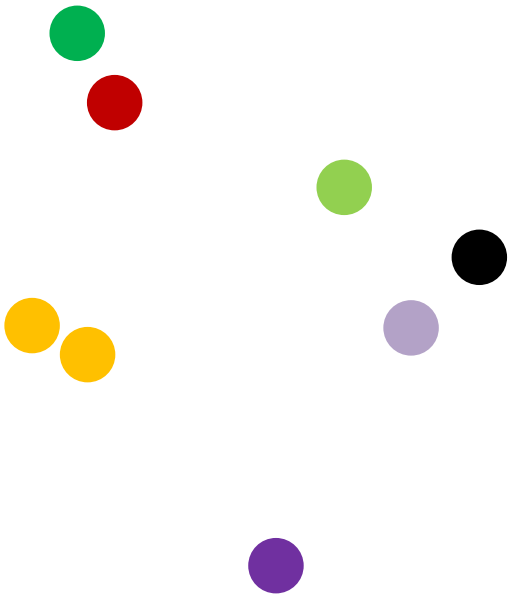

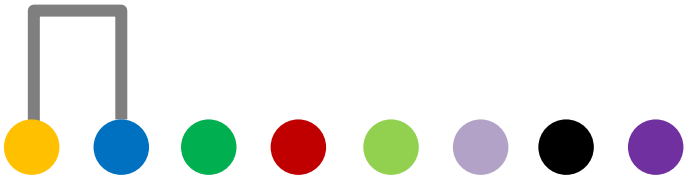

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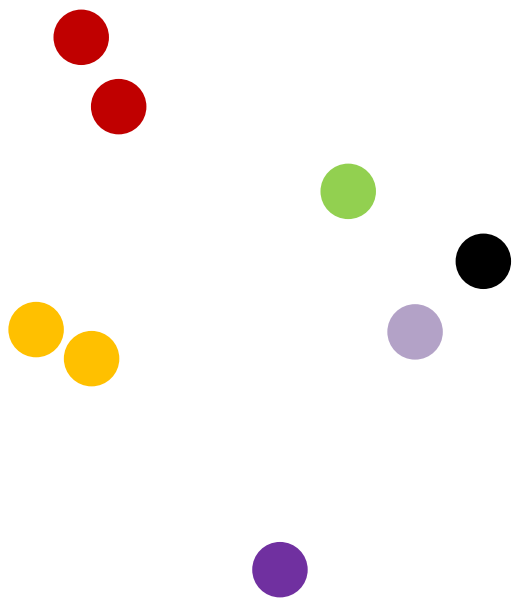
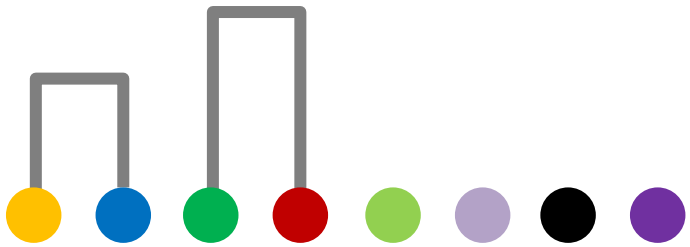
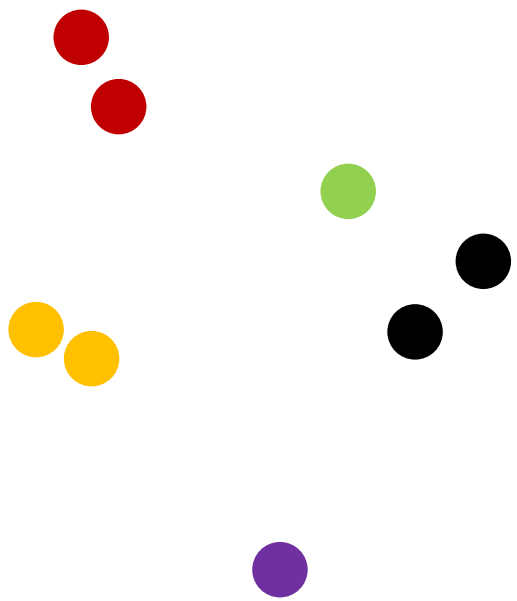
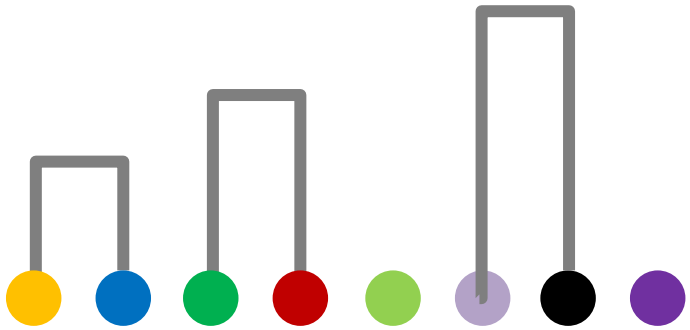


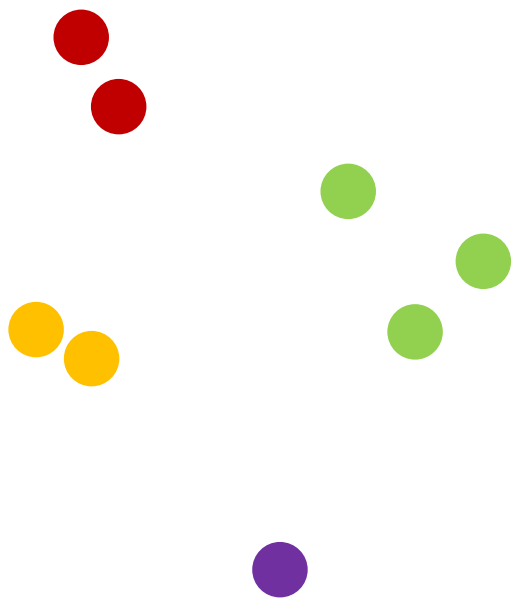


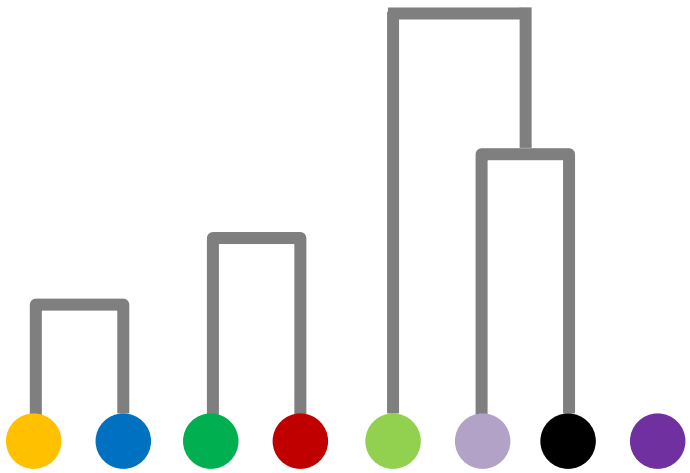
Hierarchical Clustering





Hierarchical Clustering





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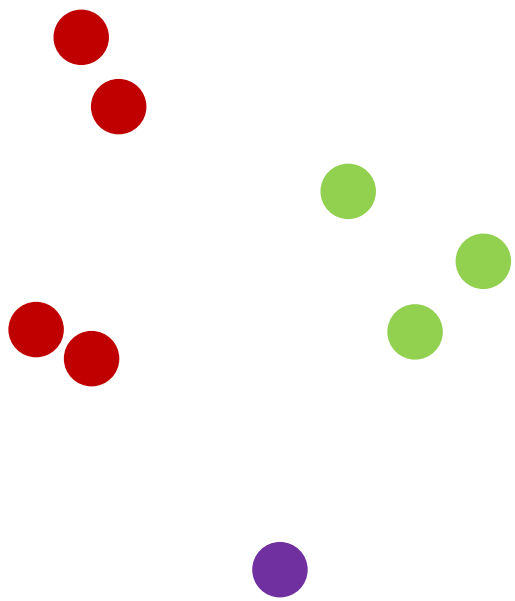

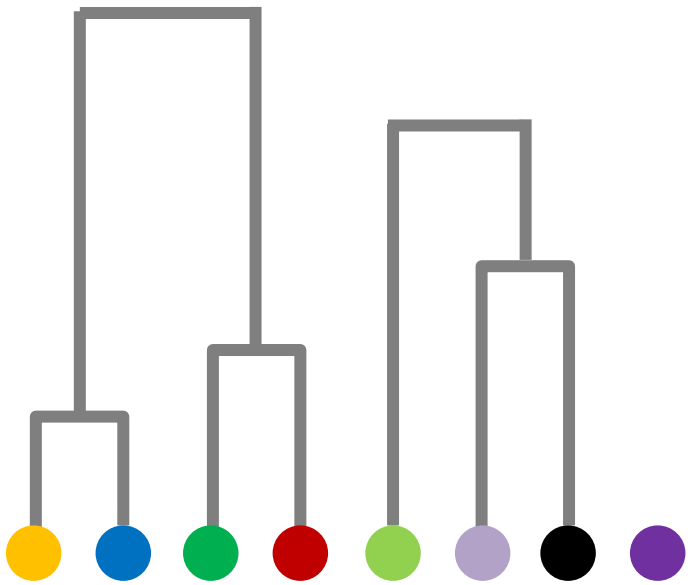

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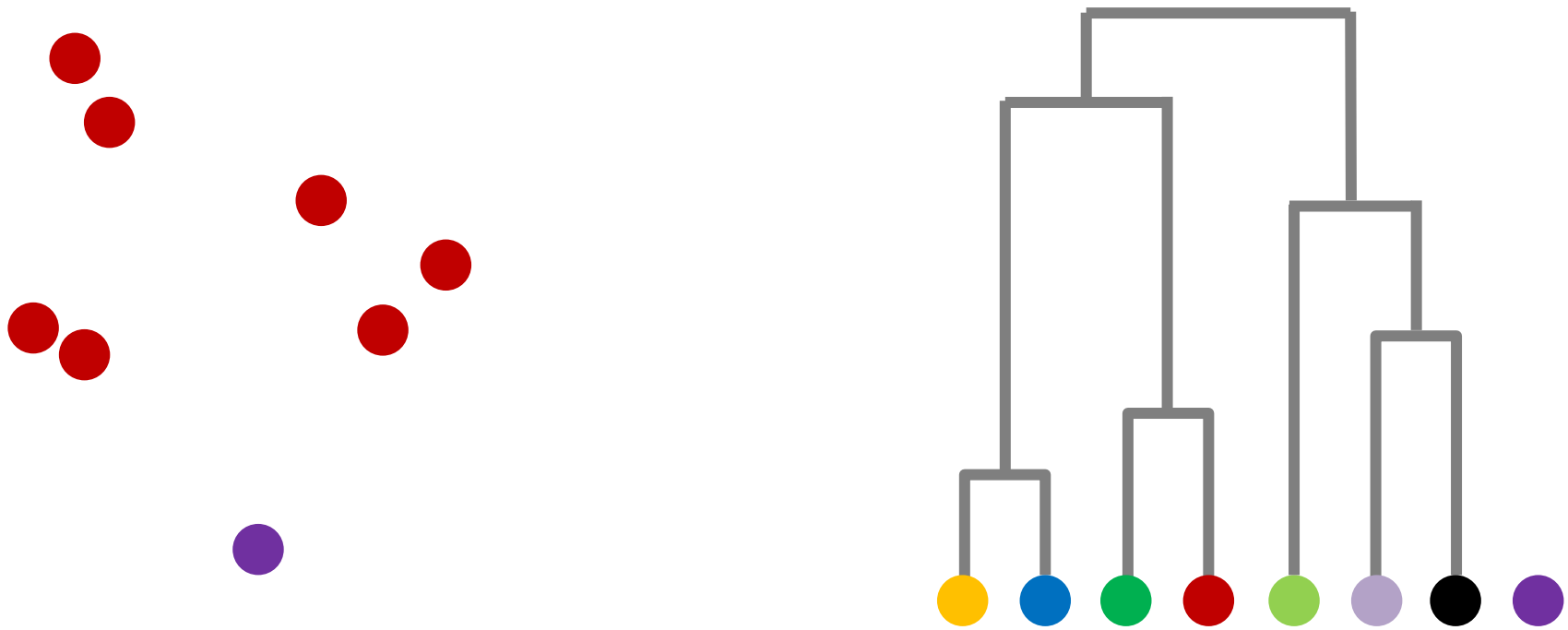

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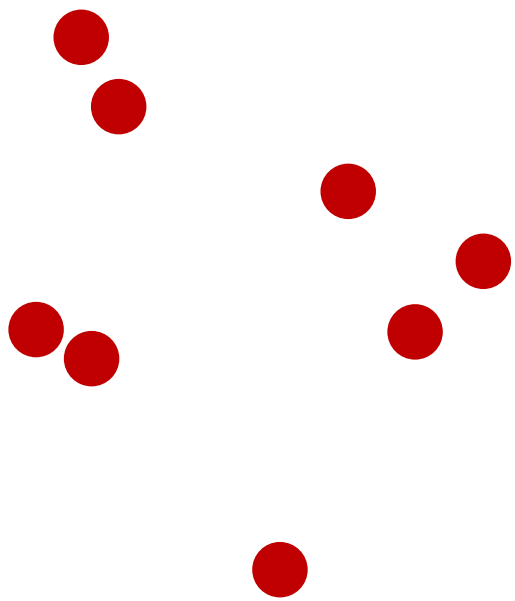

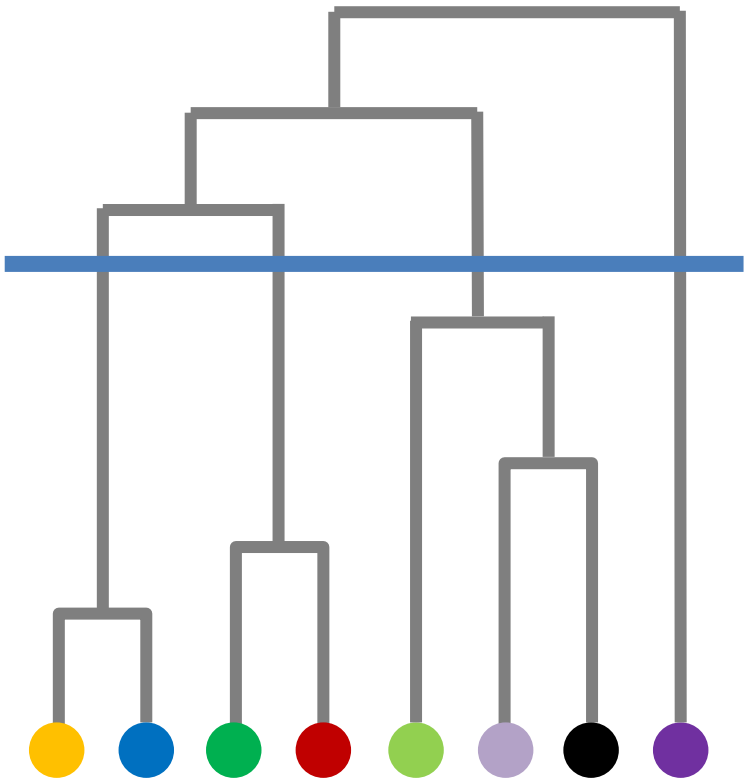

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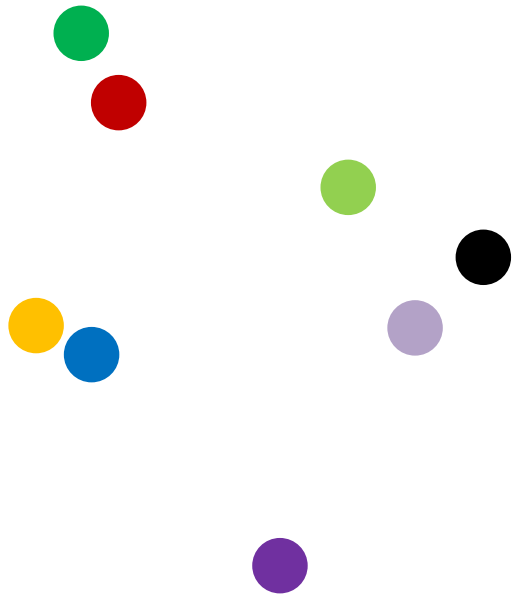
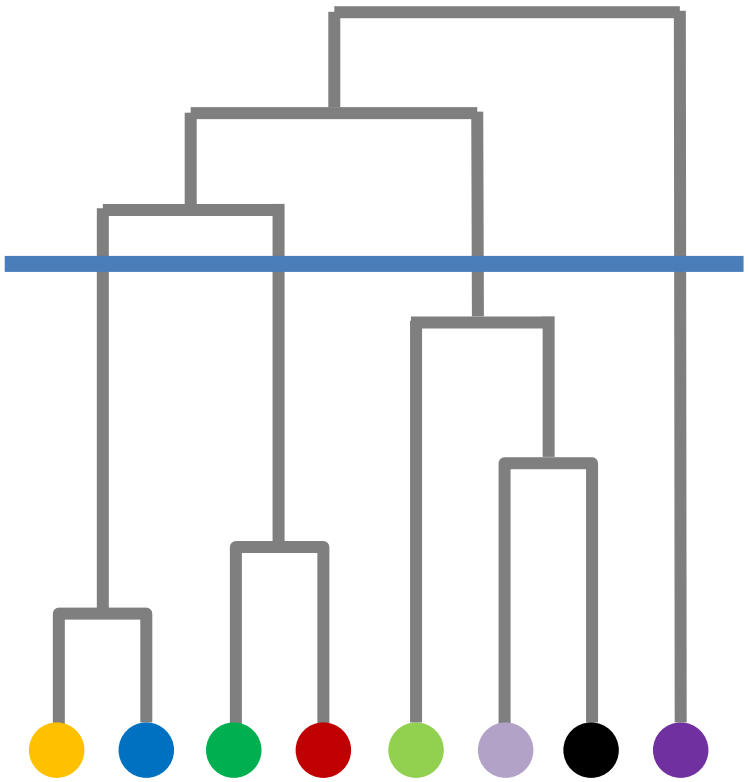


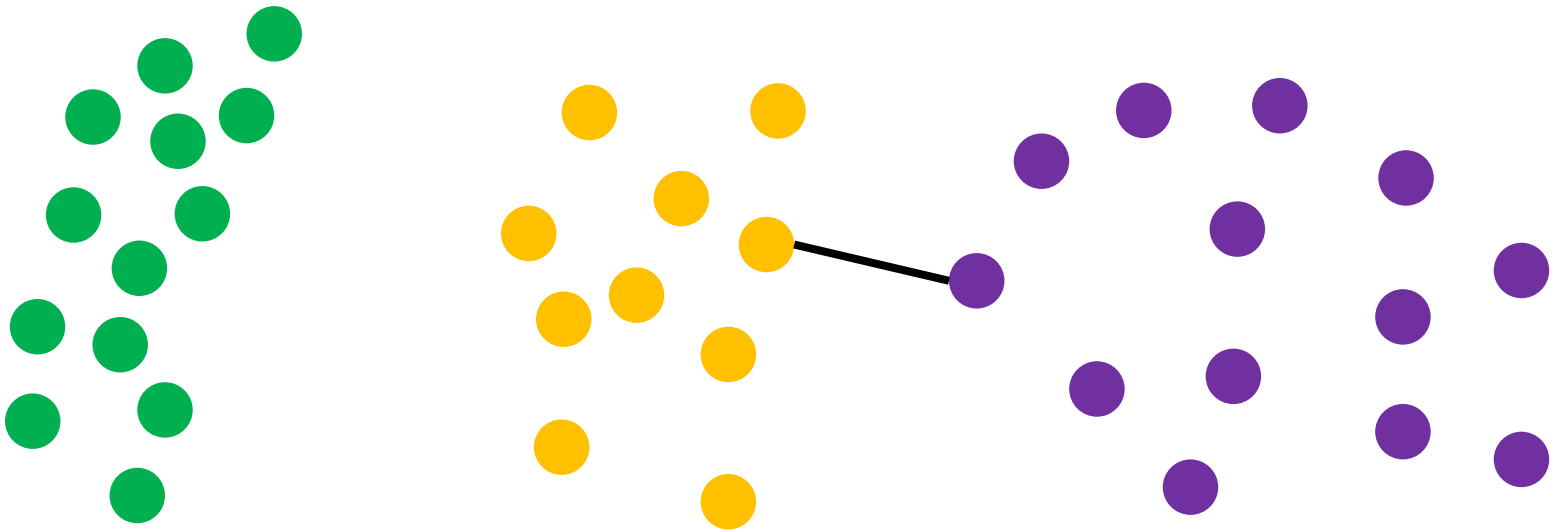


Hierarchical Clustering

- Produces complete structure
- No predefined number of clusters

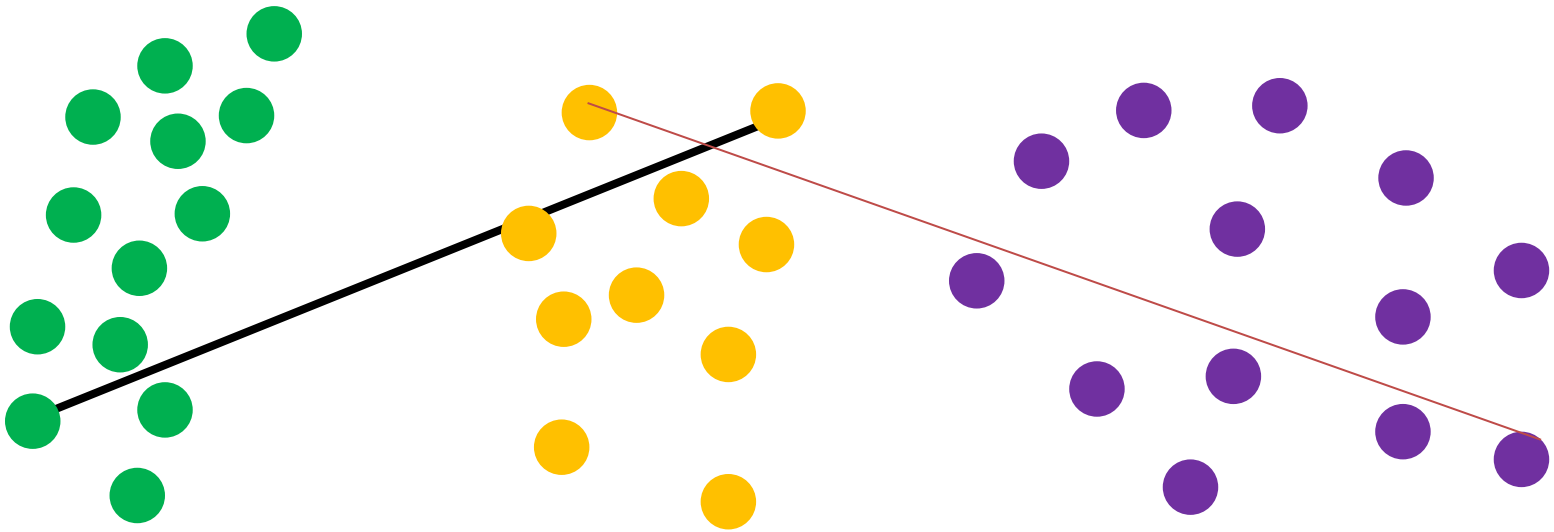
- Similarity between clusters:
  - single-linkage: $\min\{d(x,y) : x \in \mathcal{A}, y \in \mathcal{B}\}$
  - complete-linkage: $\max\{d(x,y) : x \in \mathcal{A}, y \in \mathcal{B}\}$
  - average linkage: $\frac{1}{|\mathcal{A}|\cdot|\mathcal{B}|}\sum_{x\in\mathcal{A}}\sum_{y\in\mathcal{B}} d(x,y)$

Single Linkage



$$\min\{d(x,y) : x \in \mathcal{A}, y \in \mathcal{B}\}$$

Complete Linkage

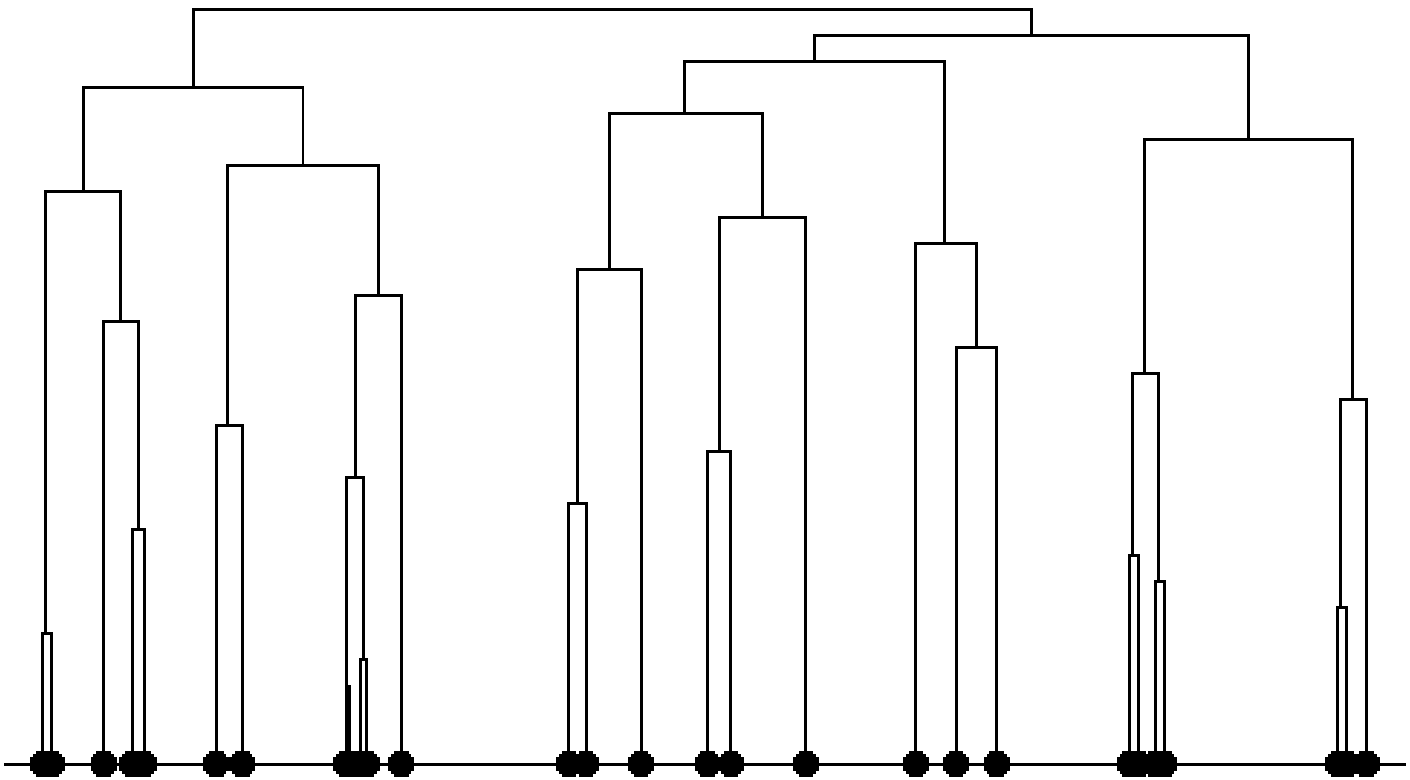


$$\max\{d(x,y) : x \in \mathcal{A}, y \in \mathcal{B}\}$$

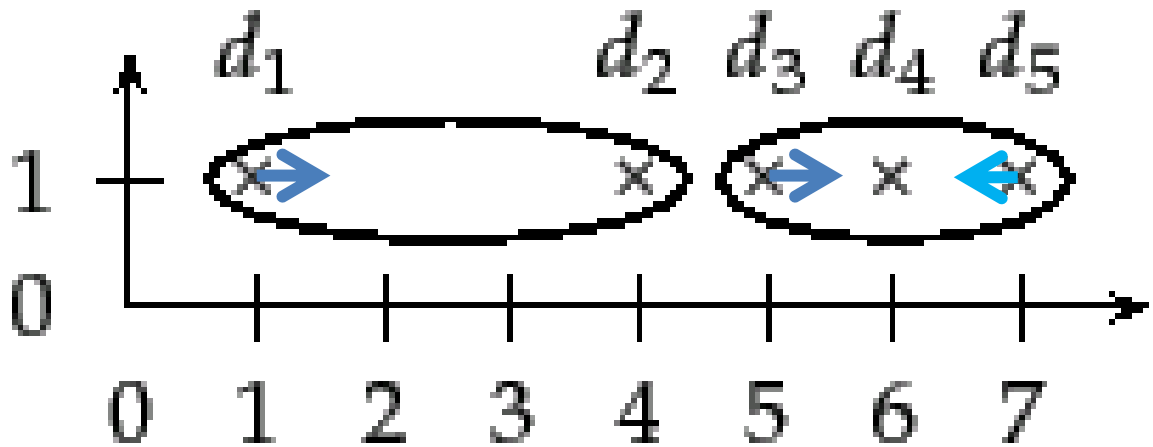
Linkage Matters

- Single linkage: tendency to form long chains
- Complete linkage: Sensitive to outliers
- Average-link: Trying to compromise between the two

Chaining Phenomenon



Outlier Sensitivity



+ 2*epsilon

- 1*epsilon

http://nlp.stanford.edu/IR-book/html/htmledition/img1569.png

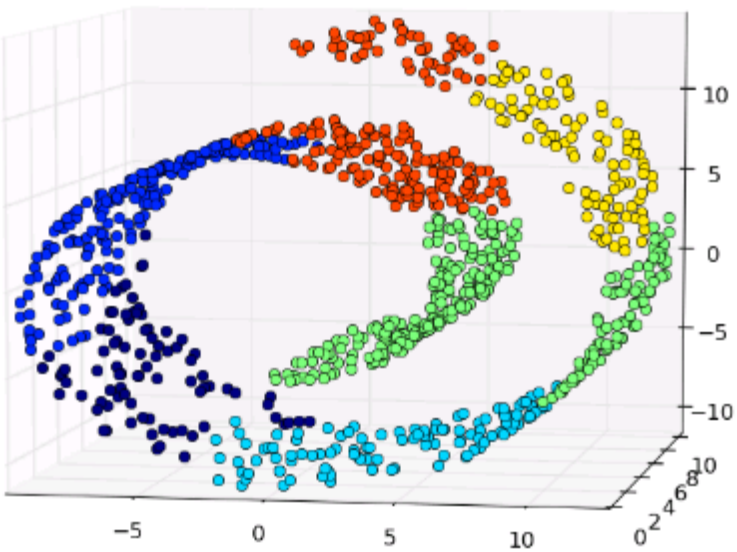
Efficient Hierarchical Graph-Based Video Segmentation

Matthias Grundmann[1,2], Vivek Kwatra[2], Mei Han[2] and Irfan Essa[1]

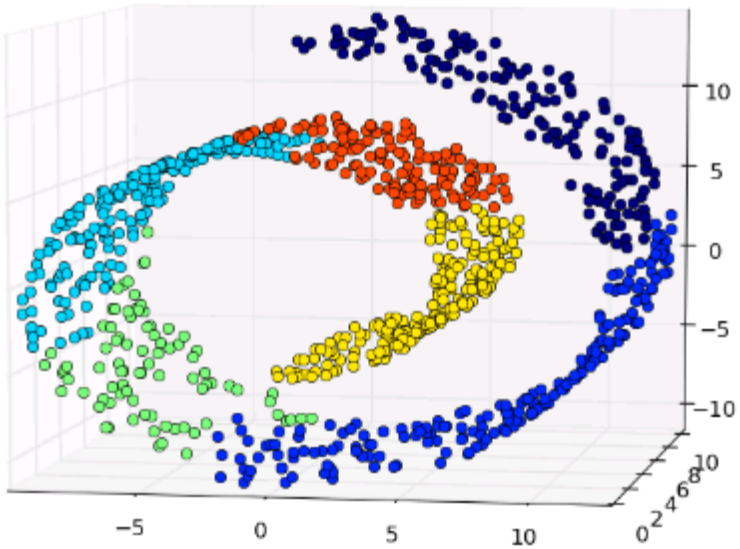
[1]Georgia Tech [2]Google Research

IEEE CVPR, San Francisco, USA, June 2010

Swiss Role Problem



without connectivity constraints



with connectivity constraints

only adjacent clusters can be merged together

http://scikit-learn.sourceforge.net/modules/clustering.html

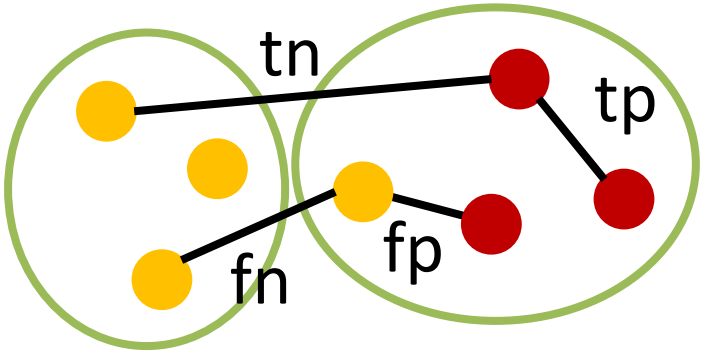
Evaluation Criteria

- Based on expert knowledge
- Debatable for real data
- Hidden Unknown structures could be present
- Do we even want to just reproduce known structure?

Rand Index

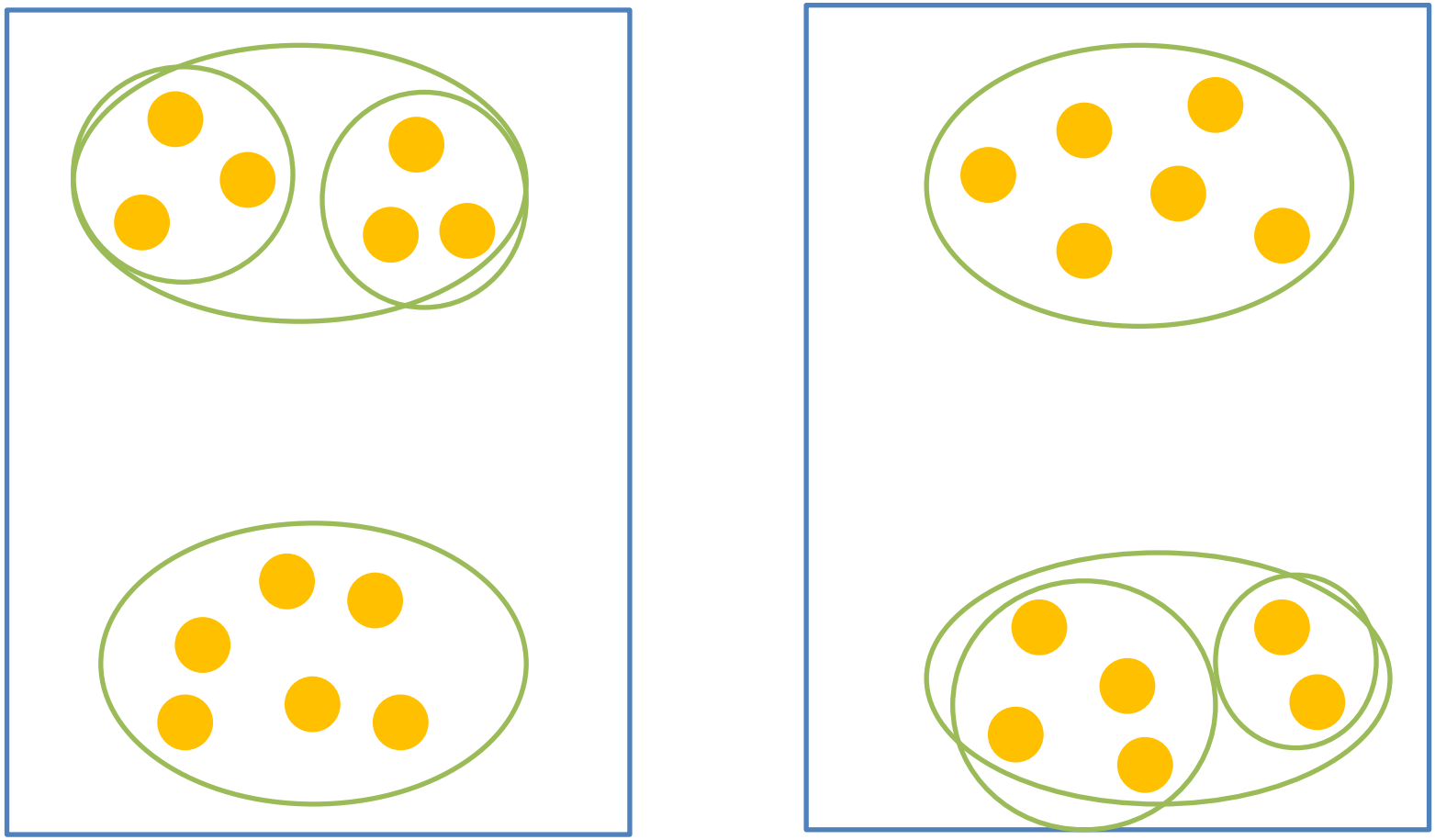
- Percentage of correct classifications
- Compare pairs of elements:

$$R = \frac{tp+tn}{tp+tn+fp+fn}$$



- Fp and fn are equally weighted

Stability

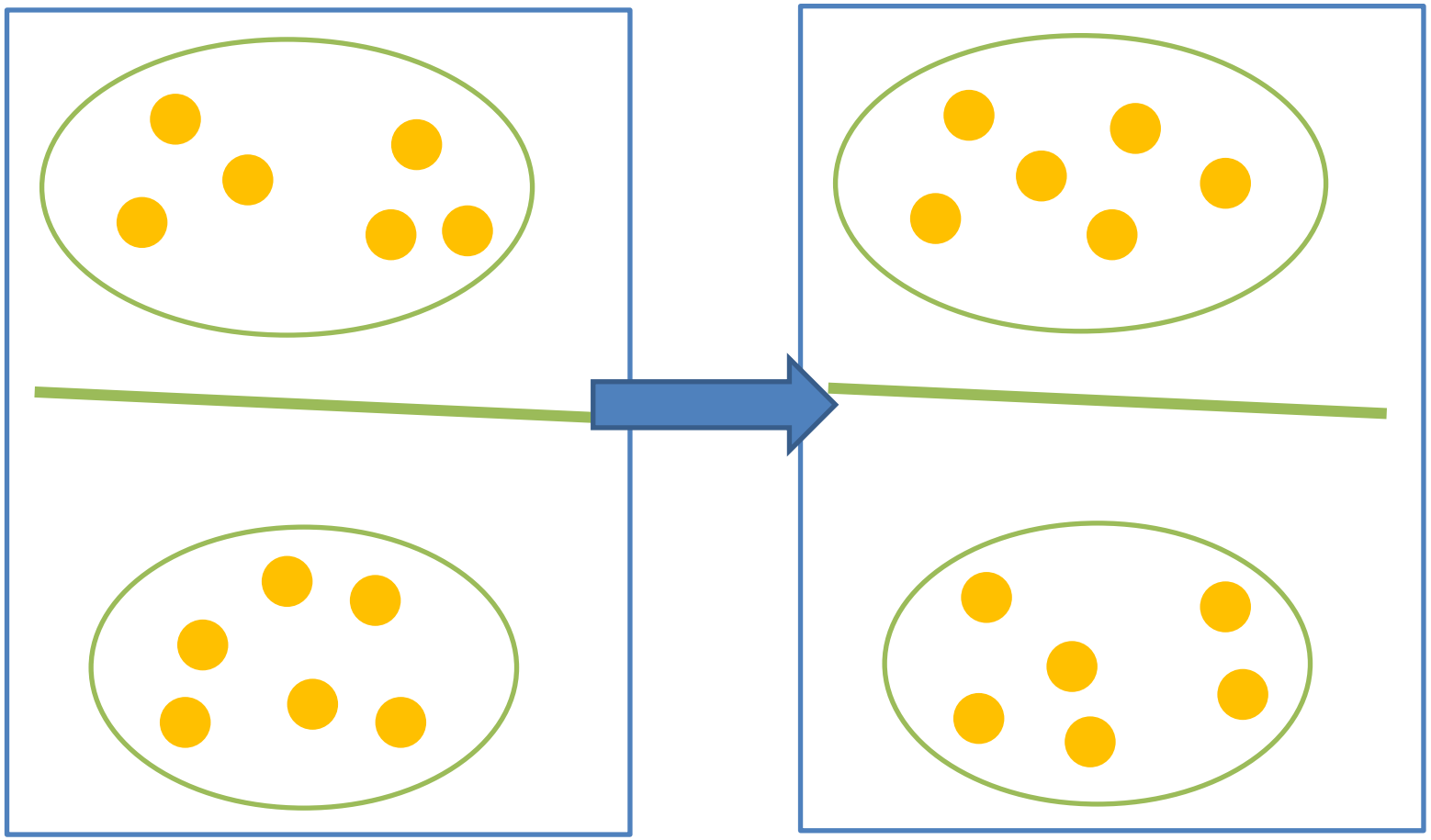


Stability

- What is the right number of clusters?
- What makes a good clustering solution?

- Clustering should generalize!

Stability



Summary

- We have covered a lot today
- Clustering
  - K-means
  - Mean-shift
  - Hierarchical clustering
- Evaluation criteria
  - Rand index
  - Stability