Unsupervised Learning

UNDERGRADUATE COURSE (SPRING 2020)

Unsupervised Learning

- What is clustering
- K-Means Clustering
- Means Shift
- Evaluations

Clustering

Document clustering

- Motivations
- Document representations
- Success criteria

Clustering algorithms

- Partitional
- Hierarchical

What is clustering?

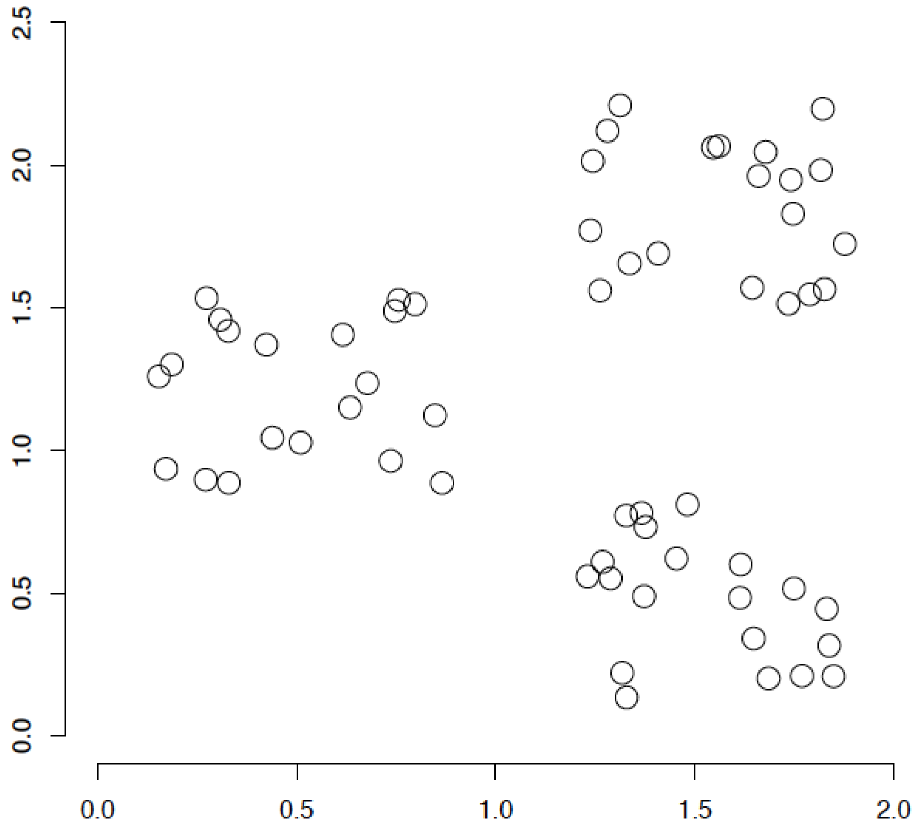
Clustering: the process of grouping a set of objects into classes of similar objects

- Documents within a cluster should be similar.
- Documents from different clusters should be dissimilar.

The commonest form of *unsupervised learning*

- Unsupervised learning = learning from raw data, as opposed to supervised data where a classification of examples is given
- A common and important task that finds many applications in information retrieval and other areas

A data set with clear cluster structure



How would you design an algorithm for finding the three clusters in this case?

Applications of clustering in IR

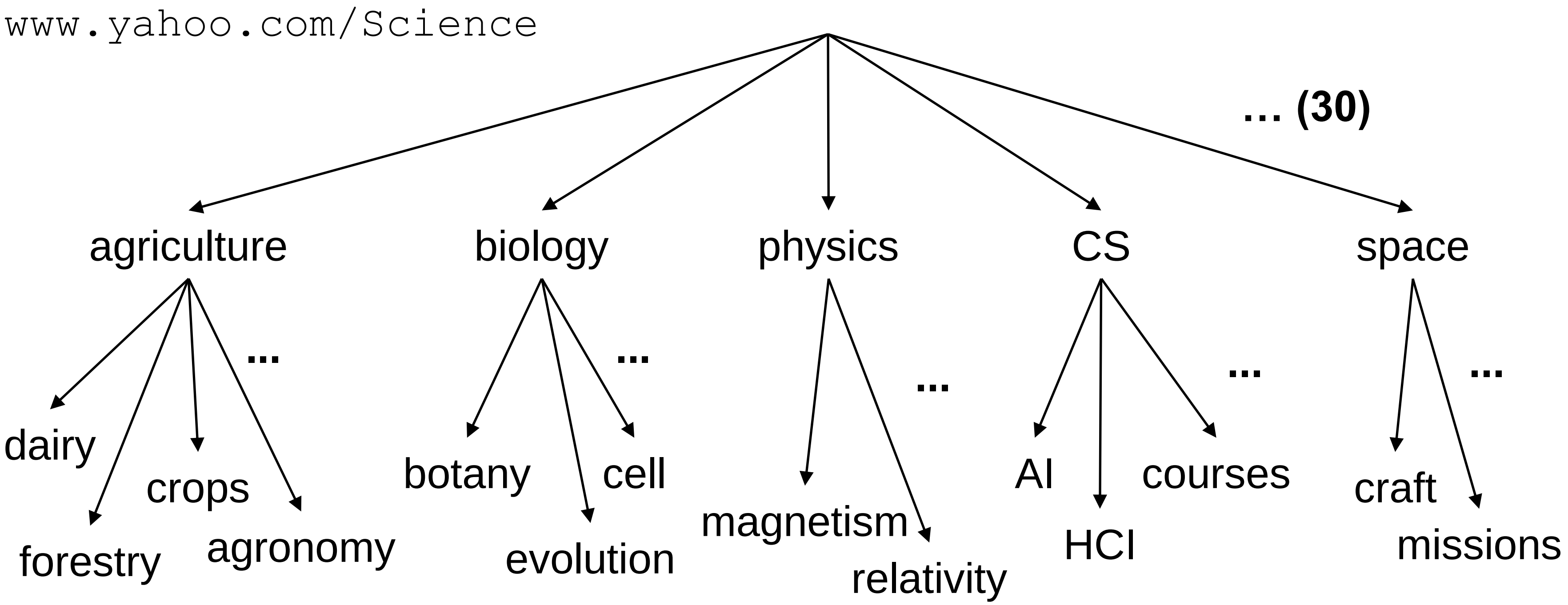
Whole corpus analysis/navigation
- Better user interface: search without typing

For improving recall in search applications
- Better search results

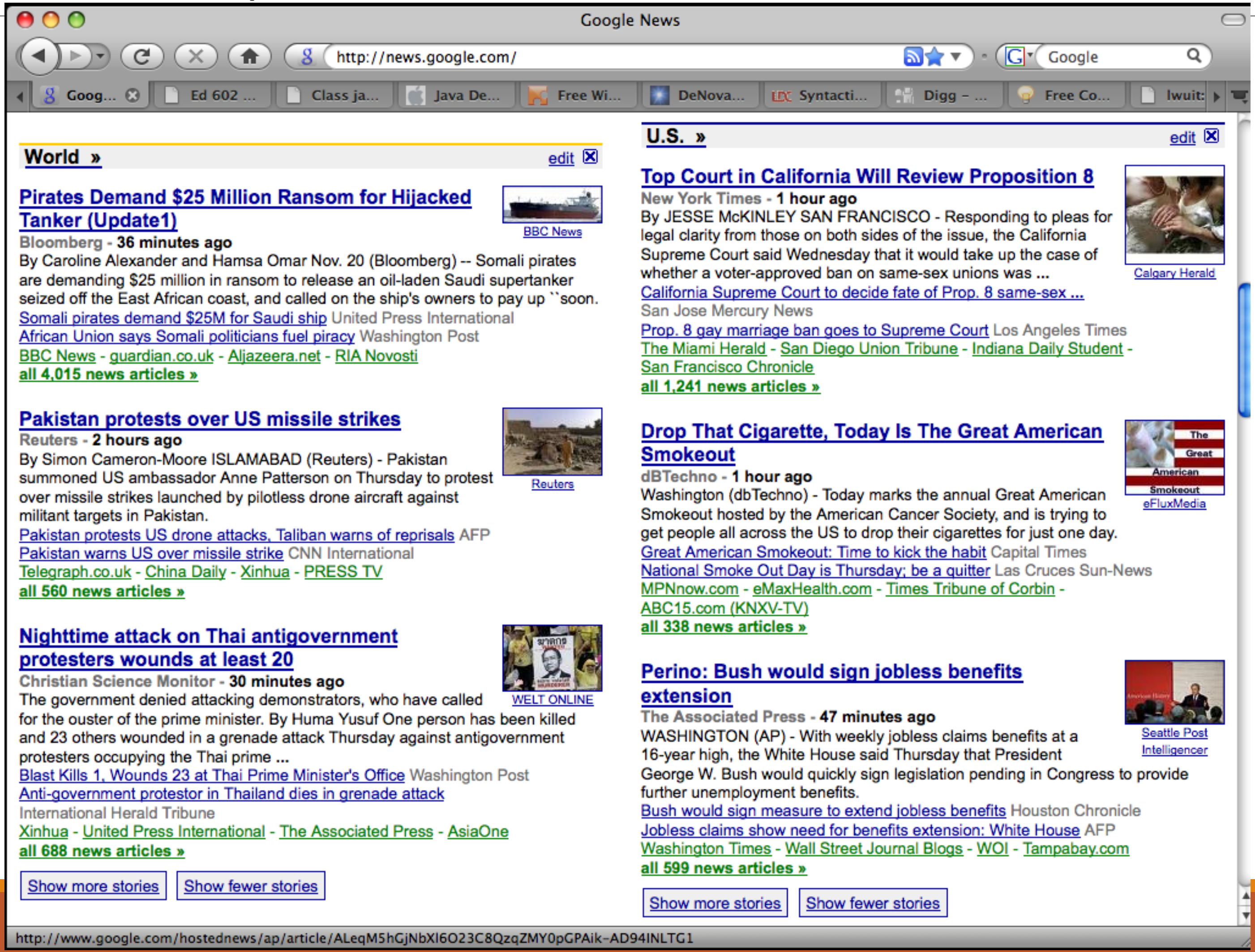
For better navigation of search results
- Effective “user recall” will be higher

For speeding up vector space retrieval
- Cluster-based retrieval gives faster search

Yahoo! Hierarchy *isn't* clustering but *is* the kind of output you want from clustering



Google News: automatic clustering gives an effective news presentation metaphor



Textual Clustering

Vector Space Model

	Doc 1	Doc 2	Doc 3
Army	1	0	0
Sensor	1	1	1
Technology	1	1	0
Help	1	0	0
Find	1	0	0
Improvise	1	0	0
Explosive	1	0	1
Device	1	0	1
ORNL	0	1	0
develop	0	1	1
homeland	0	1	1
Defense	0	1	1
Mitre	0	0	1
won	0	0	1
contract	0	0	1

TFIDF

$$W_{ij} = \log_2 (f_{ij} + 1) * \log_2\left(\frac{N}{n}\right)$$

Similarity Matrix

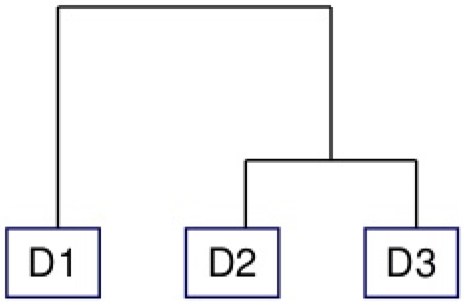
	Doc 1	Doc 2	Doc 3
Doc 1	100%	17%	21%
Doc 2		100%	36%
Doc 3			100%

Documents to Documents

Euclidean distance

$$d_2(\mathbf{x}_i, \mathbf{x}_j) = \left(\sum_{k=1}^{d} (x_{i,k} - x_{j,k})^2\right)^{1/2}$$

Cluster Analysis



Most similar documents

Time Complexity

$O(n^2 \mathrm{Log}\ n)$

Major Clustering Approaches

Partitioning algorithms: Construct various partitions and then evaluate them by some criterion

Hierarchy algorithms: Create a hierarchical decomposition of the set of data (or objects) using some criterion

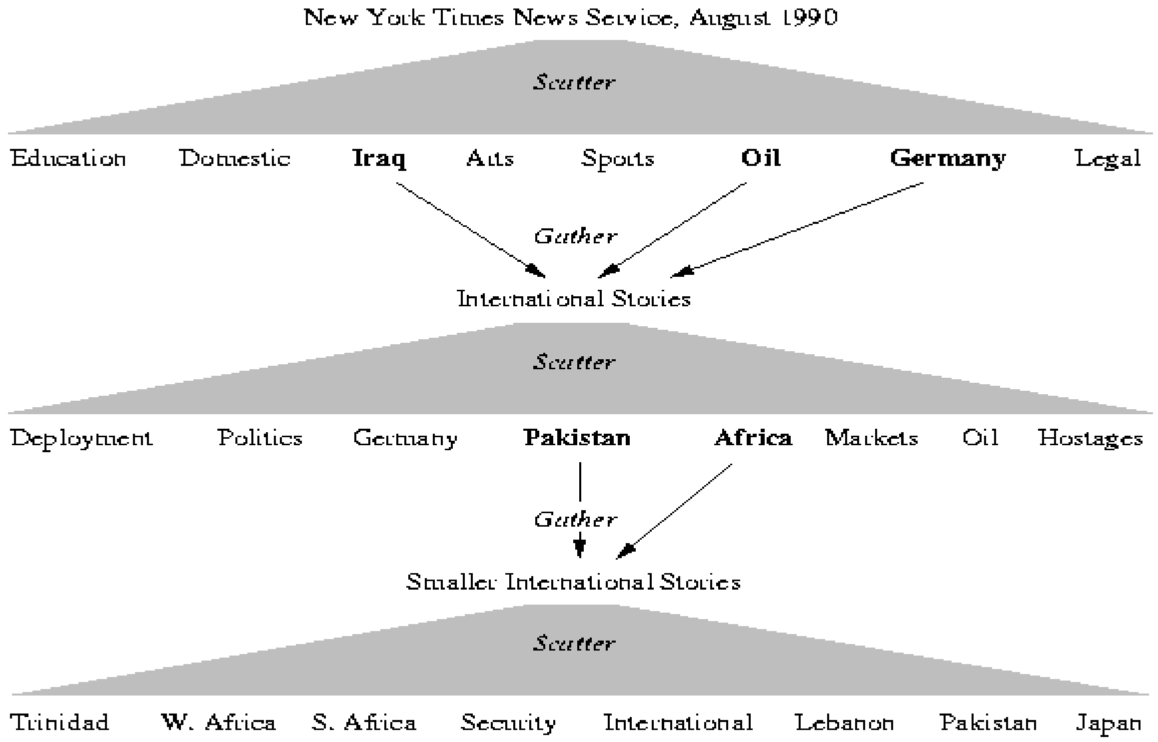
Density-based: based on connectivity and density functions

Grid-based: based on a multiple-level granularity structure

Model-based: A model is hypothesized for each of the clusters and the idea is to find the best fit of that model to each other

Scatter/Gather:

- Scatter/Gather
  - uses text clustering to group document according to the overall similarities in their content.
- Scatter/Gather
  - to scatter documents in to clusters or group
  - then gather a subset of these groups and re-scatter them to form new groups

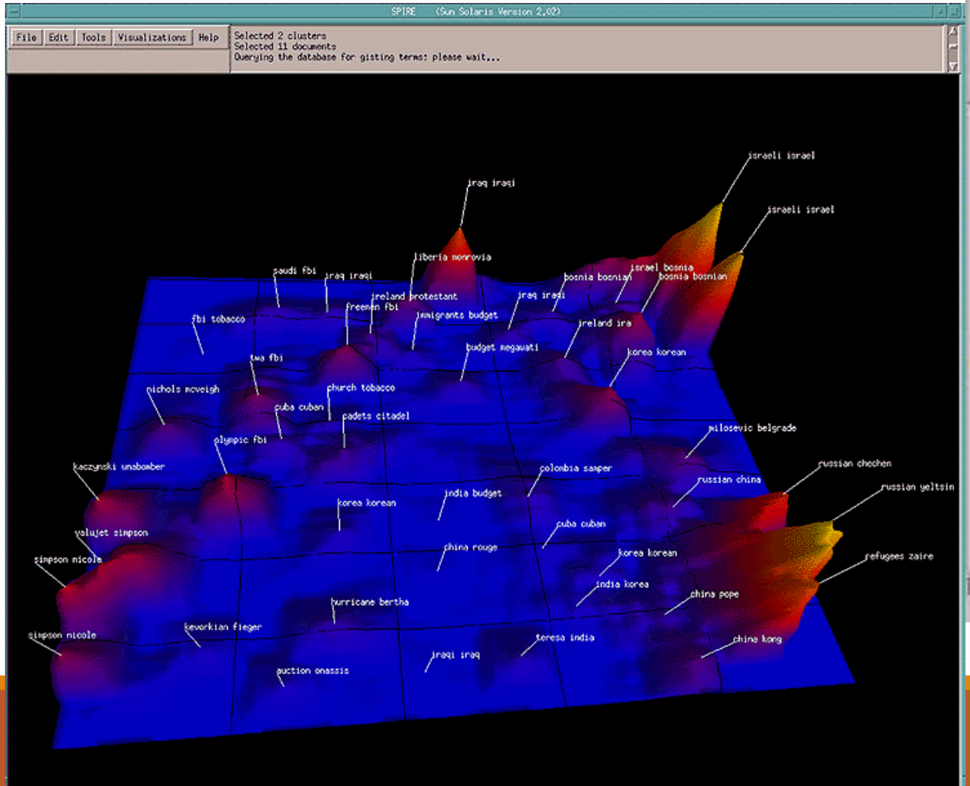


For visualizing a document collection and its themes

Wise et al, “Visualizing the non-visual” PNNL

ThemeScapes, Cartia

- [Mountain height = cluster size]



For improving search recall

Cluster hypothesis - Documents in the same cluster behave similarly with respect to relevance to information needs

Therefore, to improve search recall:

- Cluster docs in corpus a priori
- When a query matches a doc *D*, also return other docs in the cluster containing *D*

Hope if we do this: The query “car” will also return docs containing *automobile*

- Because clustering grouped together docs containing *car* with those containing *automobile.*

Why might this happen?

Issues for clustering

Representation for clustering

- Document representation
  - Vector space? Normalization?
    - Centroids aren’t length normalized
- Need a notion of similarity/distance

How many clusters?

- Fixed a priori?
- Completely data driven?
  - Avoid “trivial” clusters - too large or small
    - If a cluster's too large, then for navigation purposes you've wasted an extra user click without whittling down the set of documents much.

Notion of similarity/distance

Ideal: semantic similarity.

Practical: term-statistical similarity

- We will use cosine similarity.
- Docs as vectors.
- For many algorithms, easier to think in terms of a *distance* (rather than <u>similarity</u>) between docs.
- We will mostly speak of Euclidean distance
  - <u>But real implementations use cosine similarity</u>

Clustering Algorithms

Flat algorithms

- Usually start with a random (partial) partitioning
- Refine it iteratively
  - *K* means clustering
  - (Model based clustering)

Hierarchical algorithms

- Bottom-up, agglomerative
- (Top-down, divisive)

Hard vs. soft clustering

Hard clustering: Each document belongs to exactly one cluster

- More common and easier to do

Soft clustering: A document can belong to more than one cluster.

- Makes more sense for applications like creating browsable hierarchies
- You may want to put a pair of sneakers in two clusters: (i) sports apparel and (ii) shoes
- You can only do that with a soft clustering approach.

Focus on hard clustering

Partitioning Algorithms

Partitioning method: Construct a partition of *n* documents into a set of *K* clusters

Given: a set of documents and the number *K*

Find: a partition of *K* clusters that optimizes the chosen partitioning criterion

- Globally optimal
  - Intractable for many objective functions
  - Ergo, exhaustively enumerate all partitions
- Effective heuristic methods: *K*-means and *K*-medoids algorithms

See also Kleinberg NIPS 2002 – impossibility for natural clustering

K-Means

Assumes documents are real-valued vectors.

Clusters based on *centroids* (aka the *center of gravity* or mean) of points in a cluster, *c*:

$$\vec{\mu}(\mathrm{c}) = \frac{1}{|c|} \sum_{\vec{x} \in c} \vec{x}$$

Reassignment of instances to clusters is based on distance to the current cluster centroids.

- (Or one can equivalently phrase it in terms of similarities)

K-Means Algorithm

Select *K* random docs $\{s_1, s_2, \ldots s_K\}$ as seeds.
Until clustering *converges* (or other stopping criterion):

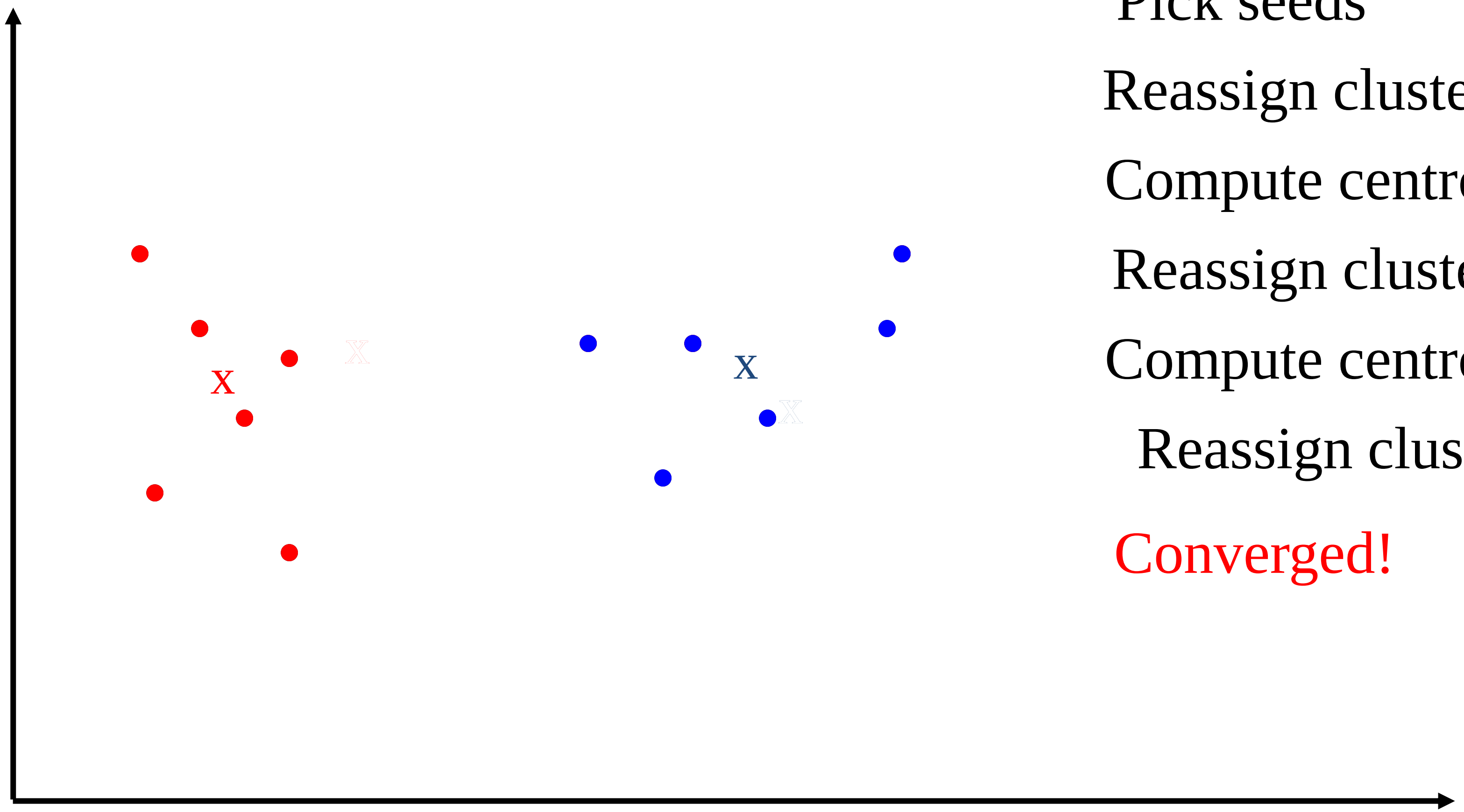
For each doc d_i:

Assign d_i to the cluster c_j such that $dist(x_i, s_j)$ is minimal.

(Next, update the seeds to the centroid of each cluster)

For each cluster c_j

$s_j = \mu(c_j)$



Pick seeds

Reassign clusters

Compute centroids

Reassign clusters

Compute centroids

Reassign clusters

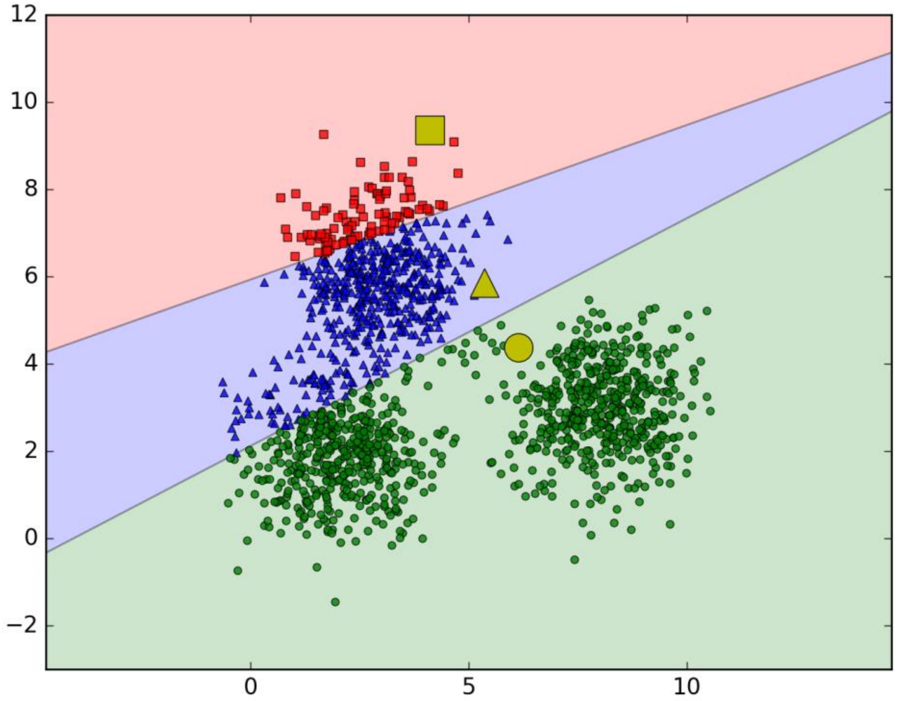
Converged!

Termination conditions

Several possibilities, e.g.,

- A fixed number of iterations.
- Doc partition unchanged.
- Centroid positions don’t change.

Does this mean that the docs in a cluster are unchanged?



iteration 0: assign points to clusters

Convergence

Why should the *K*-means algorithm ever reach a *fixed point*?

- A state in which clusters don’t change.

K-means is a special case of a general procedure known as the *Expectation Maximization (EM) algorithm*.

- EM is known to converge.
- Number of iterations could be large.
  - But in practice usually isn’t

Convergence of *K*-Means

Define goodness measure of cluster *k* as sum of squared distances from cluster centroid:

- $G_k = \Sigma_i (d_i - c_k)^2$ (sum over all d_i in cluster *k*)
- $G = \Sigma_k G_k$

Reassignment monotonically decreases G since each vector is assigned to the closest centroid.

Convergence of *K*-Means

Recomputation monotonically decreases each G_k since (m_k is number of members in cluster *k*):

- $\Sigma\,(d_i - a)^2$ reaches minimum for:

  $\Sigma\, -2(d_i - a) = 0$

  $\Sigma\, d_i = \Sigma\, a$

  $m_K\, a = \Sigma\, d_i$

  $a = (1/\, m_k)\, \Sigma\, d_i = c_k$

K-means typically converges quickly

Time Complexity

Computing distance between two docs is O*(M)* where *M* is the dimensionality of the vectors.

Reassigning clusters: O*(KN)* distance computations, or O*(KNM).*

Computing centroids: Each doc gets added once to some centroid: O*(NM).*

Assume these two steps are each done once for *I* iterations: O*(IKNM).*

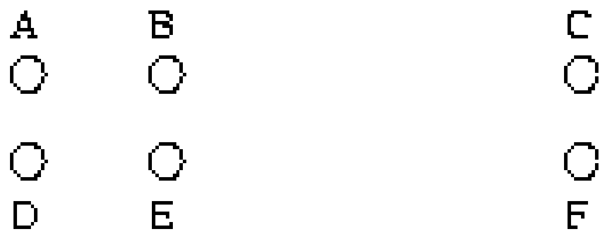
Seed Choice

Results can vary based on random seed selection.

Some seeds can result in poor convergence rate, or convergence to sub-optimal clusterings.

- Select good seeds using a heuristic (e.g., doc least similar to any existing mean)
- Try out multiple starting points
- Initialize with the results of another method.

Example showing sensitivity to seeds



In the above, if you start with B and E as centroids you converge to {A,B,C} and {D,E,F}
If you start with D and F you converge to {A,B,D,E} {C,F}

K-means issues, variations, etc.

Recomputing the centroid after every assignment (rather than after all points are re-assigned) can improve speed of convergence of *K*-means

Assumes clusters are spherical in vector space

- Sensitive to coordinate changes, weighting etc.

Disjoint and exhaustive

- Doesn’t have a notion of “outliers” by default
- But can add outlier filtering

Dhillon et al. ICDM 2002 – variation to fix some issues with small document clusters

How Many Clusters?

Number of clusters K is given

- Partition n docs into predetermined number of clusters

Finding the “right” number of clusters is part of the problem

- Given docs, partition into an “appropriate” number of subsets.
- E.g., for query results - ideal value of K not known up front - though UI may impose limits.

Can usually take an algorithm for one flavor and convert to the other.

K not specified in advance

Example, the results of a query.

Solve an optimization problem: penalize having lots of clusters

- application dependent, e.g., compressed summary of search results list.

Tradeoff between having more clusters (better focus within each cluster) and having too many clusters

K not specified in advance

Given a clustering, define the Benefit for a doc to be the cosine similarity to its centroid

Define the Total Benefit to be the sum of the individual doc Benefits.

Why is there always a clustering of Total Benefit n?

Penalize lots of clusters

For each cluster, we have a Cost C.

Thus for a clustering with K clusters, the Total Cost is KC.

Define the Value of a clustering to be =

Total Benefit - Total Cost.

Find the clustering of highest value, over all choices of K.

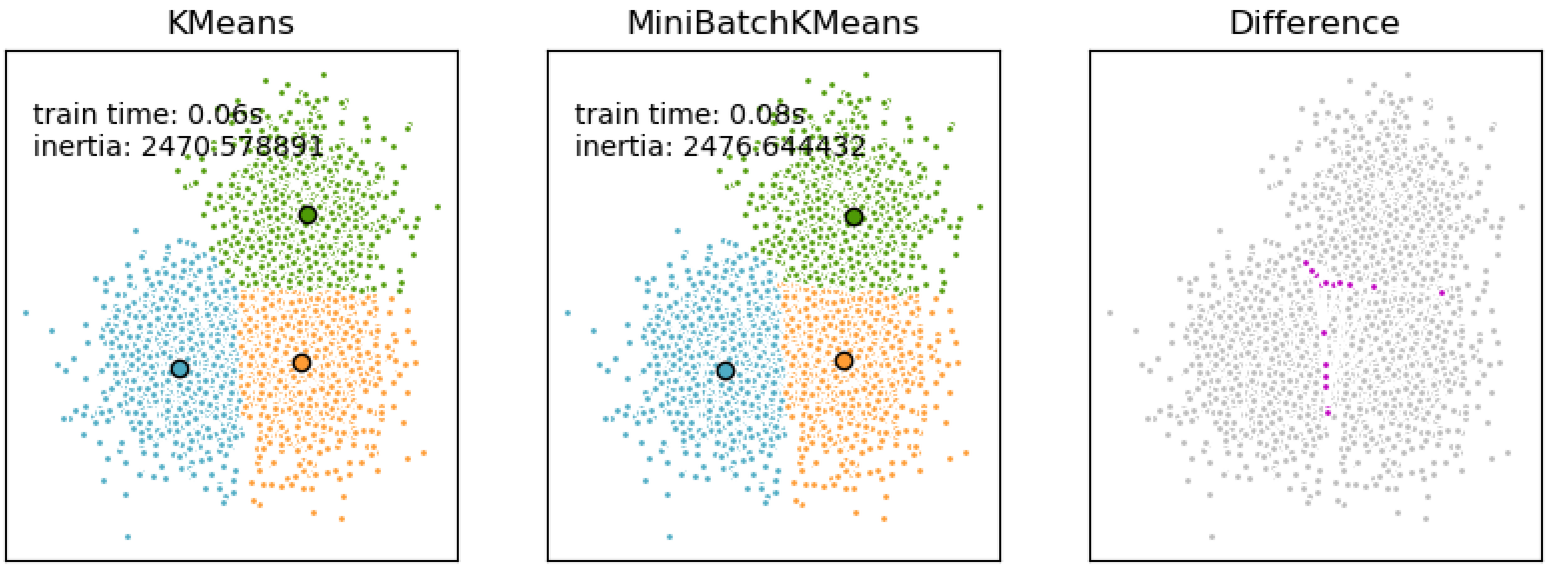
- Total benefit increases with increasing K. But can stop when it doesn't increase by "much". The Cost term enforces this.

Mini-batch K-Means

Uses mini-batches to reduce the computation time, optimize the same objective function

Mini-batches are subsets of the input data, randomly sampled in each training iteration.

Mini-Batch KMeans converges faster than KMeans, but the quality of the results is reduced



Codes and Visualization

Visualization:

http://stanford.edu/class/ee103/visualizations/kmeans/kmeans.html

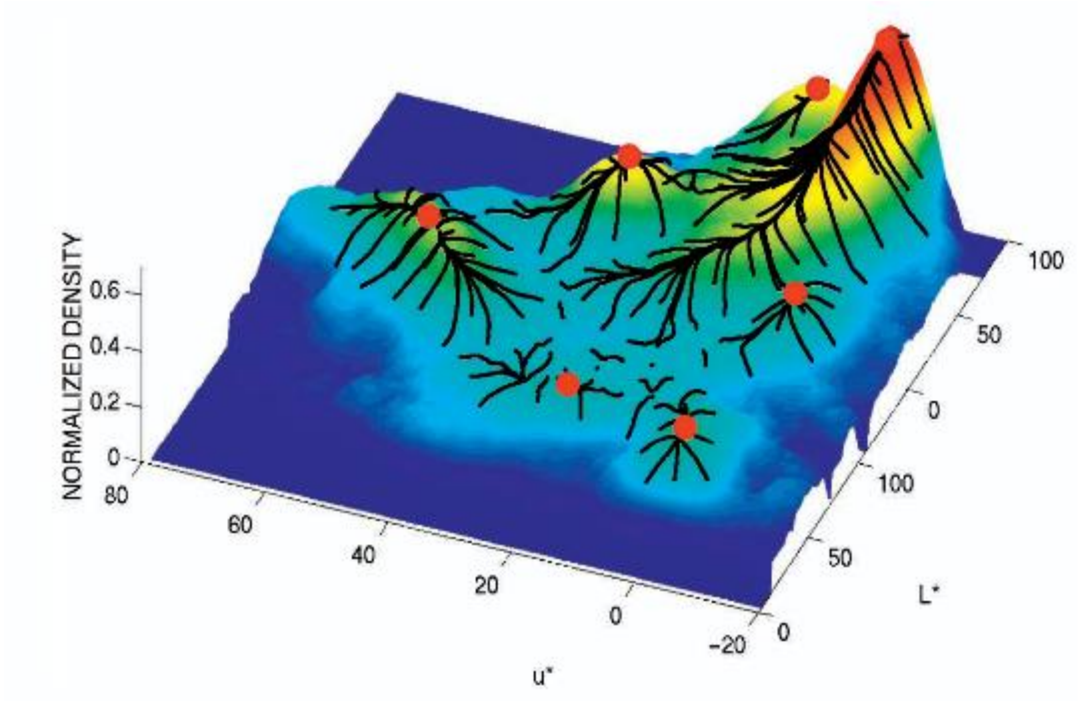
https://www.naftaliharris.com/blog/visualizing-k-means-clustering/

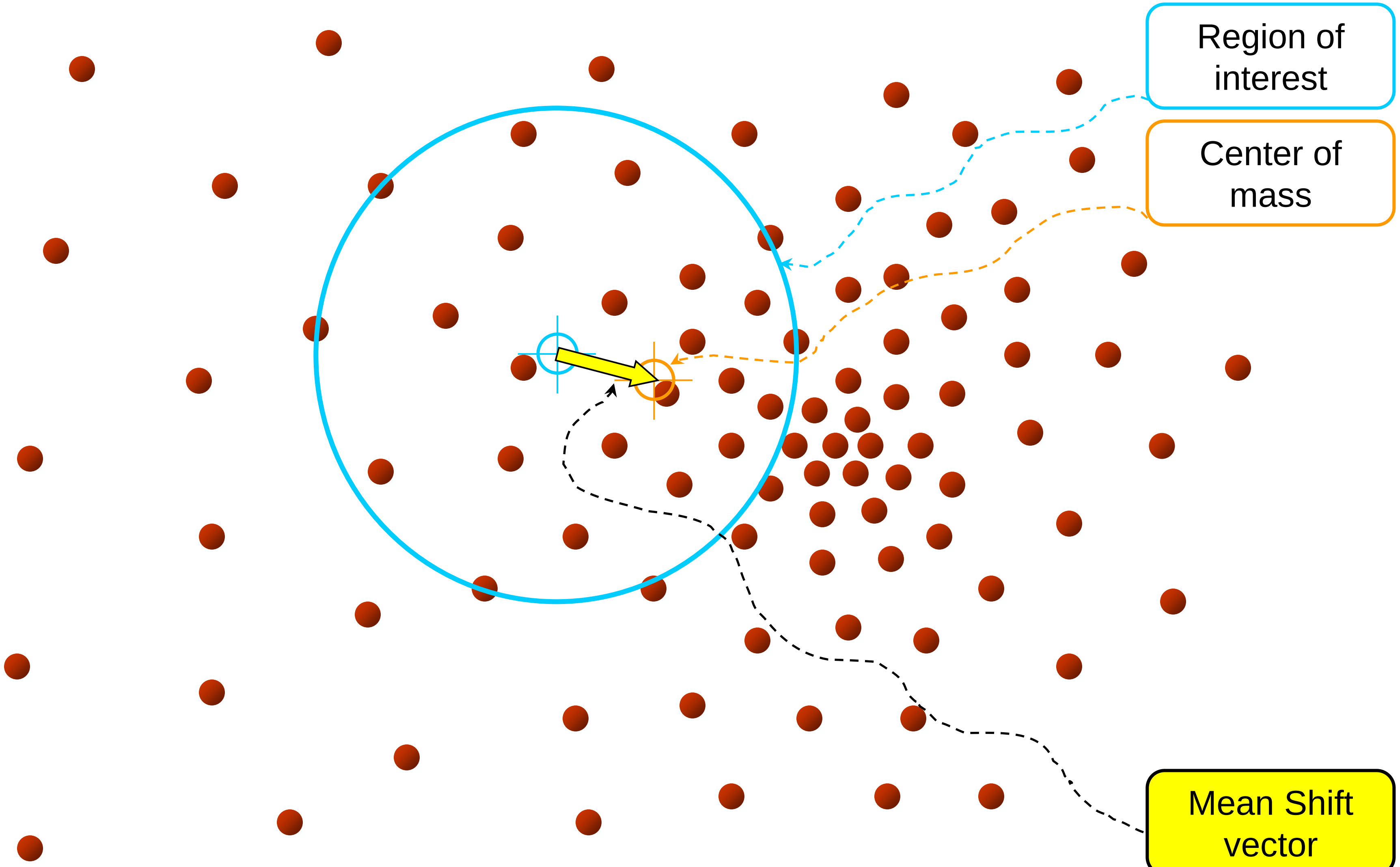
Codes:

https://github.com/tiepvupsu/tiepvupsu.github.io/blob/master/assets/kmeans/kmeans.ipynb

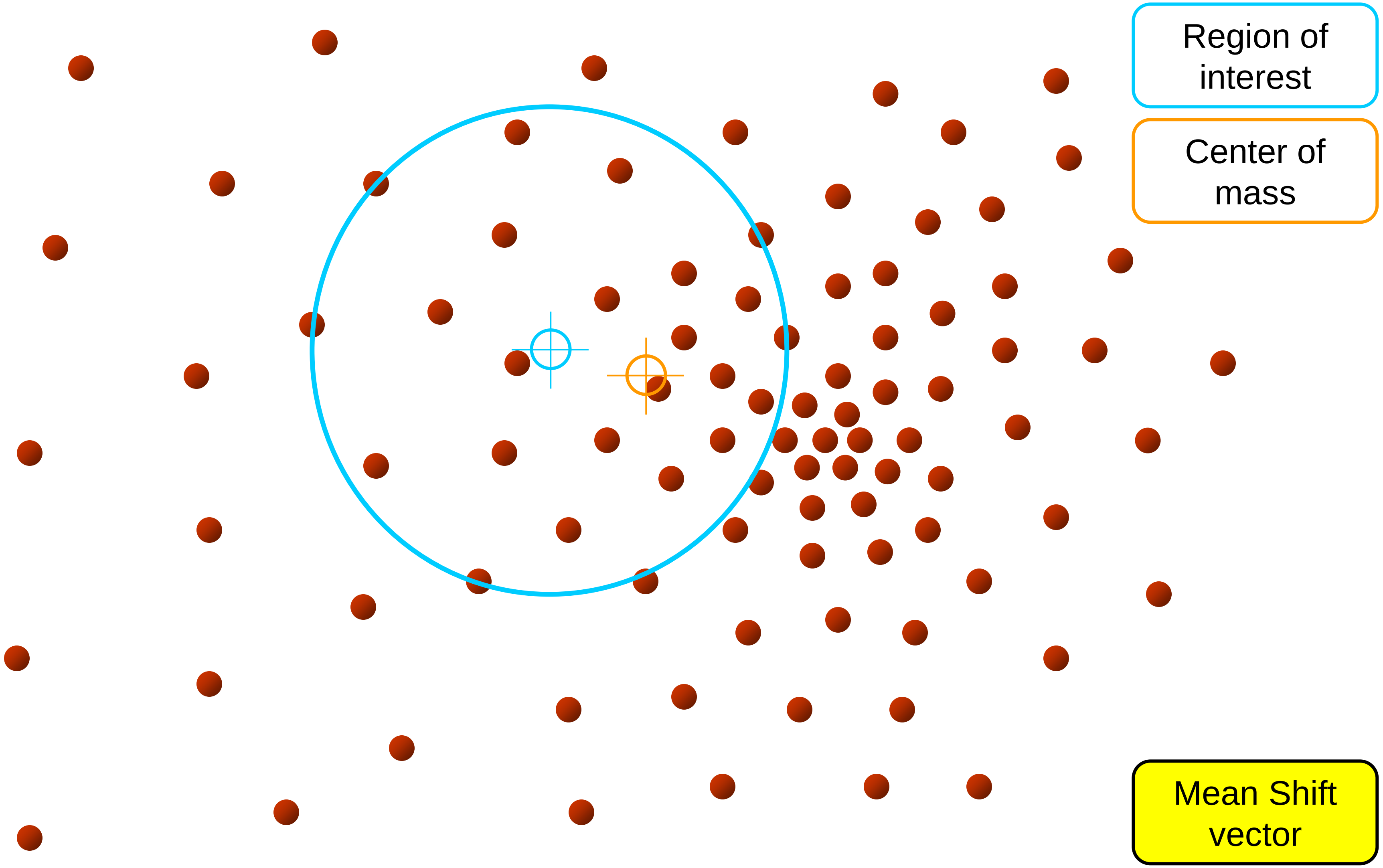
https://github.com/tiepvupsu/tiepvupsu.github.io/blob/master/assets/kmeans/Kmeans2.ipynb

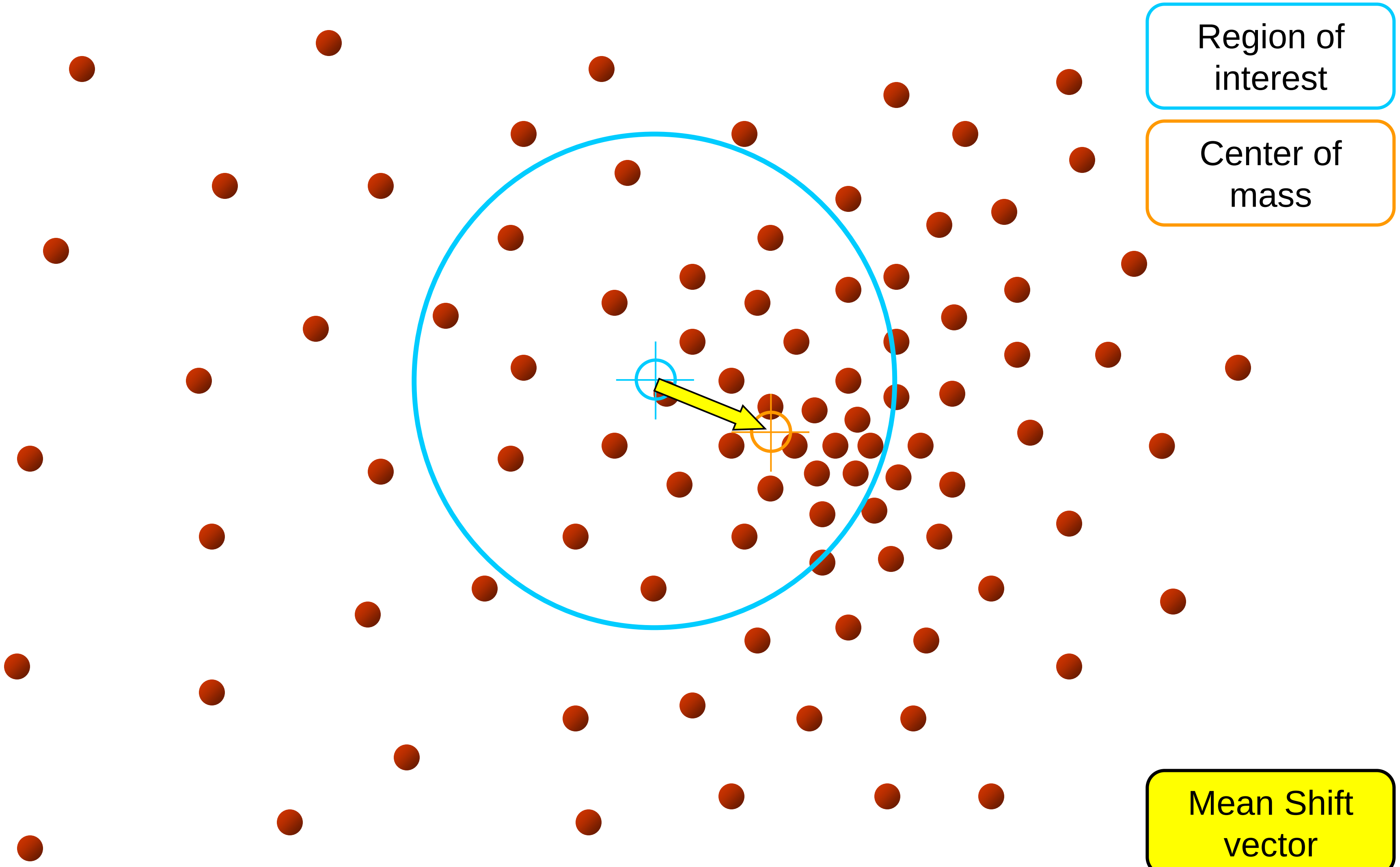
Mean Shift





Region of interest
Center of mass
Mean Shift vector


Region of interest
Center of mass
Mean Shift vector


Region of interest
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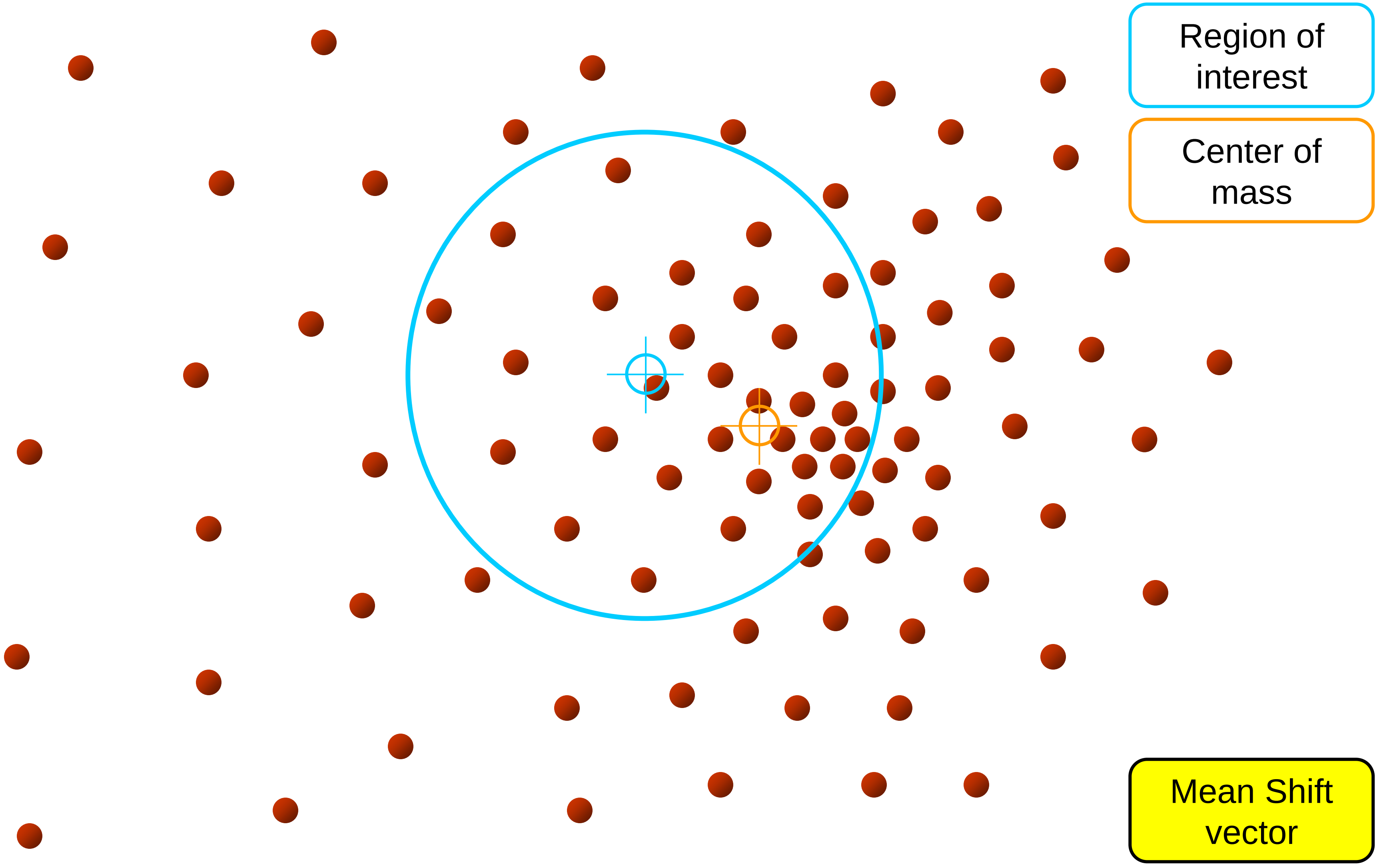
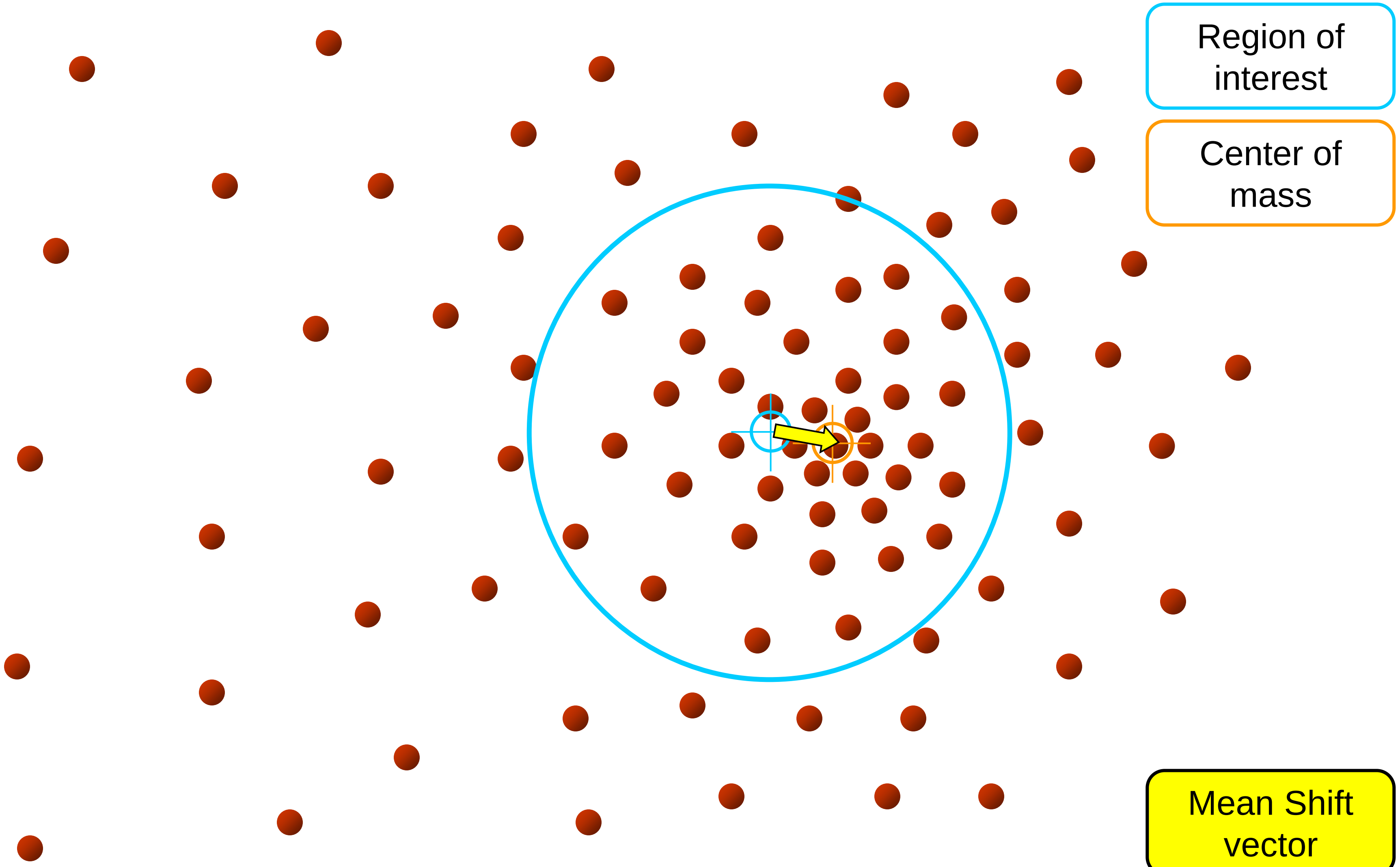
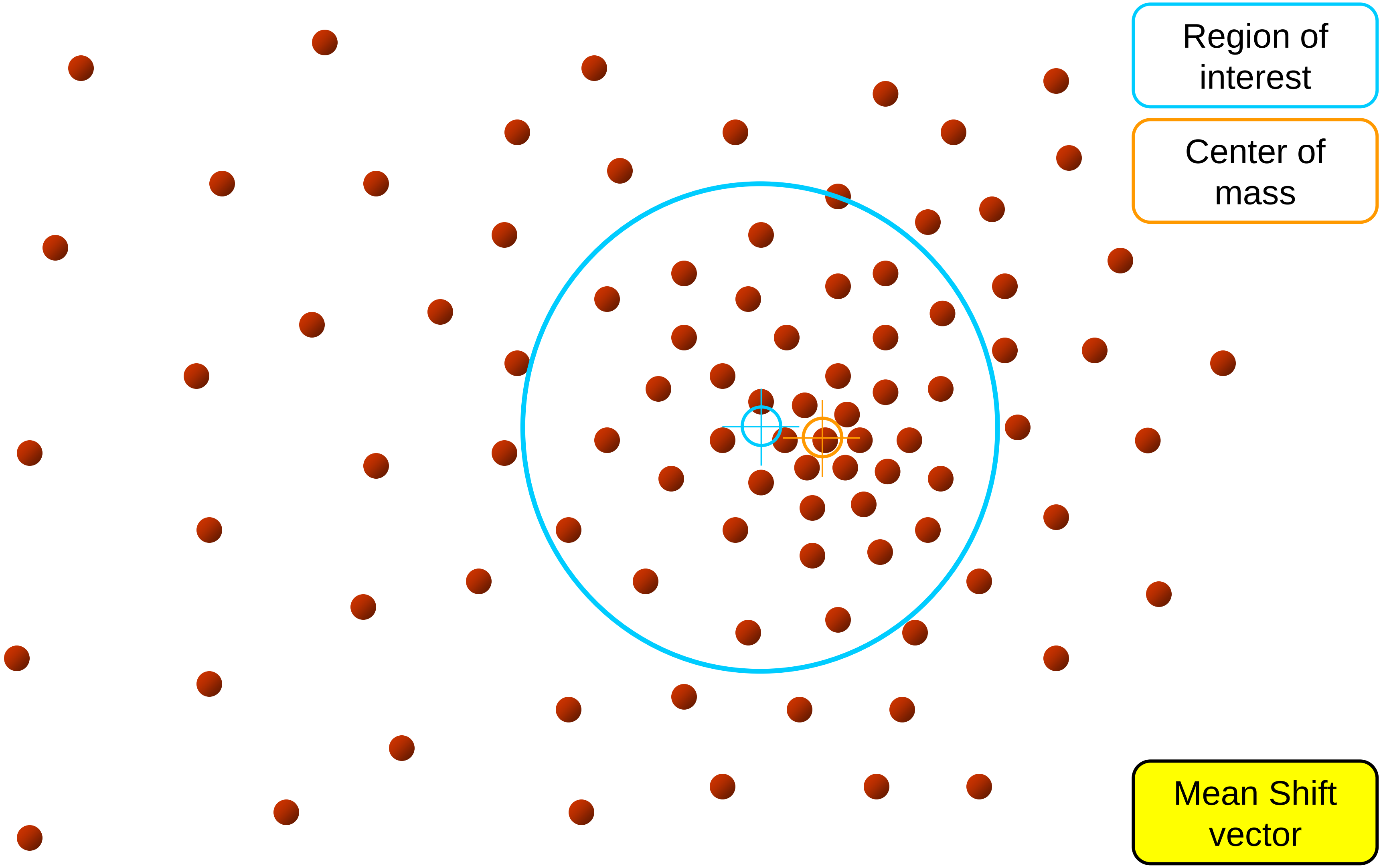
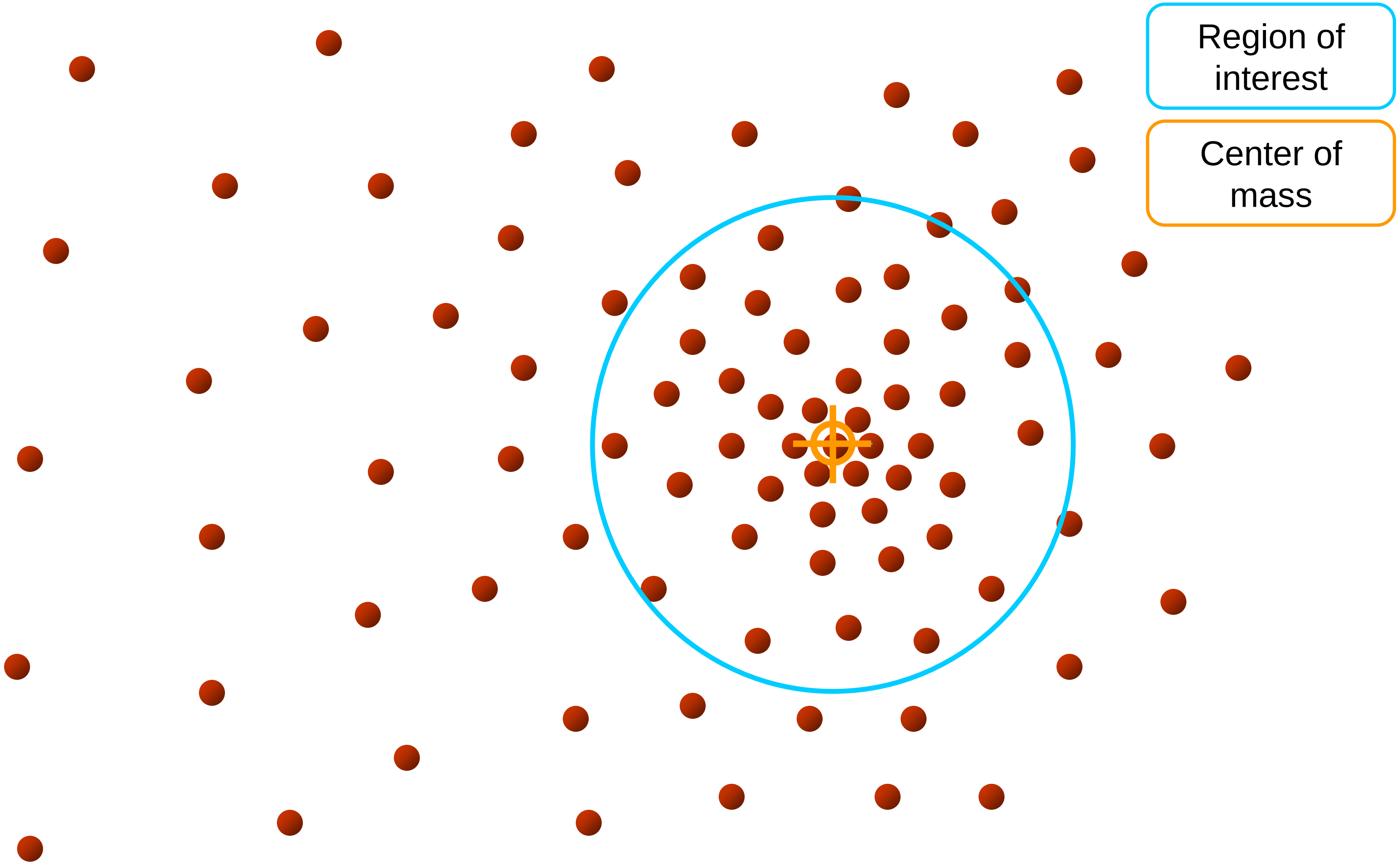

Region of interest
Center of mass
Mean Shift vector


Region of interest
Center of mass
Mean Shift vector



Slide by Y. Ukrainitz & B. Sarel


Region of interest
Center of mass

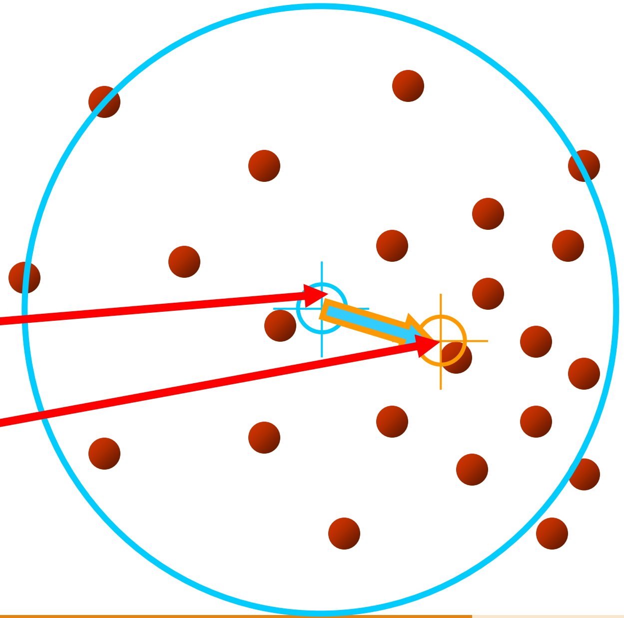
Computing the Mean Shift

<u>Simple Mean Shift procedure</u>:

• Compute mean shift vector

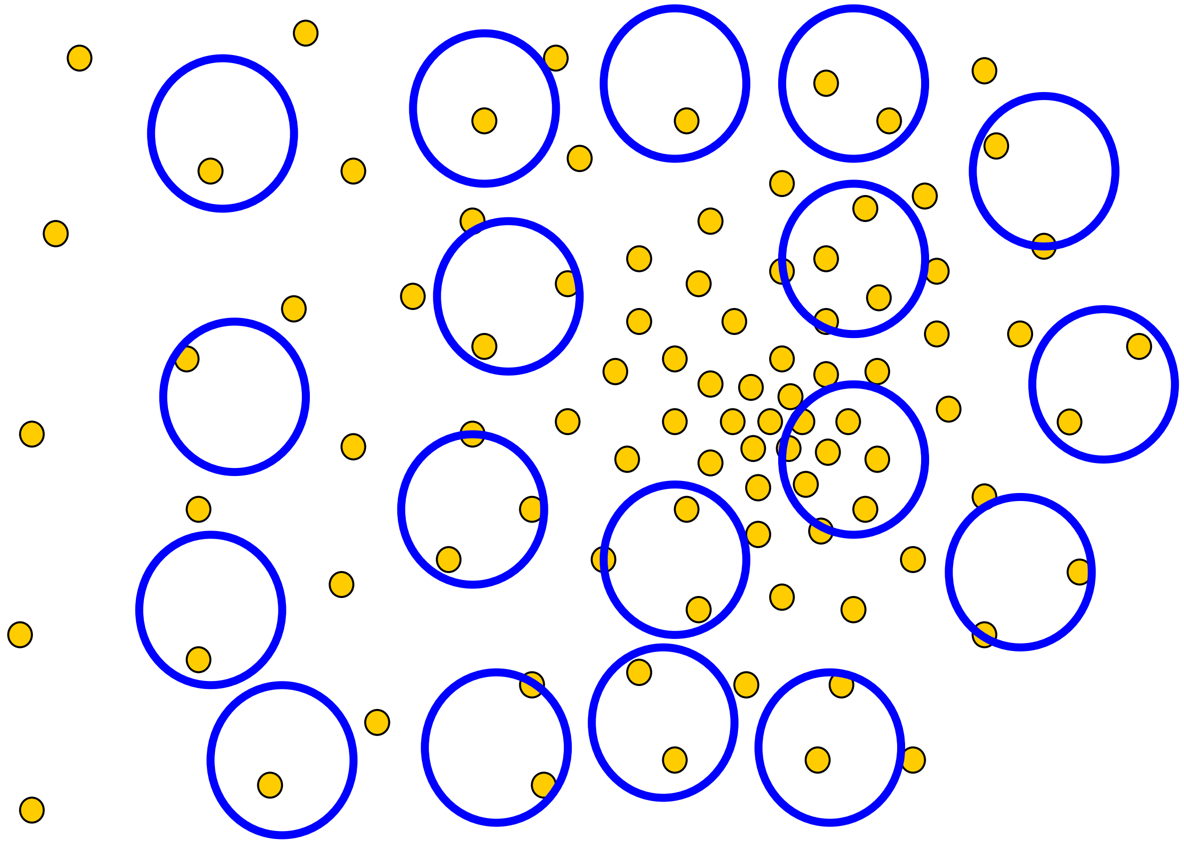
•Translate the Kernel window by **m(x)**

$$\mathbf{m}(\mathbf{x}) = \left[\frac{\sum_{i=1}^{n} \mathbf{x}_i g\left(\frac{\|\mathbf{x}-\mathbf{x}_i\|^2}{h} \right)}{\sum_{i=1}^{n} g\left(\frac{\|\mathbf{x}-\mathbf{x}_i\|^2}{h} \right)} - \boxed{\mathbf{x}} \right]$$



$$\mathrm{g}(\mathbf{x}) = -k'(\mathbf{x})$$

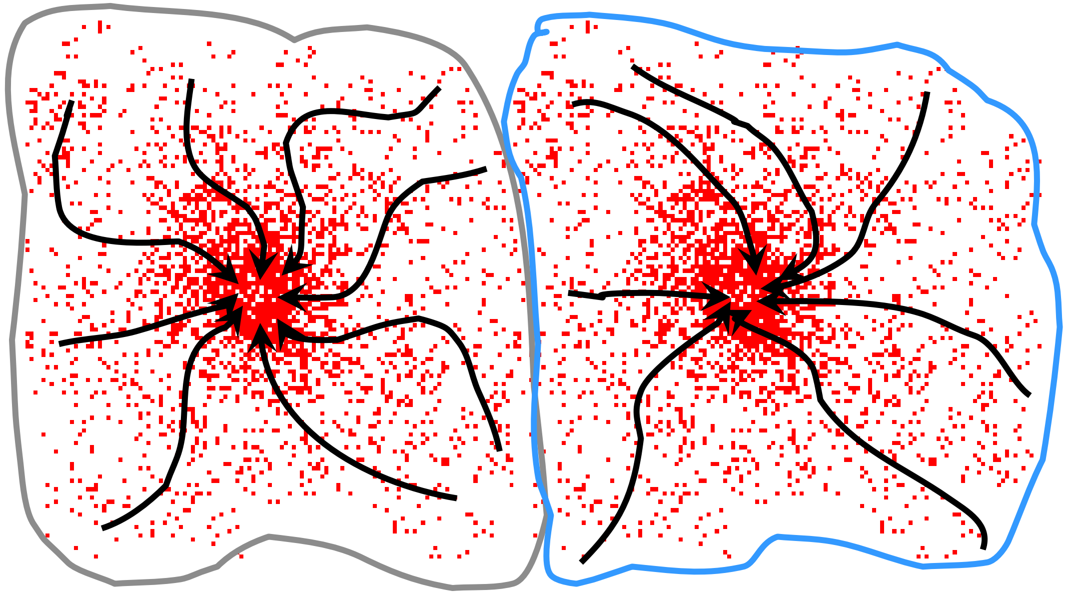
Real Modality Analysis



Attraction basin

Attraction basin: the region for which all trajectories lead to the same mode

Cluster: all data points in the attraction basin of a mode



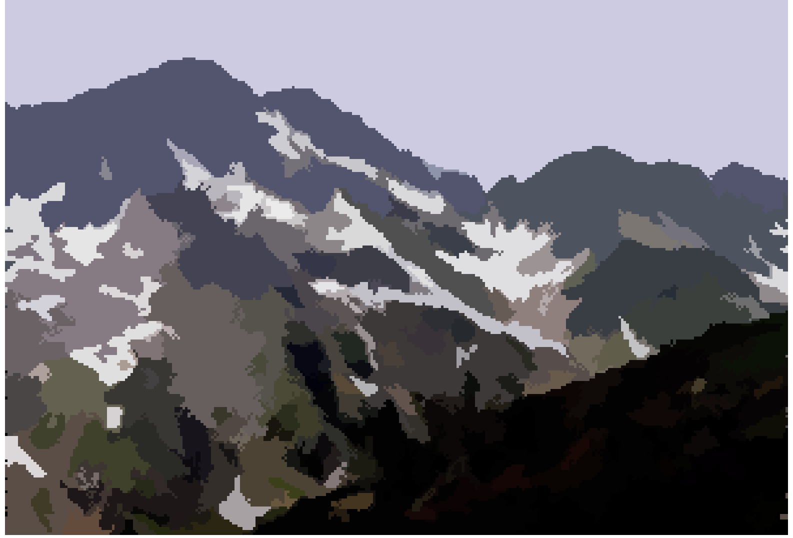
Mean shift clustering

The mean shift algorithm seeks *modes* of the given set of points

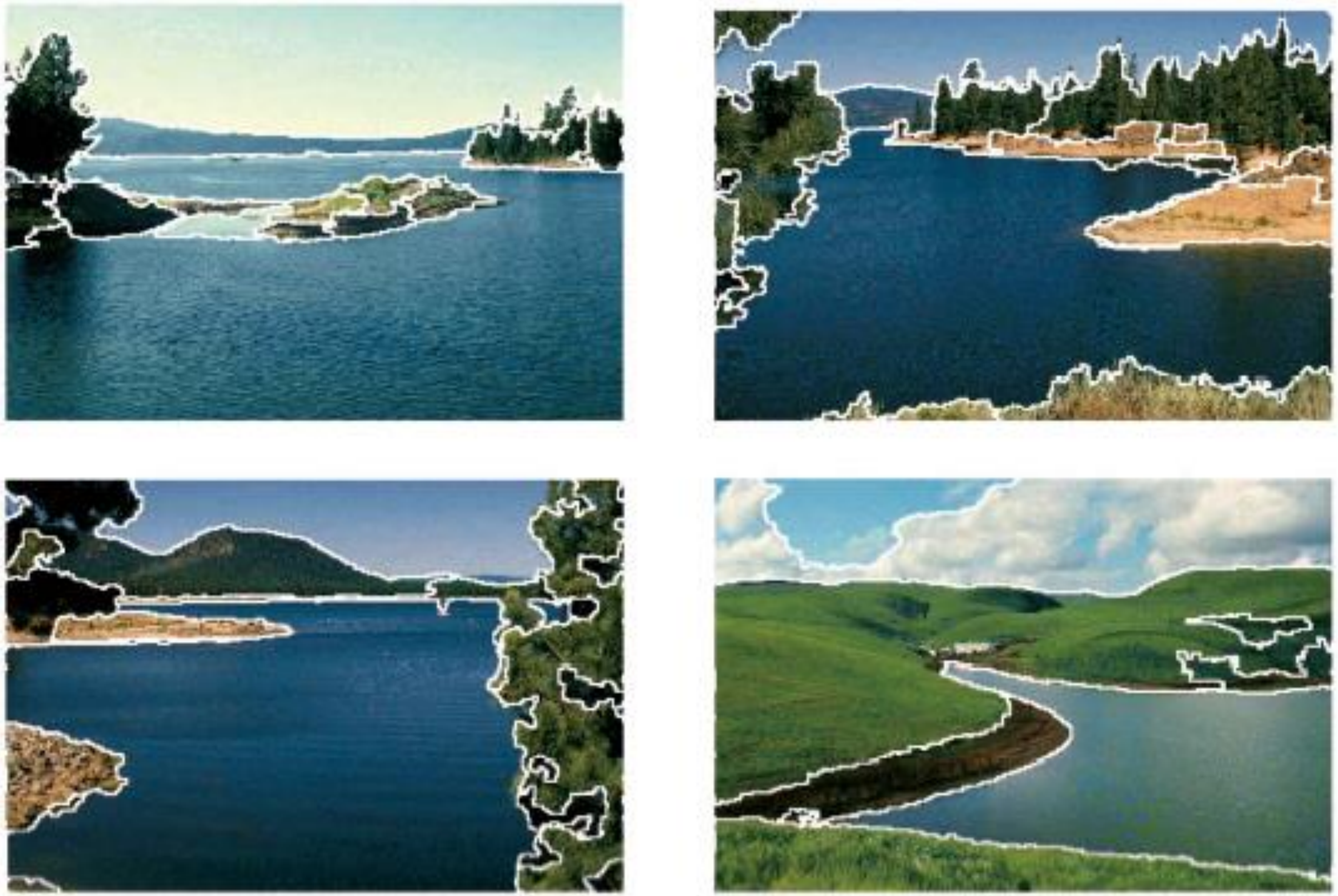
1. Choose kernel and bandwidth
2. For each point:
   a) Center a window on that point
   b) Compute the mean of the data in the search window
   c) Center the search window at the new mean location
   d) Repeat (b,c) until convergence
3. Assign points that lead to nearby modes to the same cluster

Mean shift segmentation results



http://www.caip.rutgers.edu/~comanici/MSPAMI/msPamiResults.html



http://www.caip.rutgers.edu/~comanici/MSPAMI/msPamiResults.html

Mean-shift: other issues

Speedups

- Binned estimation
- Fast search of neighbors
- Update each window in each iteration (faster convergence)

Other tricks

- Use kNN to determine window sizes adaptively

Lots of theoretical support

D. Comaniciu and P. Meer, Mean Shift: A Robust Approach toward Feature Space Analysis, PAMI 2002.

Mean shift pros and cons

Pros

- Good general-practice segmentation
- Flexible in number and shape of regions
- Robust to outliers

Cons

- Have to choose kernel size in advance
- Not suitable for high-dimensional features

When to use it

- Over-segmentation
- Multiple segmentations
- Tracking, clustering, filtering applications

Codes and Visualization

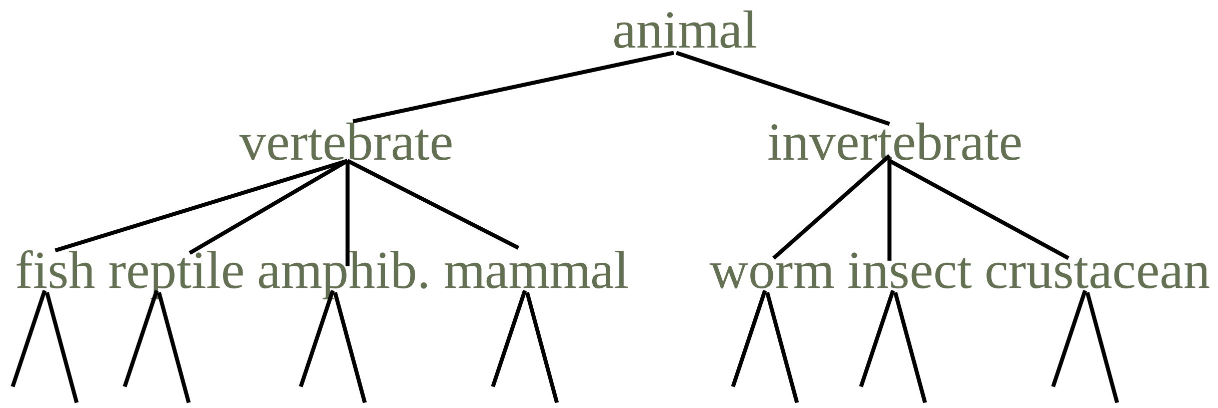
Visualization:

Codes:

https://github.com/mattnedrich/MeanShift_py

Hierarchical Clustering

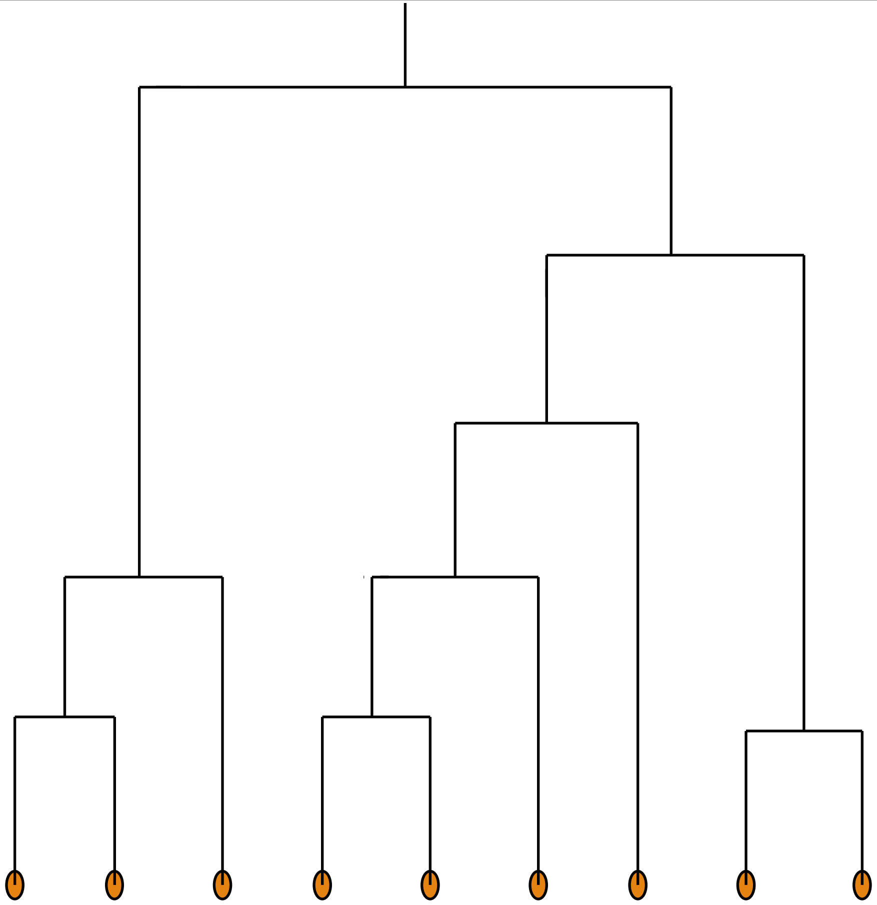
Build a tree-based hierarchical taxonomy (*dendrogram*) from a set of documents.



One approach: recursive application of a partitional clustering algorithm.

Dendrogram: Hierarchical Clustering

- Clustering obtained by cutting the dendrogram at a desired level: each connected component forms a cluster.



Hierarchical Agglomerative Clustering (HAC)

Starts with each doc in a separate cluster

- then repeatedly joins the *closest pair* of clusters, until there is only one cluster.

The history of merging forms a binary tree or hierarchy.

Note: the resulting clusters are still “hard” and induce a partition

Closest pair of clusters

Many variants to defining closest pair of clusters

Single-link

- Similarity of the *most* cosine-similar (single-link)

Complete-link

- Similarity of the “furthest” points, the *least* cosine-similar

Centroid

- Clusters whose centroids (centers of gravity) are the most cosine-similar

Average-link

- Average cosine between pairs of elements

Single Link Agglomerative Clustering

Use maximum similarity of pairs:

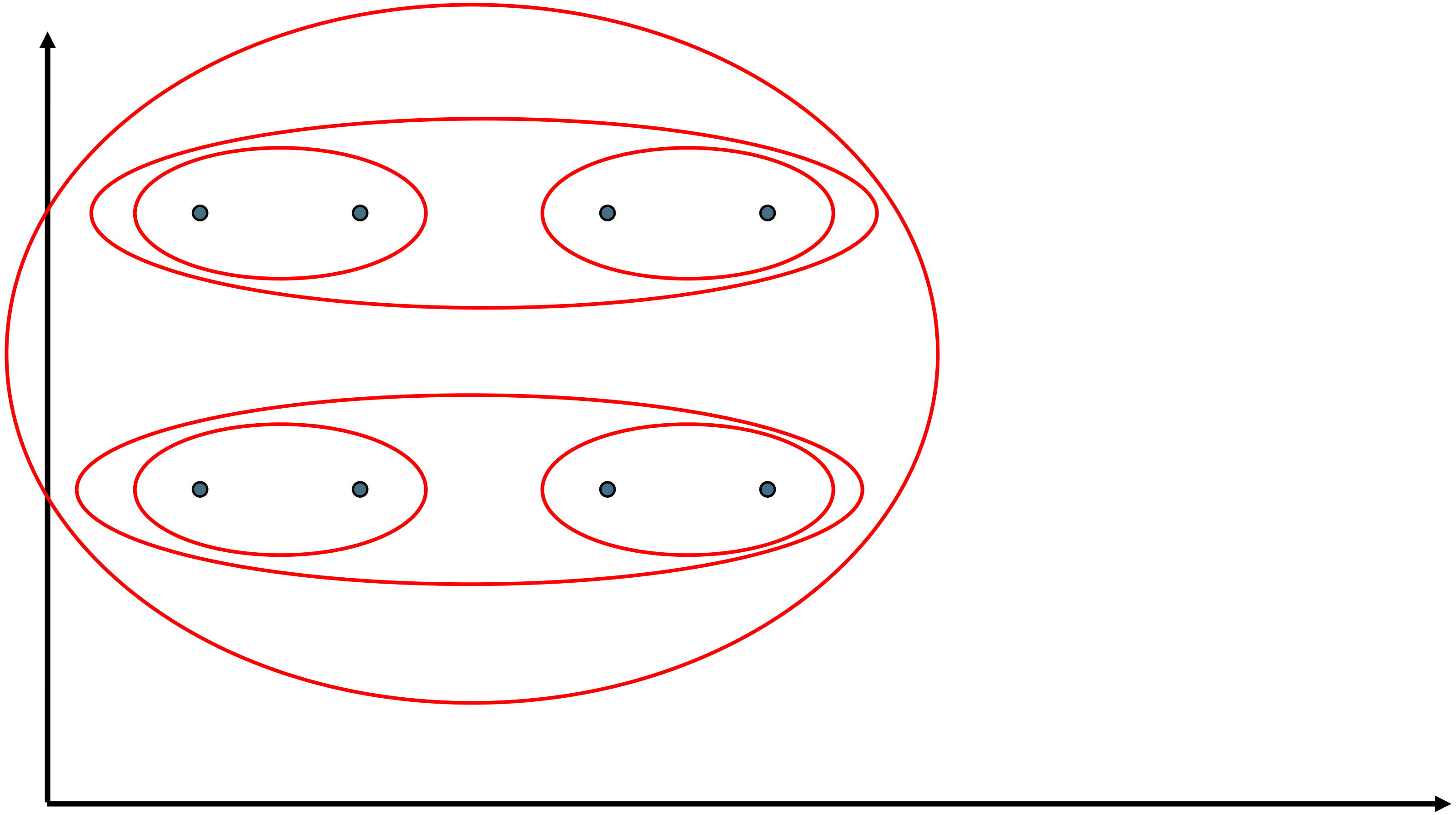
$$sim(c_i, c_j) = \max_{x \in c_i, y \in c_j} sim(x, y)$$

Can result in "straggly" (long and thin) clusters due to chaining effect.

After merging c_i and c_j, the similarity of the resulting cluster to another cluster, c_k, is:

$$sim((c_i \cup c_j), c_k) = \max(sim(c_i, c_k), sim(c_j, c_k))$$

Single Link Example



Complete Link

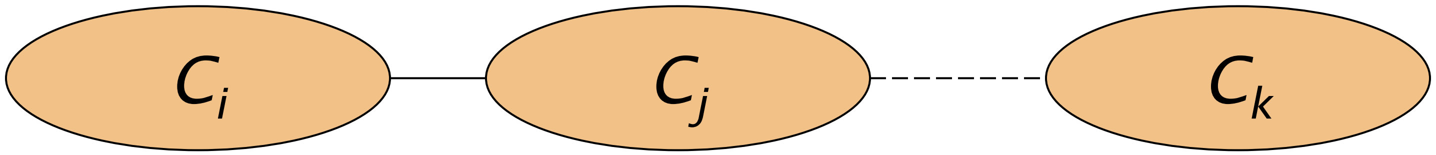
Use minimum similarity of pairs:

$$sim(c_i, c_j) = \min_{x \in c_i, y \in c_j} sim(x, y)$$

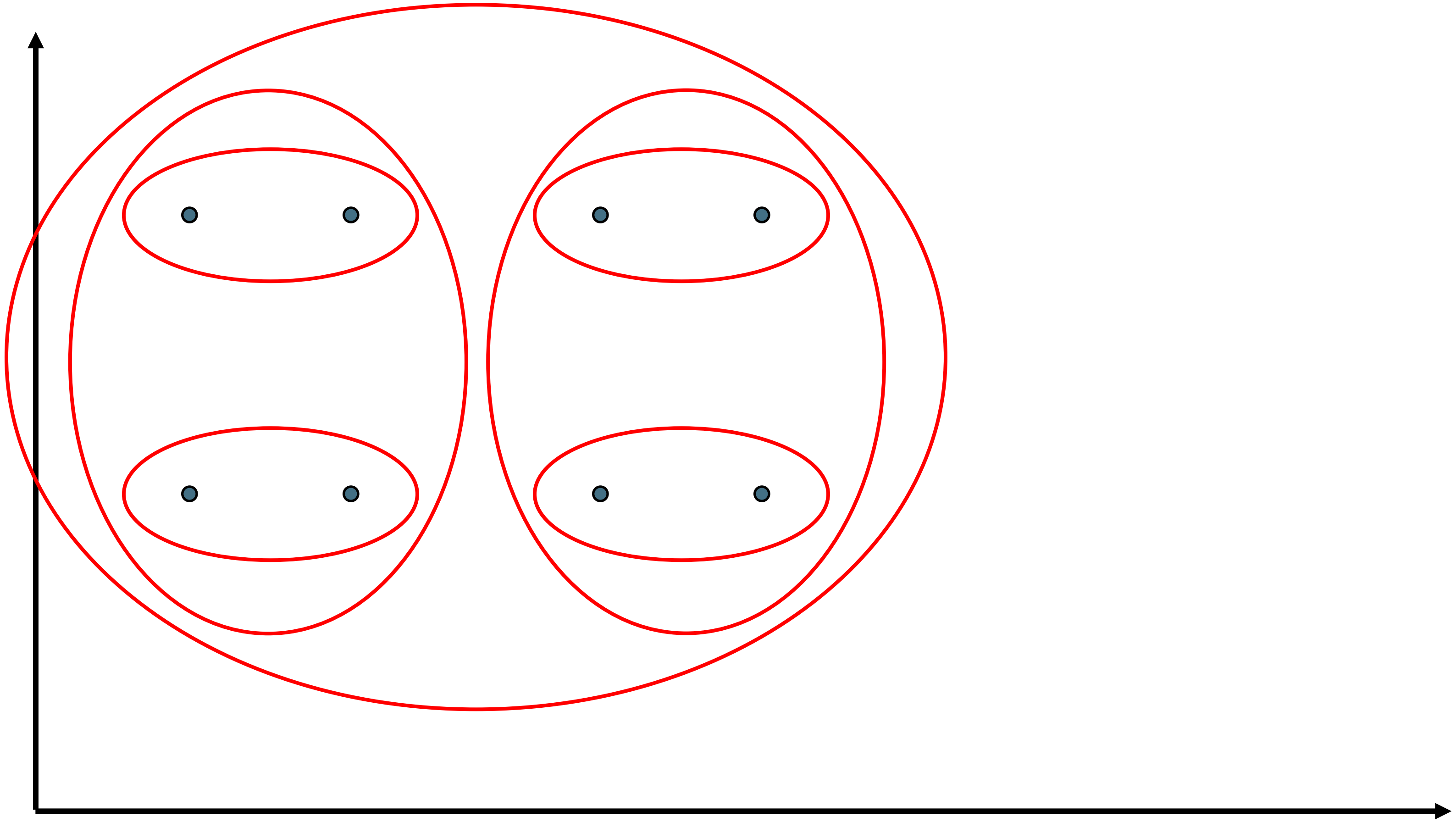
Makes "tighter," spherical clusters that are typically preferable.

After merging c_i and c_j, the similarity of the resulting cluster to another cluster, c_k, is:

$$sim((c_i \cup c_j), c_k) = \min(sim(c_i, c_k), sim(c_j, c_k))$$



Complete Link Example



Computational Complexity

- In the first iteration, all HAC methods need to compute similarity of all pairs of N initial instances, which is $O(N^2)$.
- In each of the subsequent N–2 merging iterations, compute the distance between the most recently created cluster and all other existing clusters.
- In order to maintain an overall $O(N^2)$ performance, computing similarity to each other cluster must be done in constant time.
  - Often $O(N^3)$ if done naively or $O(N^2 \log N)$ if done more cleverly

Group Average

Similarity of two clusters = average similarity of all pairs within merged cluster.

$$sim(c_i, c_j) = \frac{1}{\left|c_i \cup c_j\right|\left(\left|c_i \cup c_j\right| - 1\right)} \sum_{\vec{x} \in (c_i \cup c_j)} \; \sum_{\vec{y} \in (c_i \cup c_j) : \vec{y} \neq \vec{x}} sim(\vec{x}, \vec{y})$$

Compromise between single and complete link.

Two options:

- Averaged across all ordered pairs in the merged cluster
- Averaged over all pairs *between* the two original clusters

No clear difference in efficacy

Computing Group Average Similarity

Always maintain sum of vectors in each cluster.

$$\vec{s}(c_j) = \sum_{\vec{x} \in c_j} \vec{x}$$

Compute similarity of clusters in constant time:

$$sim(c_i, c_j) = \frac{(\vec{s}(c_i) + \vec{s}(c_j)) \bullet (\vec{s}(c_i) + \vec{s}(c_j)) - (|c_i| + |c_j|)}{(|c_i| + |c_j|)(|c_i| + |c_j| - 1)}$$

Evaluation

Cluster Validity

For supervised classification we have a variety of measures to evaluate how good our model is

- Accuracy, precision, recall

For cluster analysis, the analogous question is how to evaluate the "goodness" of the resulting clusters?

But "clusters are in the eye of the beholder"!

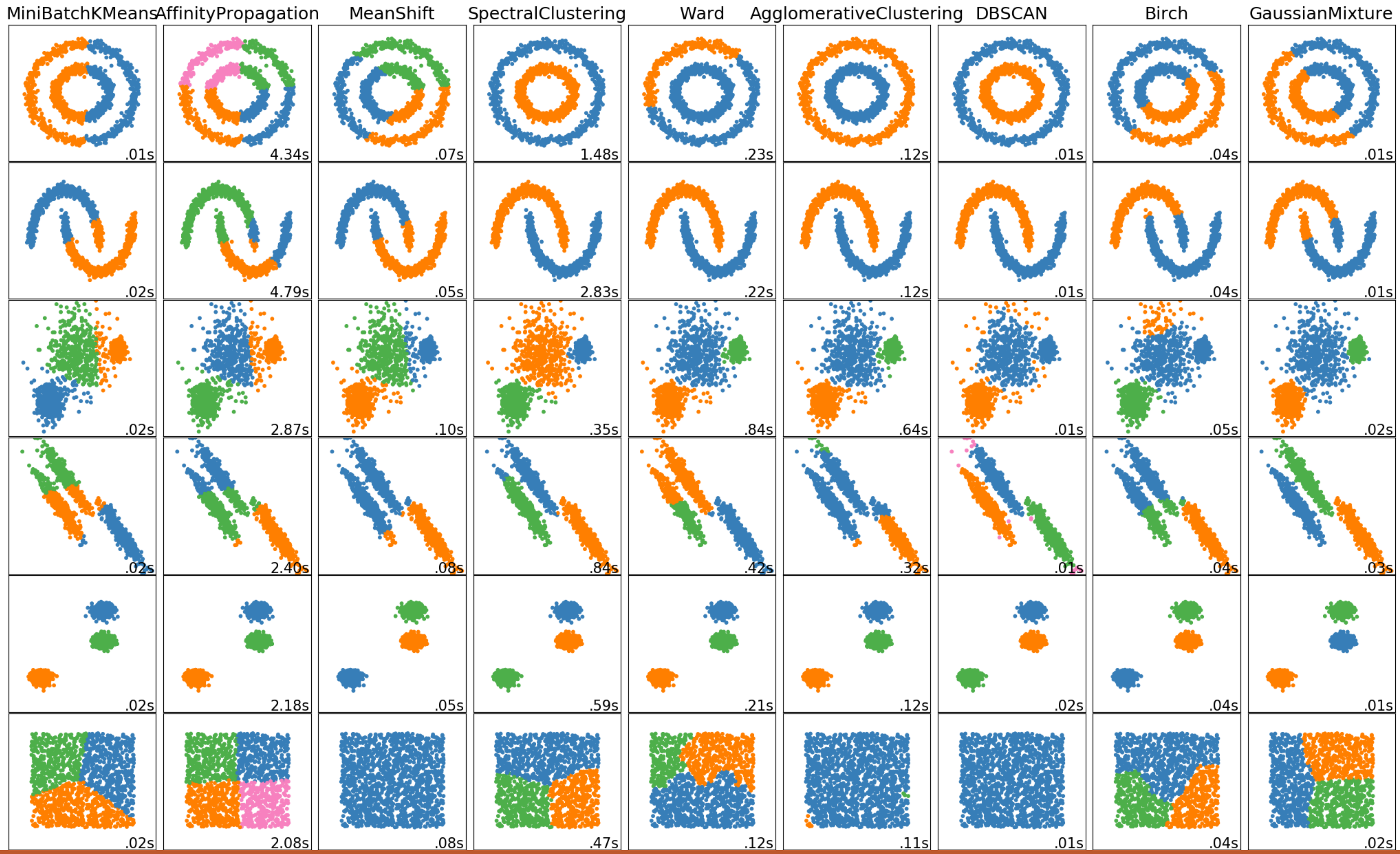
Then why do we want to evaluate them?

- To avoid finding patterns in noise
- To compare clustering algorithms
- To compare two sets of clusters
- To compare two clusters

What Is A Good Clustering?

Internal criterion: A good clustering will produce high quality clusters in which:

- the <u>intra-class</u> (that is, intra-cluster) similarity is high
- the <u>inter-class</u> similarity is low
- The measured quality of a clustering depends on both the document representation and the similarity measure used


MiniBatchKMeans
AffinityPropagation
MeanShift
SpectralClustering
Ward
AgglomerativeClustering
DBSCAN
Birch
GaussianMixture
.01s
4.34s
.07s
1.48s
.23s
.12s
.01s
.04s
.01s
.02s
4.79s
.05s
2.83s
.22s
.12s
.01s
.04s
.01s
.02s
2.87s
.10s
.35s
.84s
.64s
.01s
.05s
.02s
.02s
2.40s
.08s
.84s
.42s
.32s
.01s
.04s
.03s
.02s
2.18s
.05s
.59s
.21s
.12s
.02s
.04s
.01s
.02s
2.08s
.08s
.47s
.12s
.11s
.01s
.04s
.02s

External criteria for clustering quality

- Quality measured by its ability to discover some or all of the hidden patterns or latent classes in gold standard data
- Assesses a clustering with respect to ground truth … requires *labeled data*
- Assume documents with C gold standard classes, while our clustering algorithms produce K clusters, $\omega_1, \omega_2, \ldots, \omega_K$ with n_i members.

External Evaluation of Cluster Quality

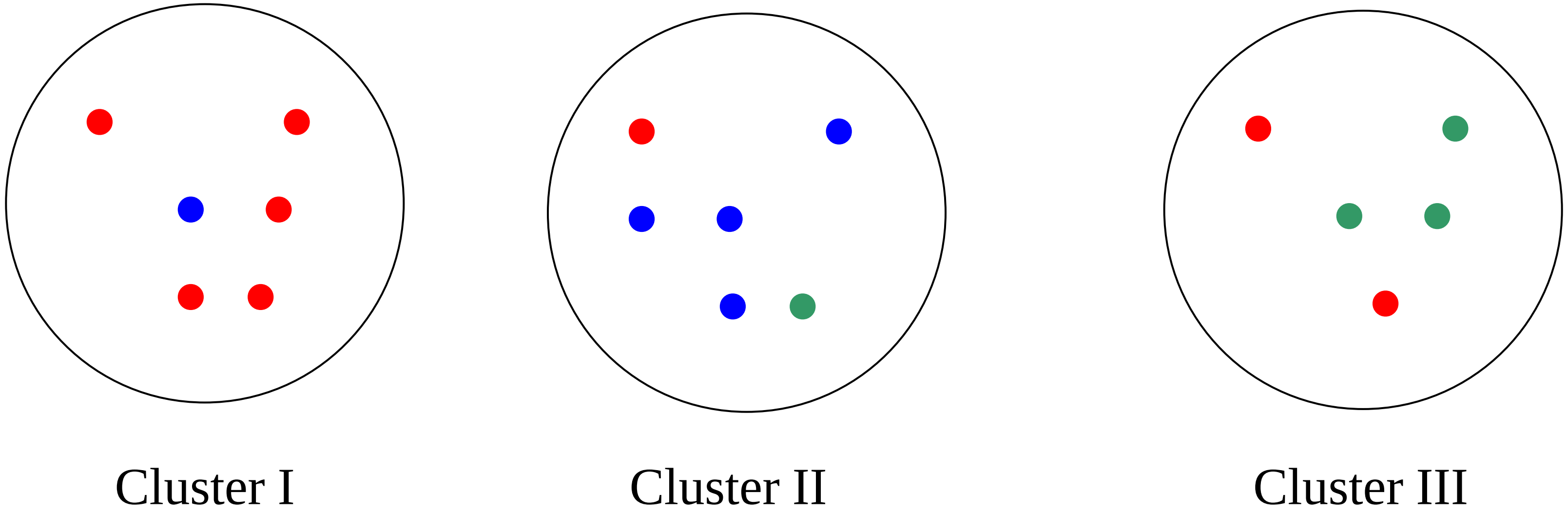
Simple measure: <u>purity</u>, the ratio between the dominant class in the cluster π_i and the size of cluster ω_i

$$Purity(\omega_i) = \frac{1}{n_i} \max_j (n_{ij}) \quad j \in C$$

Biased because having *n* clusters maximizes purity

Others are entropy of classes in clusters (or mutual information between classes and clusters)

Purity example



Cluster I: Purity = 1/6 (max(5, 1, 0)) = 5/6

Cluster II: Purity = 1/6 (max(1, 4, 1)) = 4/6

Cluster III: Purity = 1/5 (max(2, 0, 3)) = 3/5

Rand Index measures between pair decisions. Here RI = 0.68

Number of points	Same Cluster in clustering	Different Clusters in clustering
Same class in ground truth	20	24
Different classes in ground truth	20	72

Rand index and Cluster F-measure

$$RI = \frac{A+D}{A+B+C+D}$$

Compare with standard Precision and Recall:

$$P = \frac{A}{A+B} \qquad R = \frac{A}{A+C}$$

People also define and use a cluster F-measure, which is probably a better measure.

Issues in Machine Learning

What algorithms can approximate functions well and when?

How does the number of training examples influence accuracy?

How does the complexity of hypothesis representation impact it?

How does noisy data influence accuracy?

What are the theoretical limits of learnability?

Machine vs. Robot Learning

Machine Learning

Learning in vaccum

Statistically well-behaved data

Mostly off-line

Informative feed-back

Computational time not an issue

Hardware does not matter

Convergence proof

Robot Learning

- Embedded learning
- Data distribution not homegeneous
- Mostly on-line
- Qualitative and sparse feed-back
- Time is crucial
- Hardware is a priority
- Empirical proof