More Clustering Algorithms

Week 7

March 4, 2024

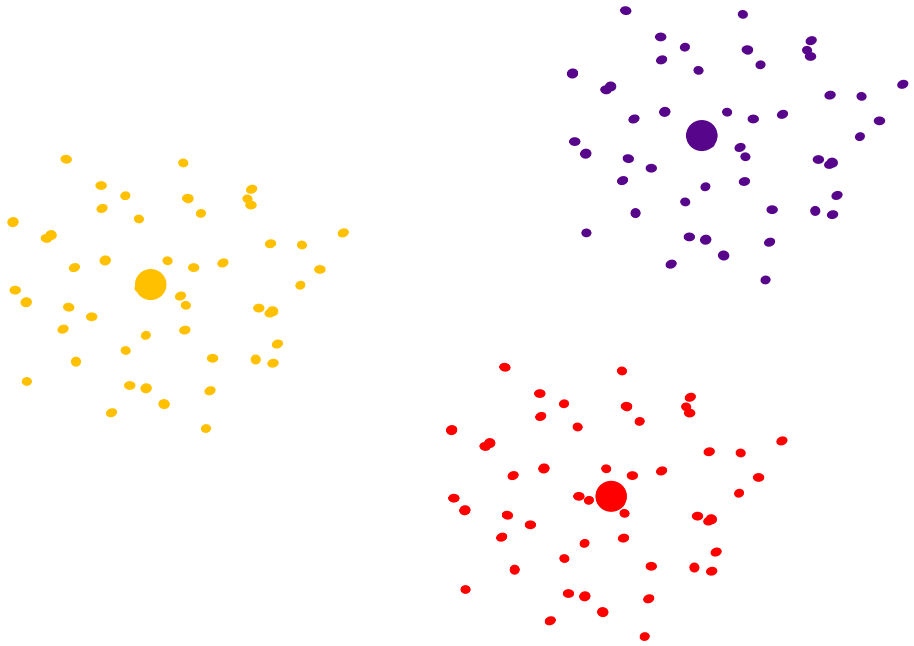
Today’s Outline

- Brief conversation: clustering as a search problem
- ***Hierarchical clustering***: bottom-up and top-down
- ***K-means clustering***
- ***Leader clustering*** for massive streaming data
- Lab: Clustering in Python

Recap from Last Week

We saw how Bayesian methods (Naïve Bayes/EM) could be used for a range of applications, including **supervised learning** (classification), **semi-supervised learning** (classification with labeled and unlabeled data), and **unsupervised learning** (clustering).

Today we will take a step back to better understand clustering- what it is and why it is useful- and examine a variety of other clustering methods.



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Clustering Data

Main goal: Given a dataset of N records, we wish to partition the dataset into k << N groups such that records in the same group are similar to each other, and records in different groups are dissimilar.

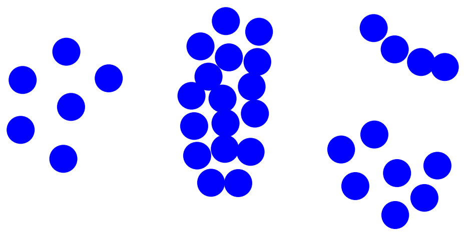
Given a population of individuals, we want to **identify** and **characterize** the underlying subgroups (or “clusters”) of individuals, and possibly use these subgroups for **prediction**.

We want to explain the data in terms of its natural groupings.

How many groups are there?
Who belongs to which group?
Characteristics of each group?

Example: identify congressional voting blocs.

How well do blocs correspond to party affiliation?
Are there relevant blocs within a party?
Are there “mavericks” that vote across party lines?
How much do blocs vary with proposed legislation?



2-D example

Clustering Data

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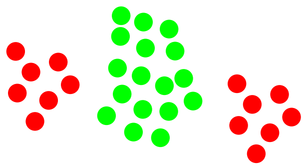
How does clustering differ from prediction?

There may not be any single output that we are trying to predict.

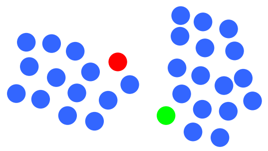
We are interested in an underlying **structure** that explains or predicts many characteristics of the population.

Clustering can sometimes improve prediction performance.

Improve model-based classification by learning multiple models per class.

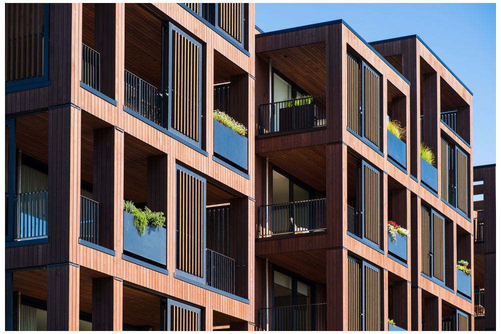


We may have little or no labeled training data for learning class models but lots of unlabeled data.



Supervised vs Unsupervised

1. Supervised learning

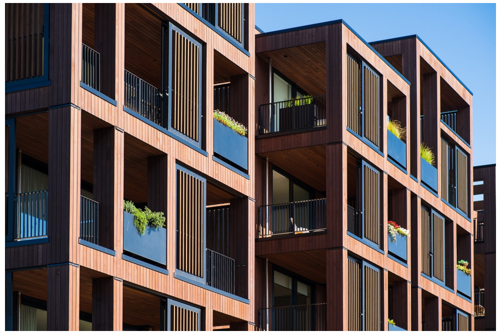


This is a house

This is a car

What is this?

2. It is an <u>unsupervised</u> learning technique that segment instances into “known” number of clusters

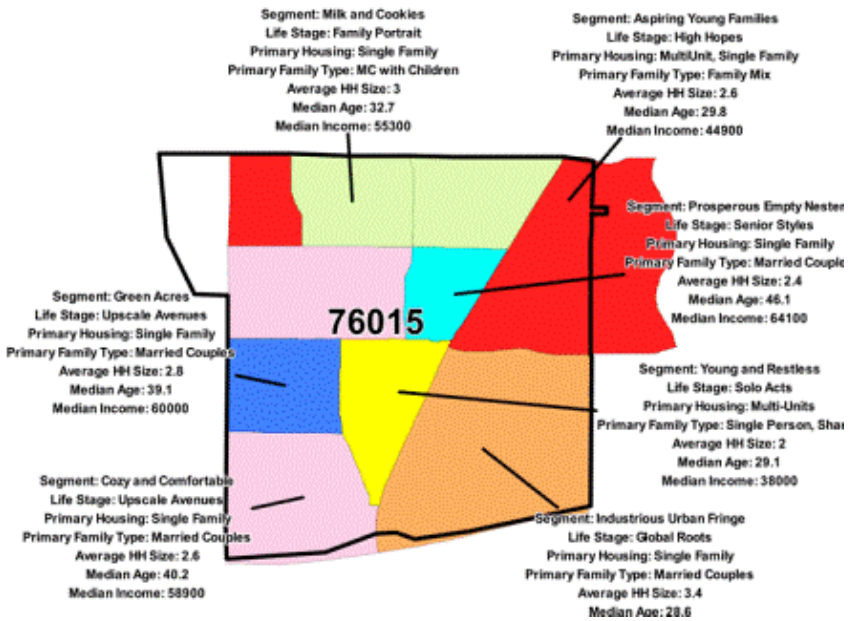


There are two objects in this set of images. Separate them into “two” groups

Application of Clustering

Main goal: Given a dataset of N records, we wish to partition the dataset into k << N groups such that records in the same group are similar to each other, and records in different groups are dissimilar.

An important application of clustering is to improve **prediction** of an individual’s characteristics or behavior, using information obtained from other members of their inferred group.



Customer database segmentation: To which subgroups should I market my product, and how should I target them? (Similarly, voter database segmentation)

Census outreach activities: Different subgroups of the population should have different targeted outreach strategies.

Patient database segmentation: Different subgroups of patients may benefit from different treatment regimens.

Application of Clustering

<u>Main goal</u>: Given a dataset of N records, we wish to partition the dataset into k << N groups such that records in the same group are similar to each other, and records in different groups are dissimilar.

Group-based trajectory modeling identifies subgroups of the population and uses these subgroups to predict how an individual's behavior will change over the course of their life.

Daniel Nagin (CMU) developed these methods and applied them to **predict** juvenile delinquency and criminal behavior.

This figure shows the predicted and actual trajectories of an individual's number of criminal convictions, varying with age. Three trajectory groups were identified: never (71%), limited to adolescence (22%), and chronic offenders (7%).

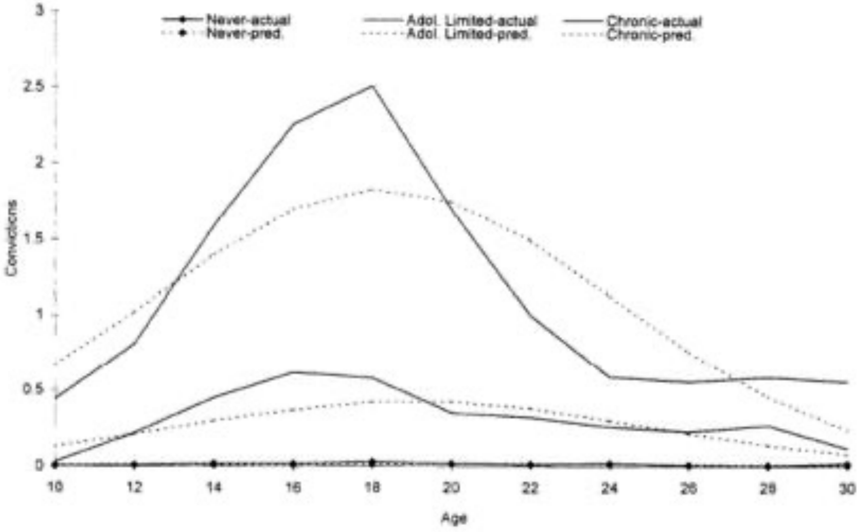


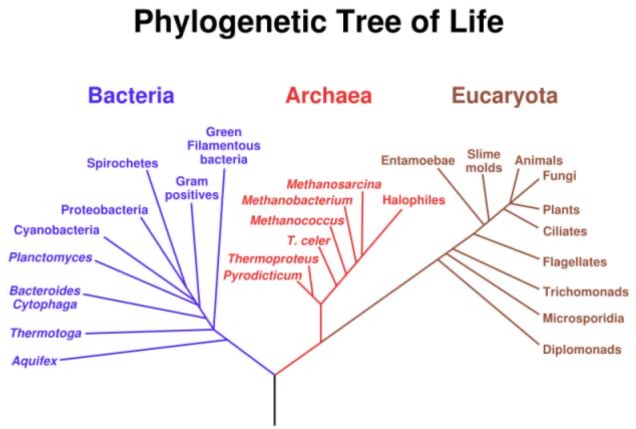
Figure 1. Trajectories of number of convictions (Cambridge sample). Adol. = adolescent; pred. = predicted.

Nagin, D. S. 1999. "Analyzing Developmental Trajectories: A Semi-parametric, Group-based Approach." *Psychological Methods*, 4: 139-177.

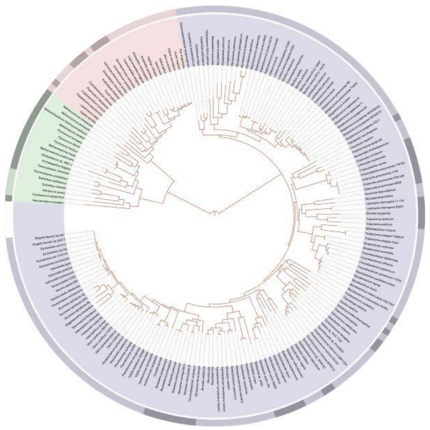
Application of Clustering

Main goal: Given a dataset of N records, we wish to partition the dataset into k << N groups such that records in the same group are similar to each other, and records in different groups are dissimilar.

Clustering is also very commonly used in **evolutionary biology** to create “phylogenetic trees” relating different species and showing when the species diverged from a common ancestor.



Here is a simple phylogenetic tree developed manually by evolutionary biologists.



Now, much more detailed trees can be generated automatically by clustering DNA sequences, enhancing our understanding of evolution.

Here, we are interested in learning the **hierarchy** of clusters!

Real-World Example

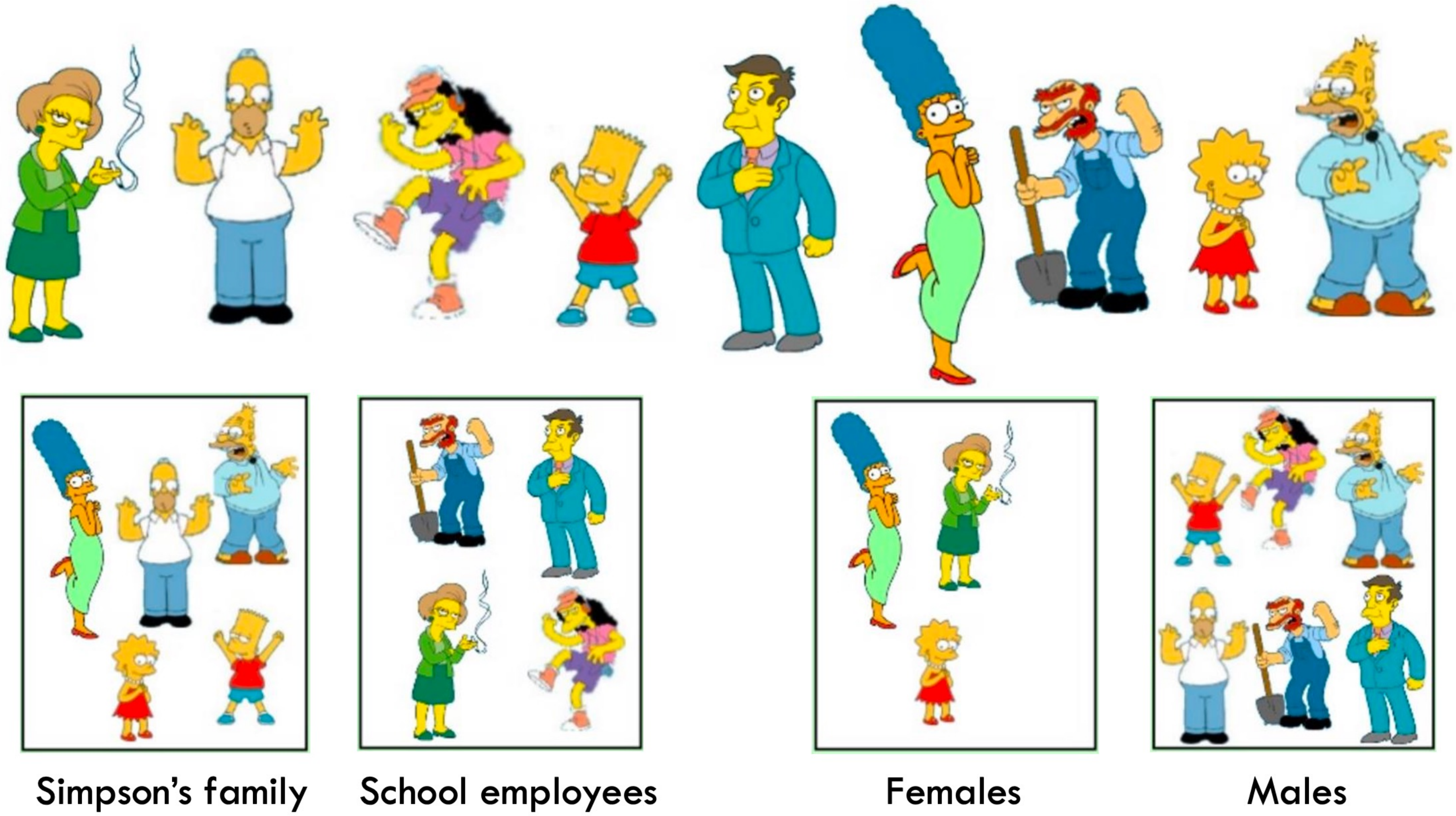
- Clustering images based on their perceptual similarities
- Image segmentation (clustering pixel)

- Clustering webpages based on their content
- Clustering web-search results
- Clustering people in social networks based on user properties/preferences

Reference: N. Soheili (UIC), Z. Joesph and I. Nourbakhsh (CMU) and K. Chen and T. Mu (The Univ of Manchester), V. Lavrenko (Univ of Edinburgh)

Non-Real-World Example

Different similarity criteria can lead to different clustering



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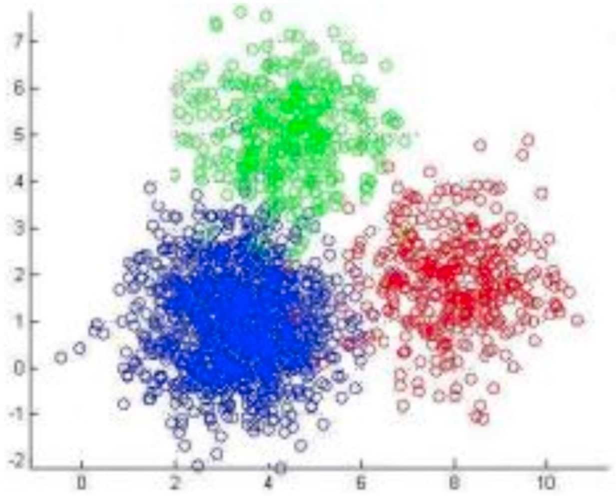
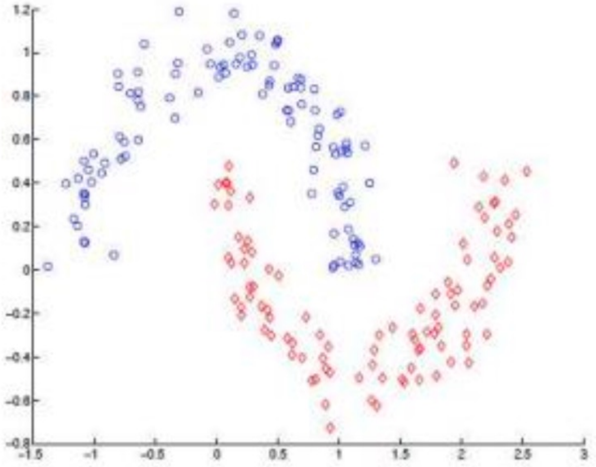
Notion of Similarity

- Choice of the similarity measure is very important for clustering
- Similarity is inversely related to distance
- Different ways exist to measure distances. Some examples:
  - Euclidean distance: $d(x,y) = ||x-y|| = \sqrt{\sum_i (x_i - y_i)^2}$
  - Manhattan distance: $d(x,y) = \sum_i |x_i - y_i|$
  - Kernelized (non-linear) distance: $d(x,y) = ||\varphi(x) - \varphi(y)||$



For this figure, Euclidean distance may be reasonable



For this figure, Kernelized distance seems more reasonable

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Hierarchical Clustering

Hierarchical Clustering

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2 real-valued
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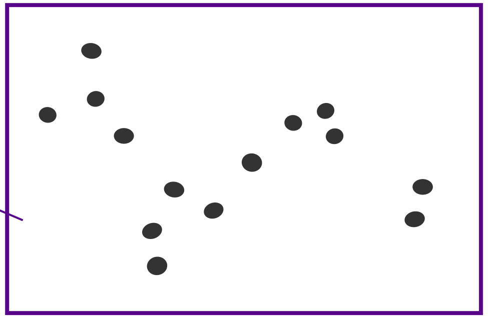

Given a set of records $x_1..x_N$ and
a distance metric $d(x_i, x_j)$.

Records can have real and
discrete-valued attributes.

We will create a **hierarchy** of clusters
by merging similar records.

How to define "nearest" clusters?

$$D(C,C') = \min_{x \in C, x' \in C'} d(x,x')$$

Bottom-up hierarchical clustering

(1) Start with N clusters, each containing one record.

(2) Choose the two "nearest" clusters and merge them into a single cluster.

(3) Repeat until all points are merged into a single cluster.

Single-Link Clustering

14 records,
2 real-valued
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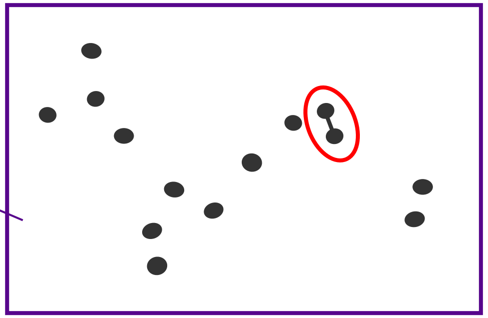

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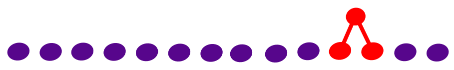
(After 1 merge)



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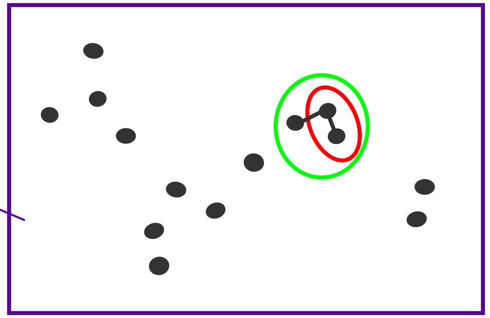

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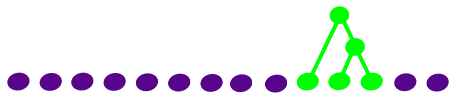
(After 2 merges)



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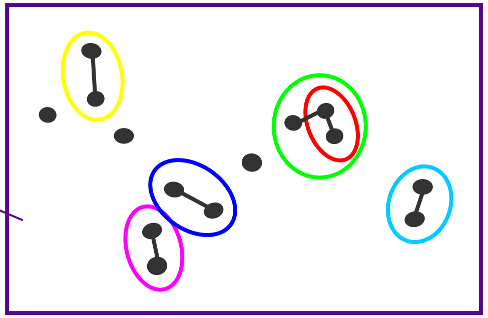

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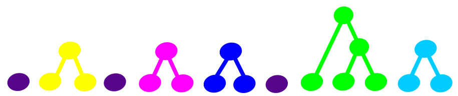
(After 6 merges)



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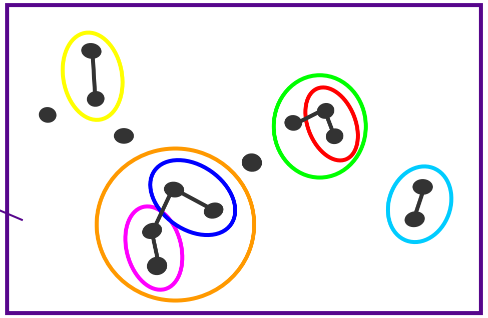

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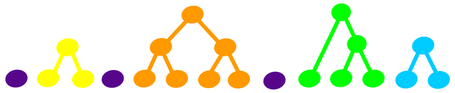
(After 7 merges)



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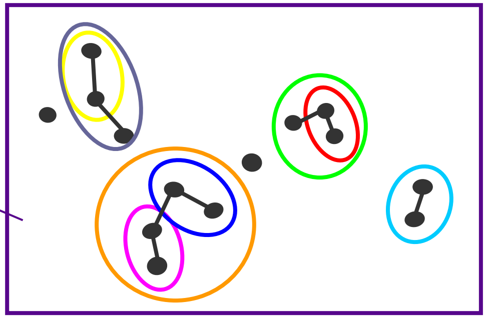

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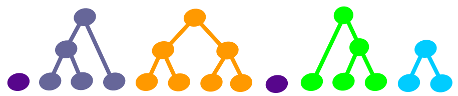
(After 8 merges)



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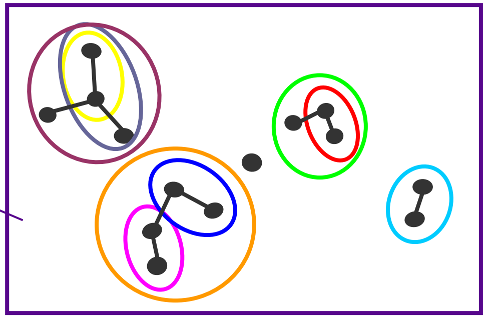

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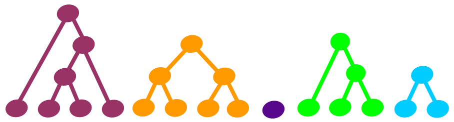
(After 9 merges)



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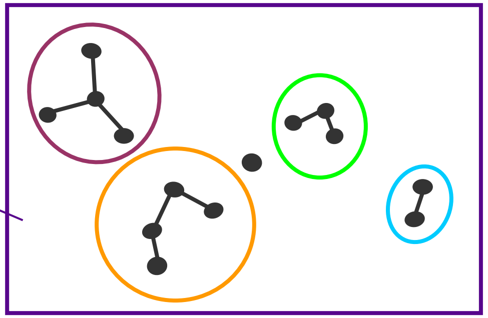

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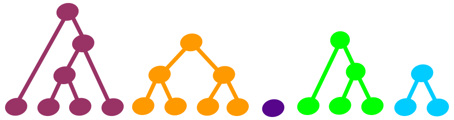

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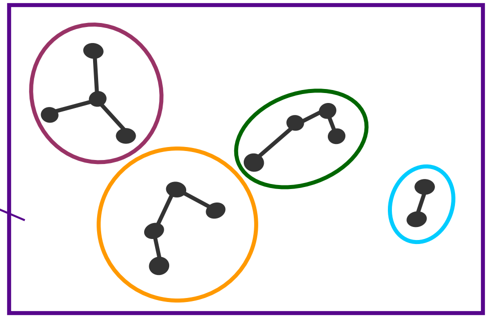

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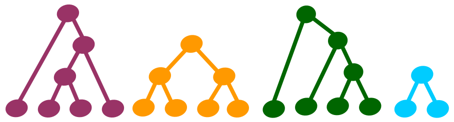
(After 10 merges)



Single-Link Clustering

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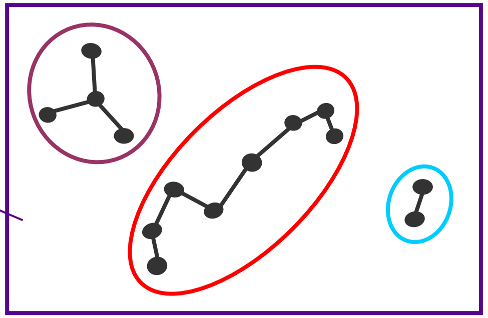

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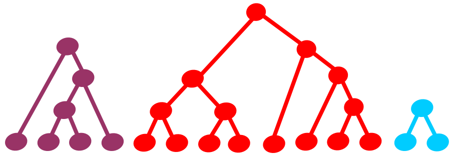
(After 11 merges)



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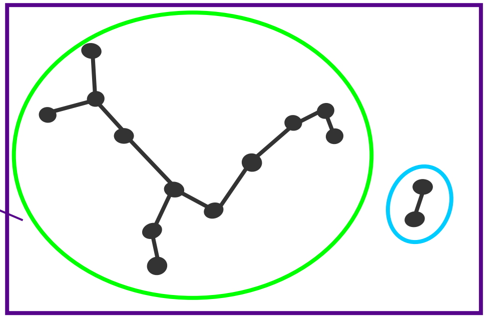

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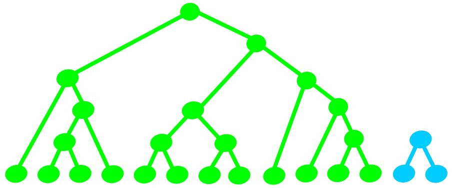
(After 12 merges)



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Single-Link Clustering

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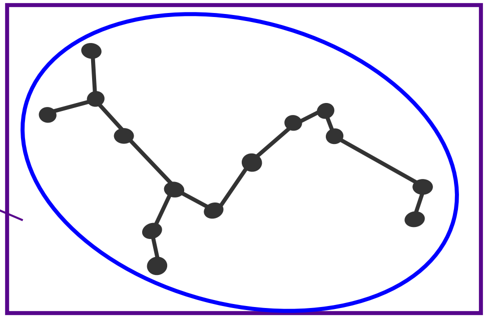

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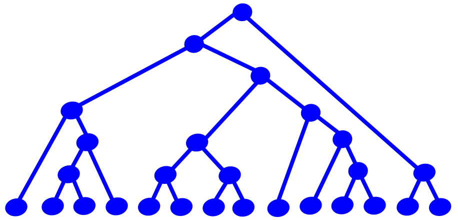

Done!

Single-Link Clustering

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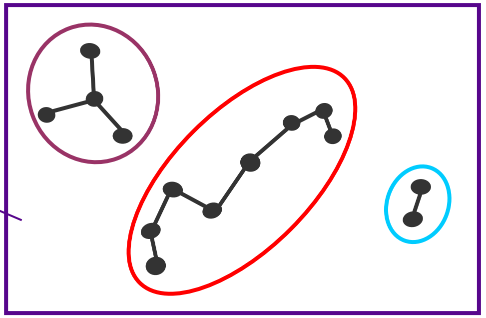

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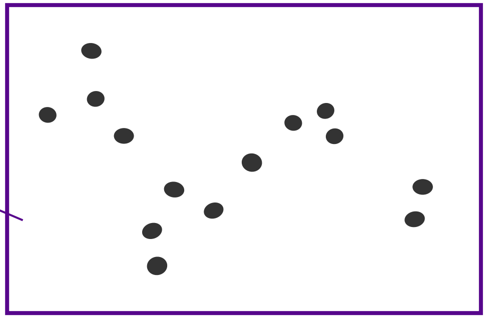
(3) Repeat until all points are merged into a single cluster.

Note that single-link clustering tends to produce highly elongated groups (or "chains") as shown above.

If we want to produce more spherical groups, we can instead consider the **maximum** distance between clusters.

Complete-Link Clustering

14 records,
2 real-valued
attributes,
Euclidean
distance



Given a set of records $x_1..x_N$ and
a distance metric $d(x_i, x_j)$.

Records can have real and
discrete-valued attributes.

We will create a **hierarchy** of clusters
by merging similar records.

How to define “nearest” clusters?

$$D(C, C') = \max_{x \in C,\, x' \in C'} d(x, x')$$

<u>Bottom-up hierarchical clustering</u>

(1) Start with N clusters, each containing one record.

(2) Choose the two “nearest” clusters and merge them into a single cluster.

(3) Repeat until all points are merged into a single cluster.

Complete-Link Clustering

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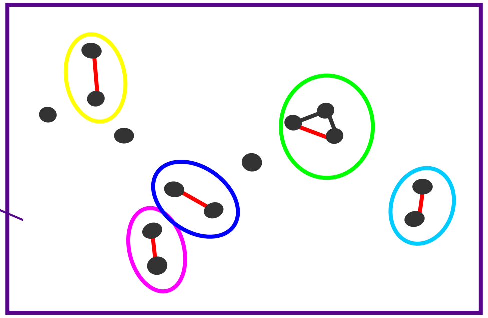

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(After 6 merges)

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Complete-Link Clustering

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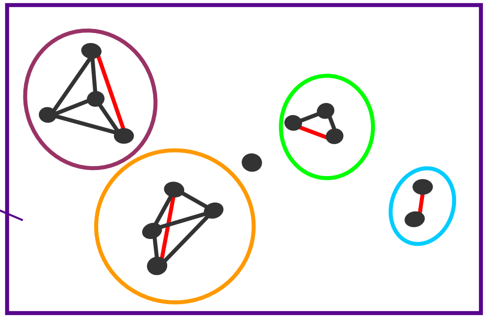
Euclidean
distance



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(After 9 merges)

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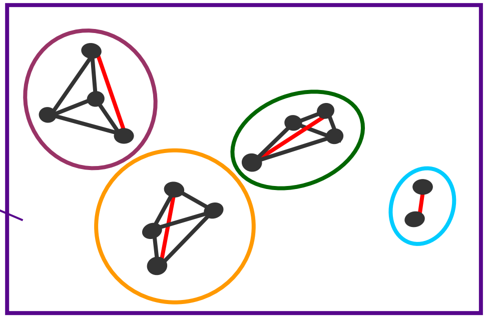
distance



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(After 10 merges)

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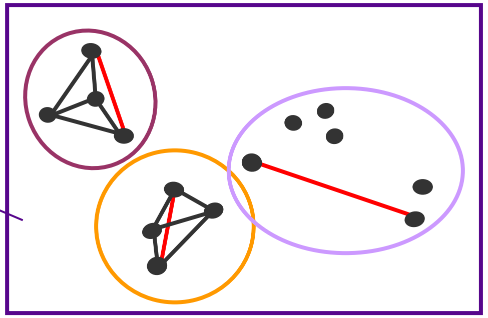

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Bottom-up hierarchical clustering

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(After 11 merges)

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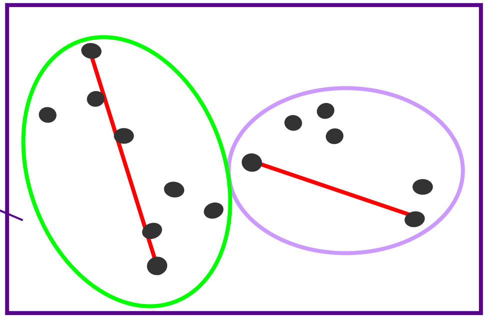

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Bottom-up hierarchical clustering

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(2) Choose the two "nearest" clusters and merge them into a single cluster.

(3) Repeat until all points are merged into a single cluster.

(After 12 merges)

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Hierarchical Clustering

Top-down hierarchical clustering

- Start with one cluster containing all N records.
- Choose the "worst" cluster, and optimally partition it into two distinct clusters.
- Repeat until all points are in separate clusters.

Bottom-up hierarchical clustering

- Start with N clusters, each containing one record.
- Choose the two "nearest" clusters and merge them into a single cluster.
- Repeat until all points are merged into a single cluster.

Top-down clustering is hard, so we focus on the bottom-up approach.

Some fancy hierarchical clustering algorithms alternate bottom-up and top-down stages.

Advantages of hierarchical clustering

You get an entire cluster hierarchy, not just a single clustering.

Easy to compare different numbers of clusters k: just cut the longest k-1 links and optimize some measure of "goodness" (more on that later).

(Any disadvantages?)

K-means Clustering

K-means Clustering

Hierarchical clustering is a simple, useful clustering method, but it gives you no guarantees on the quality of the resulting groups.

An alternative is to define some <u>objective function</u> that describes the quality of the groups and attempt to optimize that function.

Assume that all attributes are real-valued, so we can compute the <u>centroid</u> of any cluster (i.e. the mean value of each attribute)

Possible objective:
minimize distortion

$$\sum_{C_k} \sum_{x_i \in C_k} (x_i - \mu_k)^2$$

This is the sum of squared errors for each data point x_i, assuming that each x_i is mapped to the closest cluster center μ_k.

<u>Possible moves for state-space search</u>
Change position of cluster center μ_k
Change mapping of point x_i to center μ_k
Change number of clusters K

How to perform this search efficiently?

K-means Clustering

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This is the sum of squared errors for each data point x_i, assuming that each x_i is mapped to the closest cluster center μ_k.

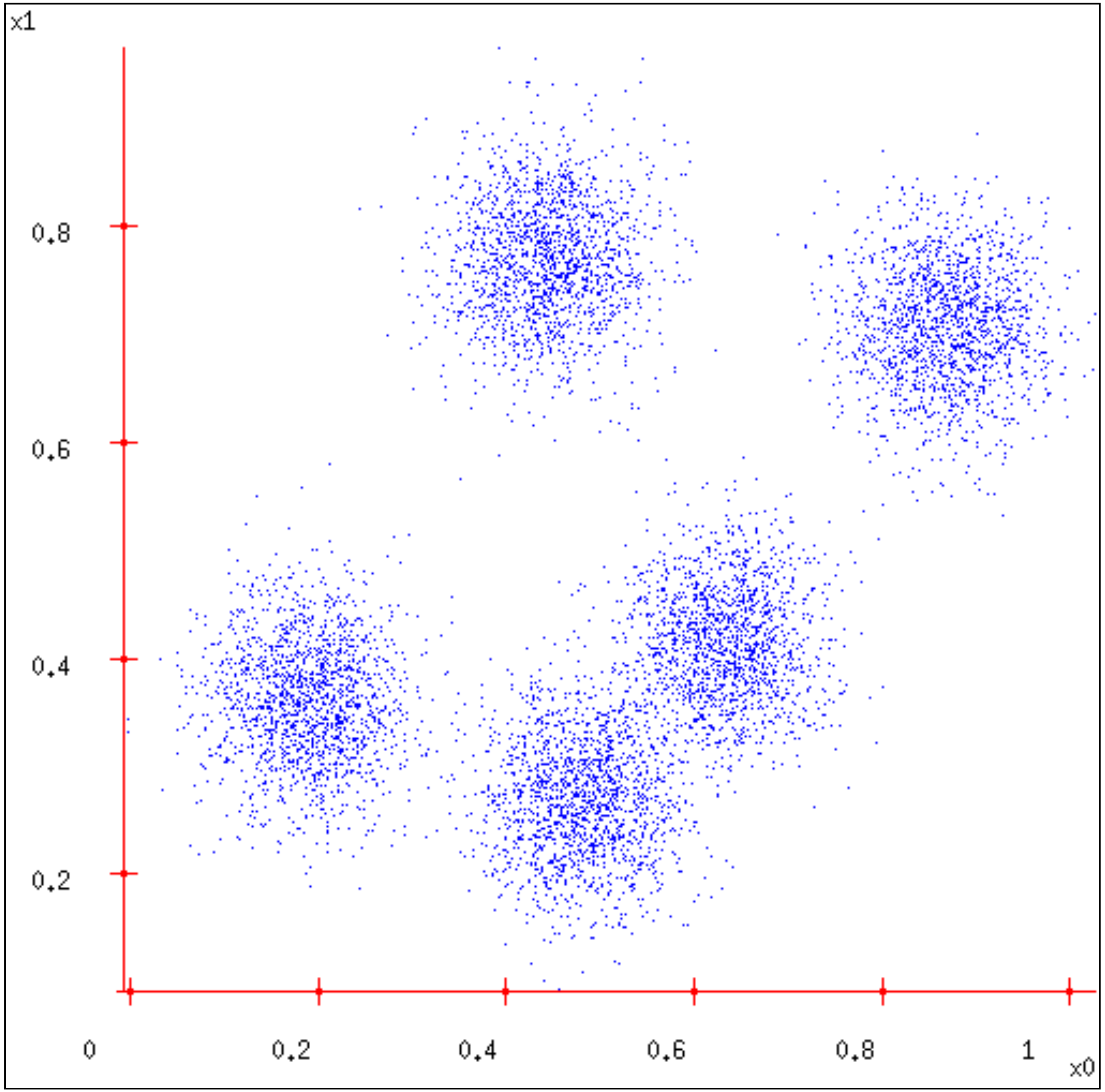
1. Moving μ_k to centroid of all points in C_k reduces distortion
2. Mapping point x_i to nearest center μ_k reduces distortion.

Possible moves for state-space search
Change position of cluster center μ_k
Change mapping of point x_i to center μ_k
Change number of clusters K

Keep a number of centers fixed, and alternate between these two moves.

K-means

1. Ask users how many clusters they'd like. (e.g. k = 5)



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Thanks to Andrew Moore for providing this example.

K-means

1. Ask users how many clusters they'd like. (e.g. k = 5)
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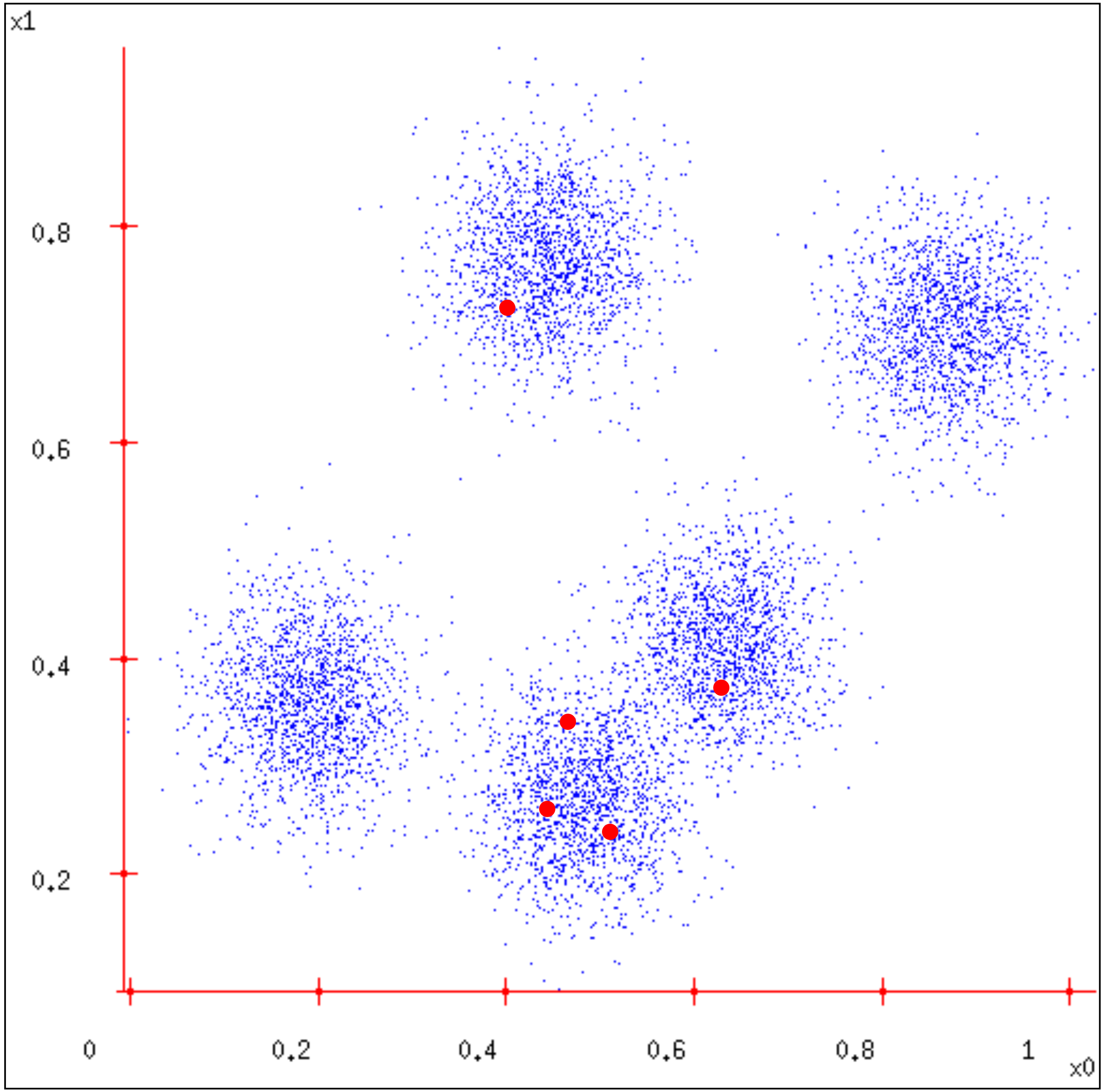

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K-means

1. Ask users how many clusters they'd like. (e.g. k = 5)
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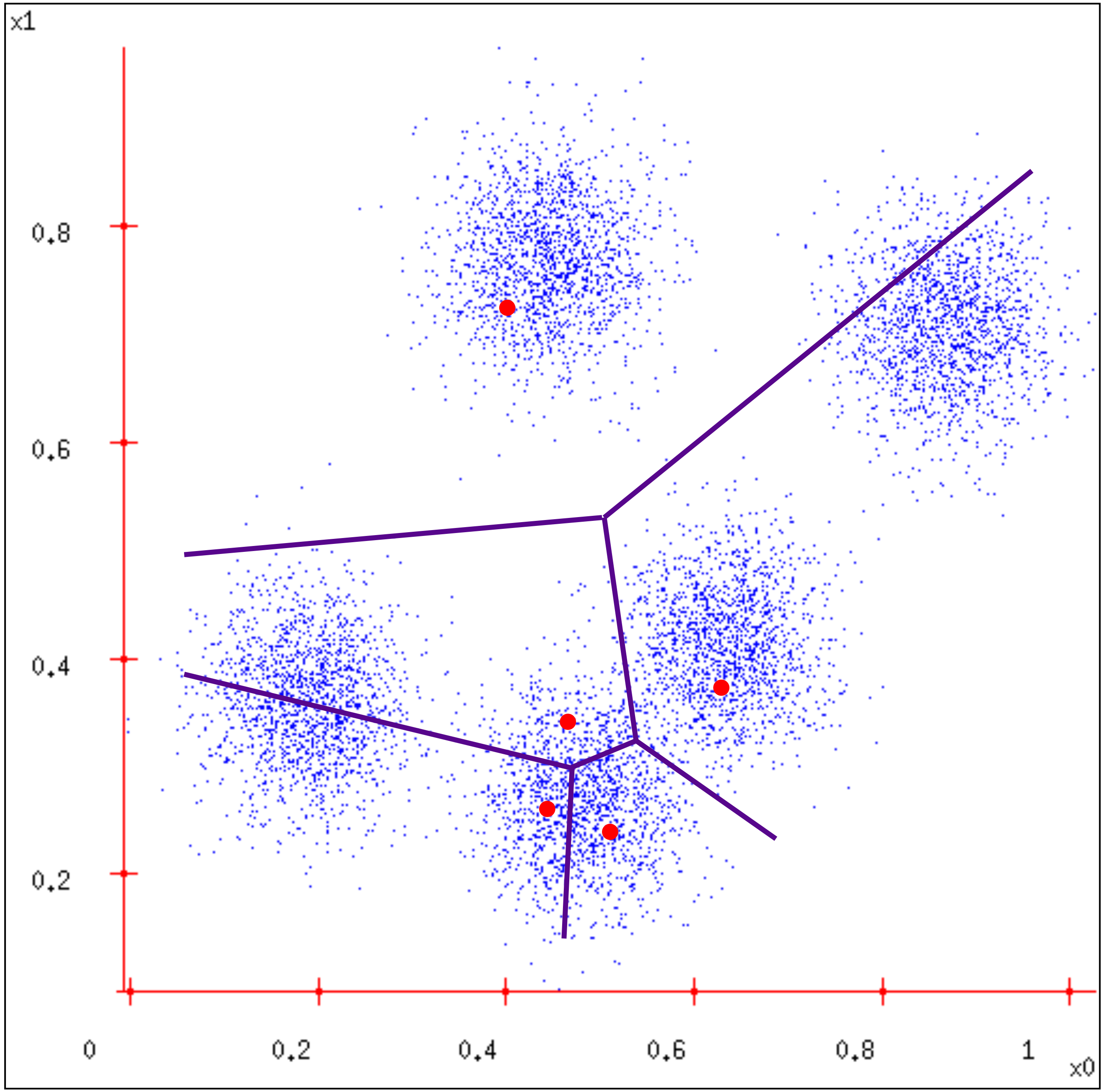
3. Each datapoint finds out which center it's closest to



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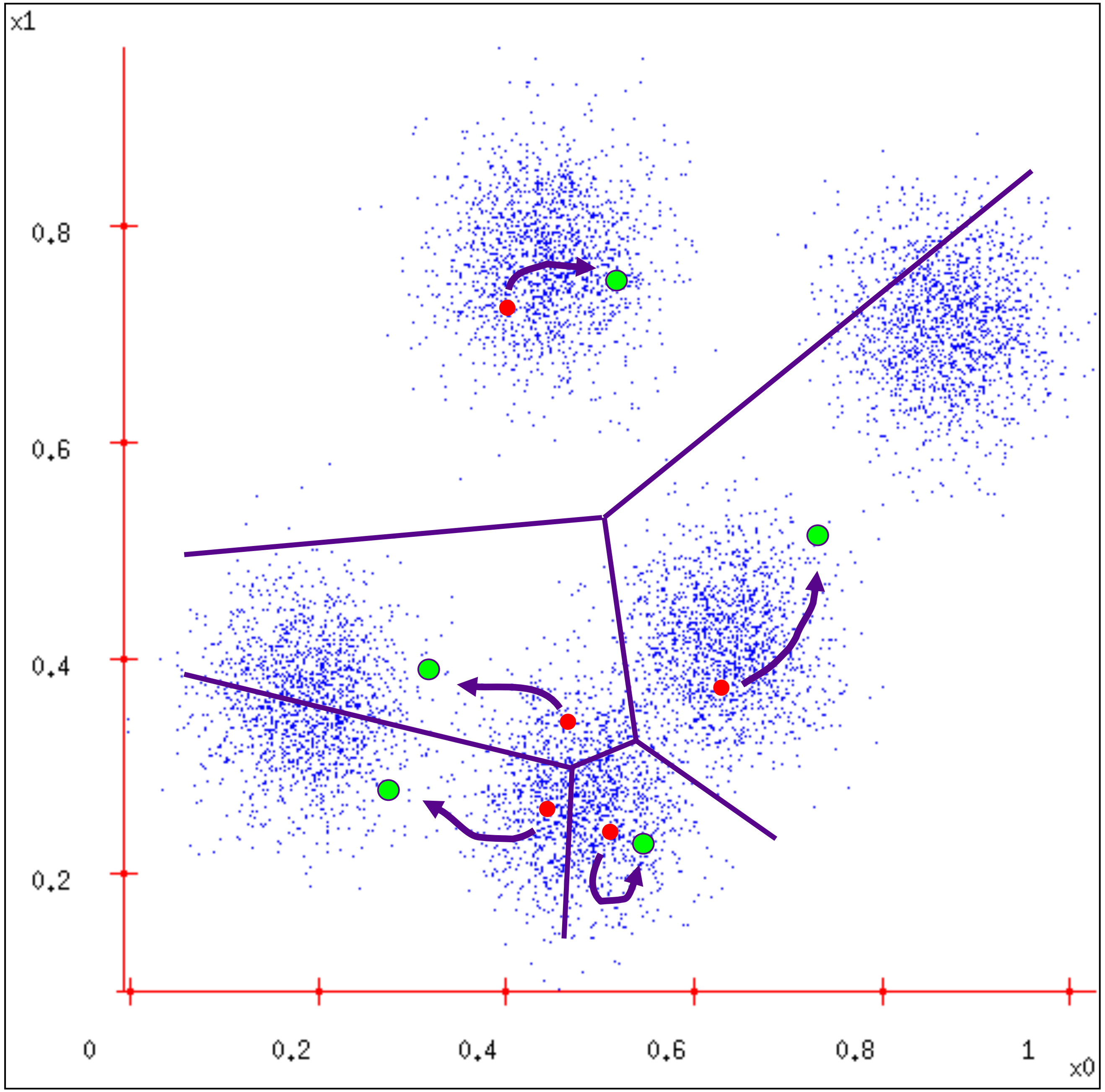
4. Each center finds the centroid of the points it owns and moves there.



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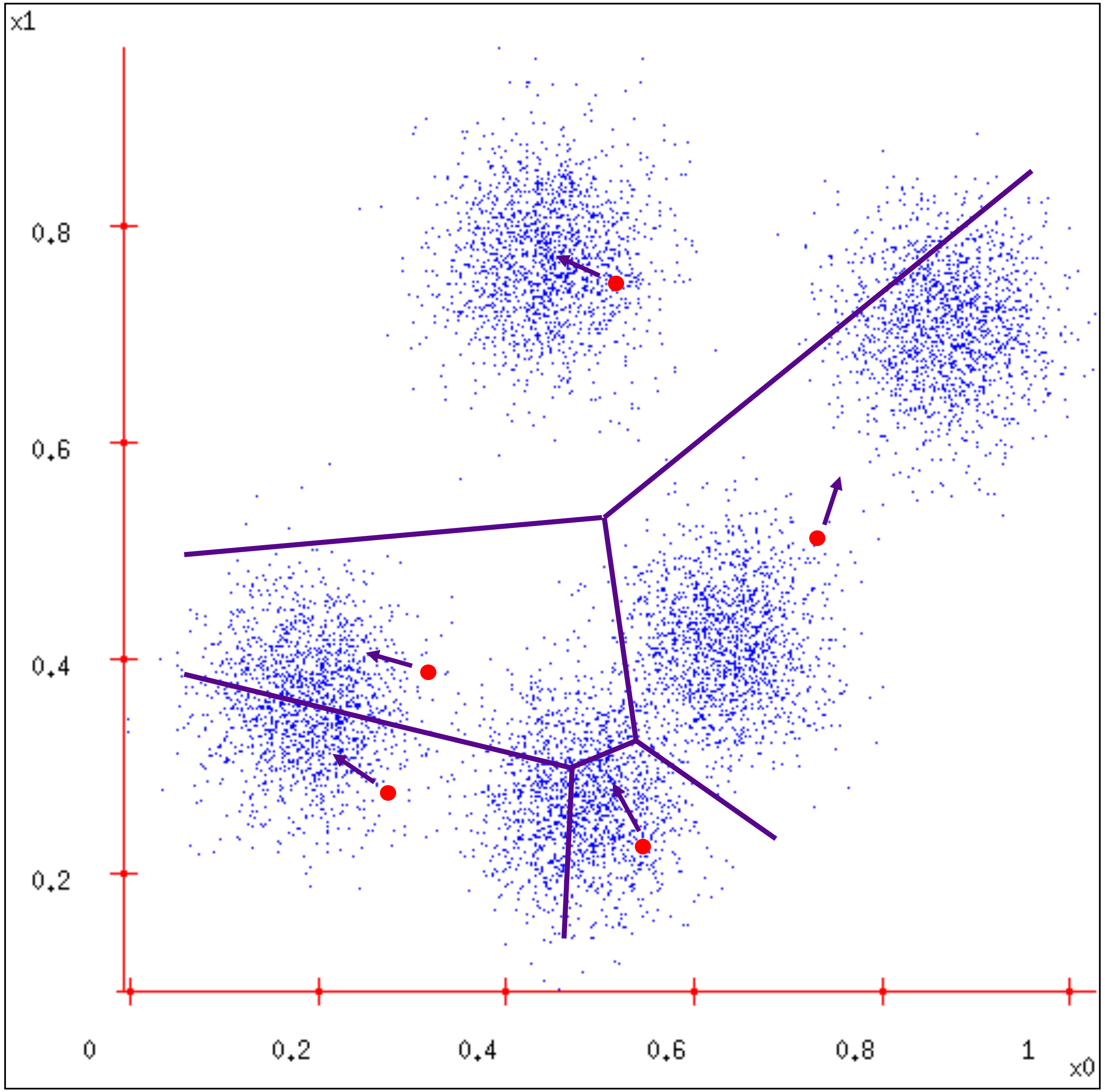
Repeat steps 3-4 until convergence!



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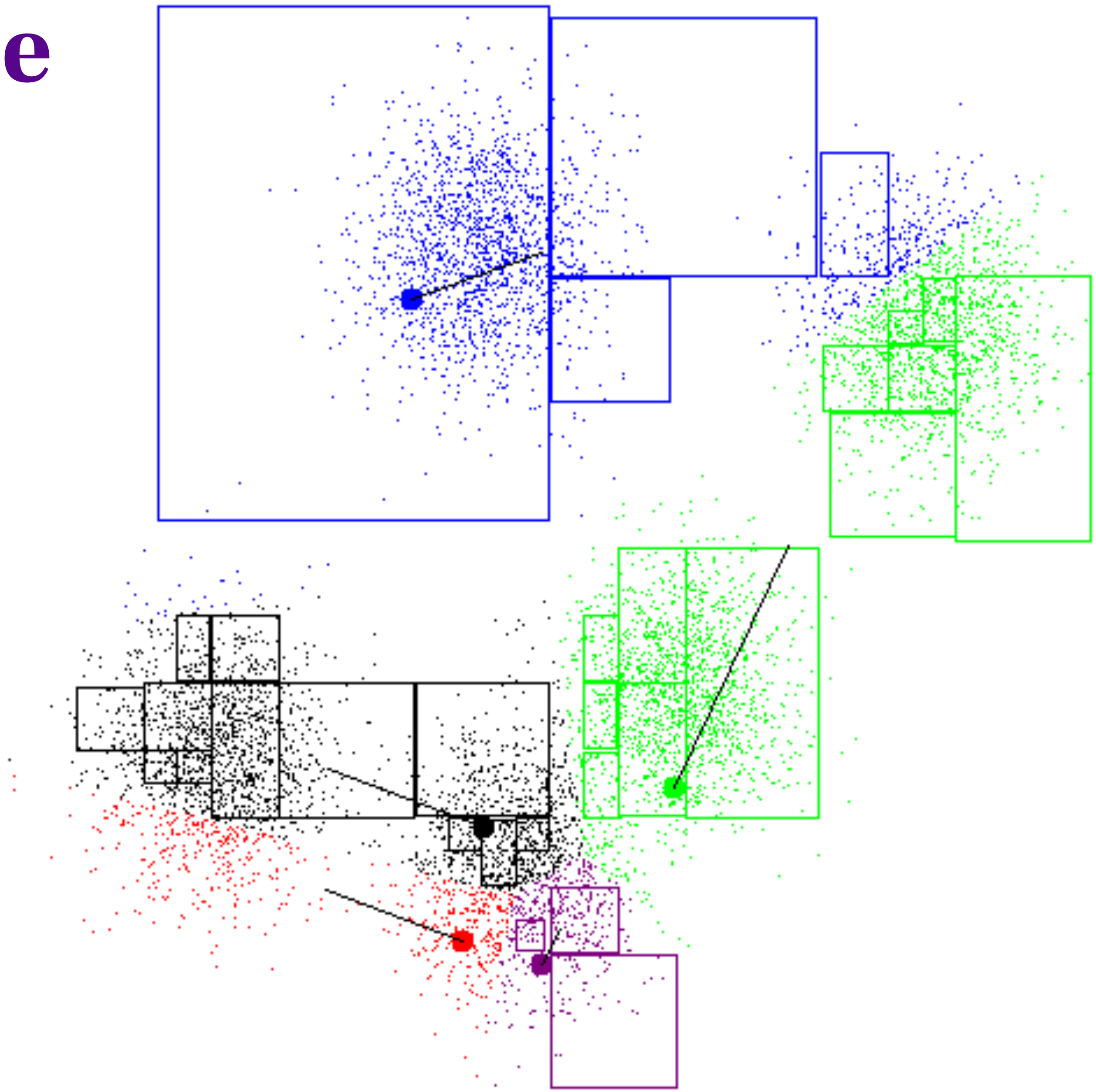
K-means real example

Here's an example run of k-means, generated by a software.



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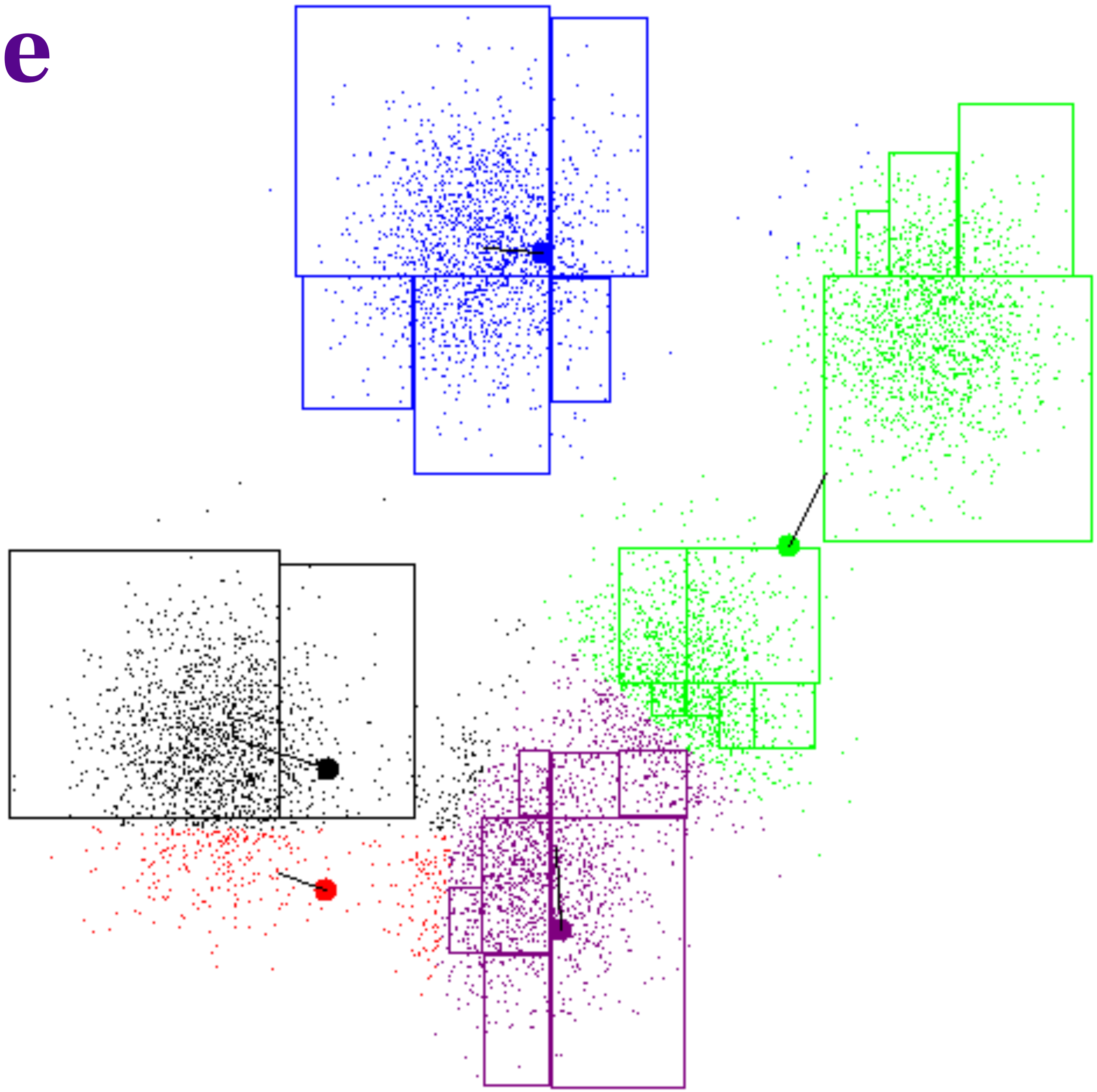

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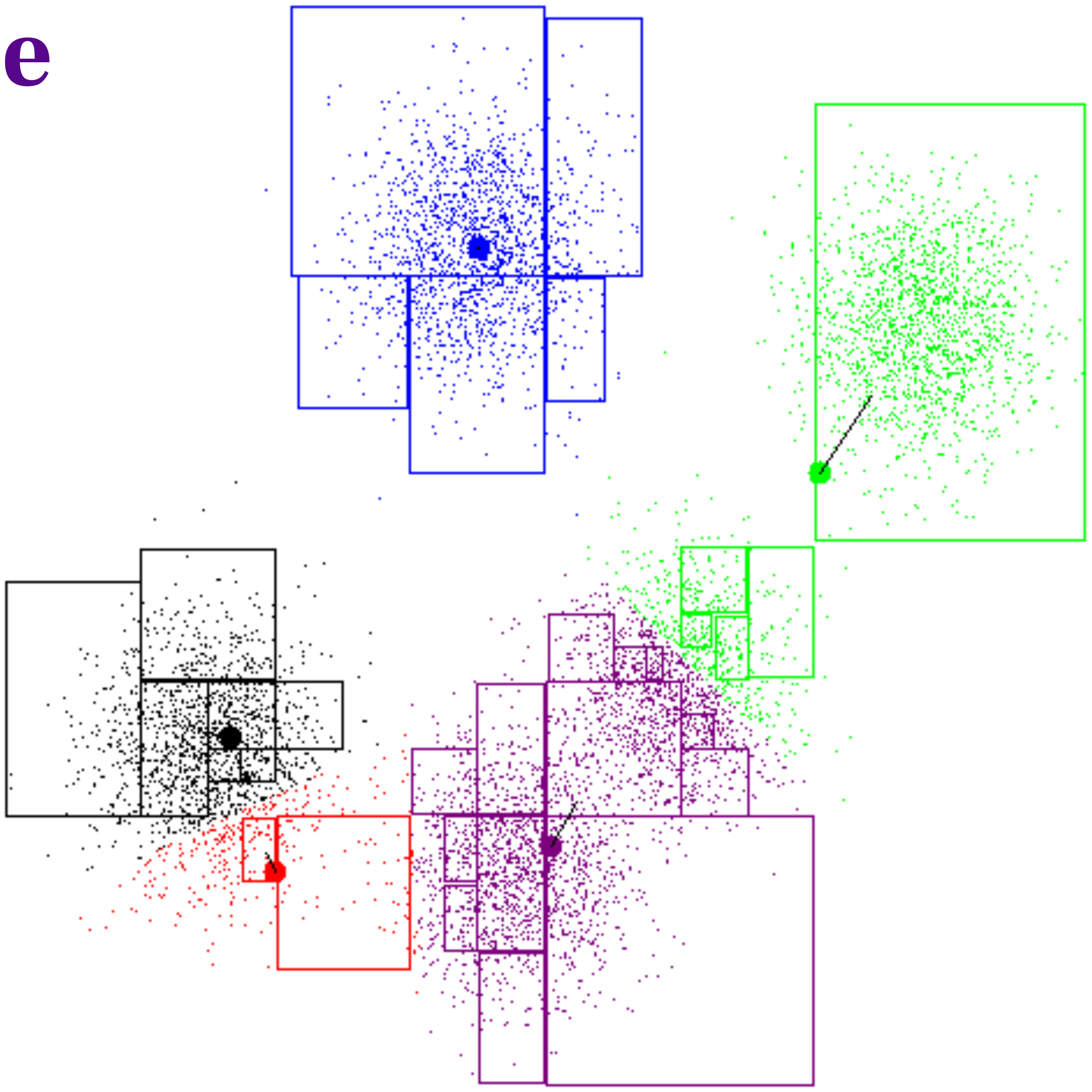

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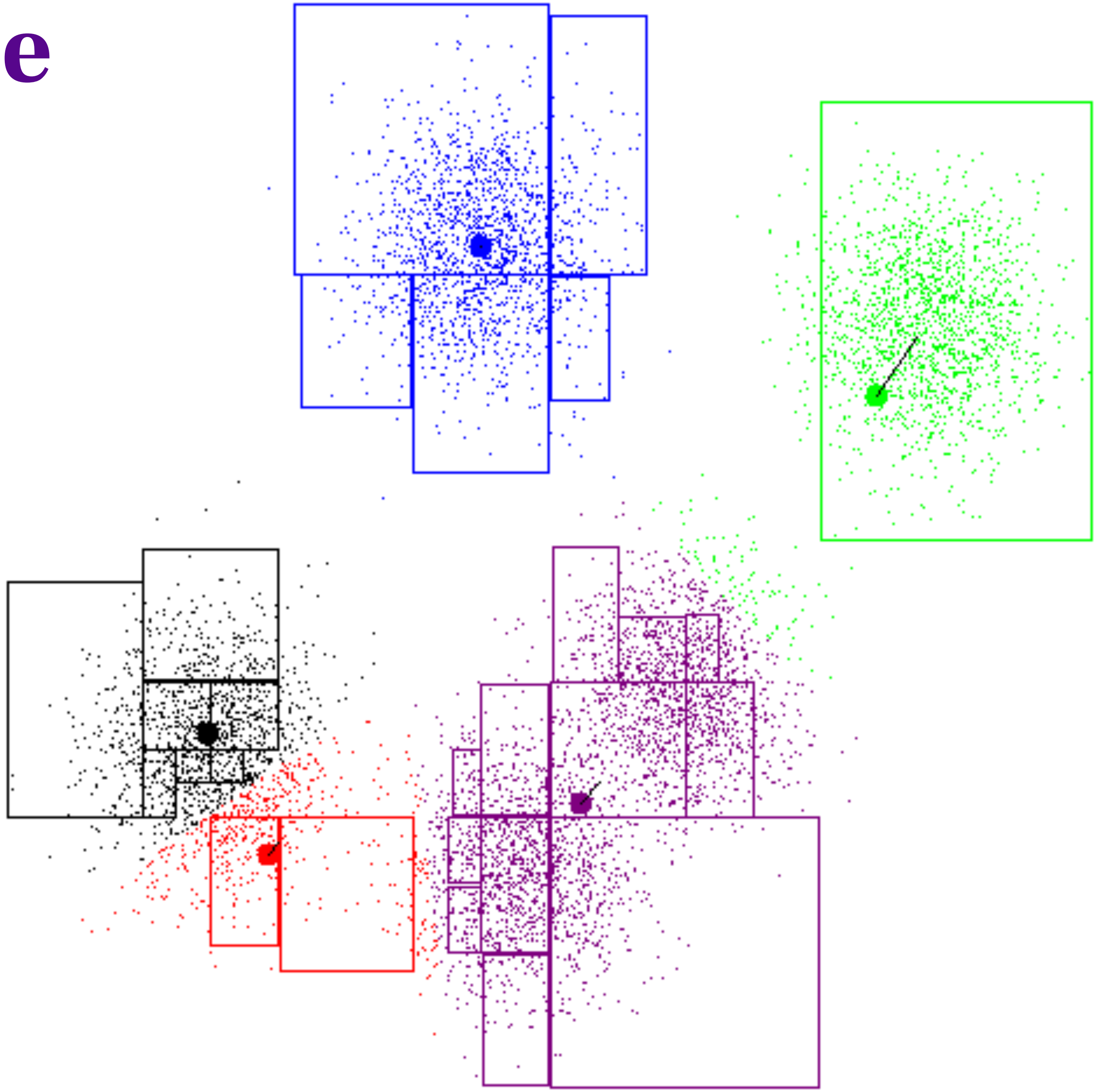

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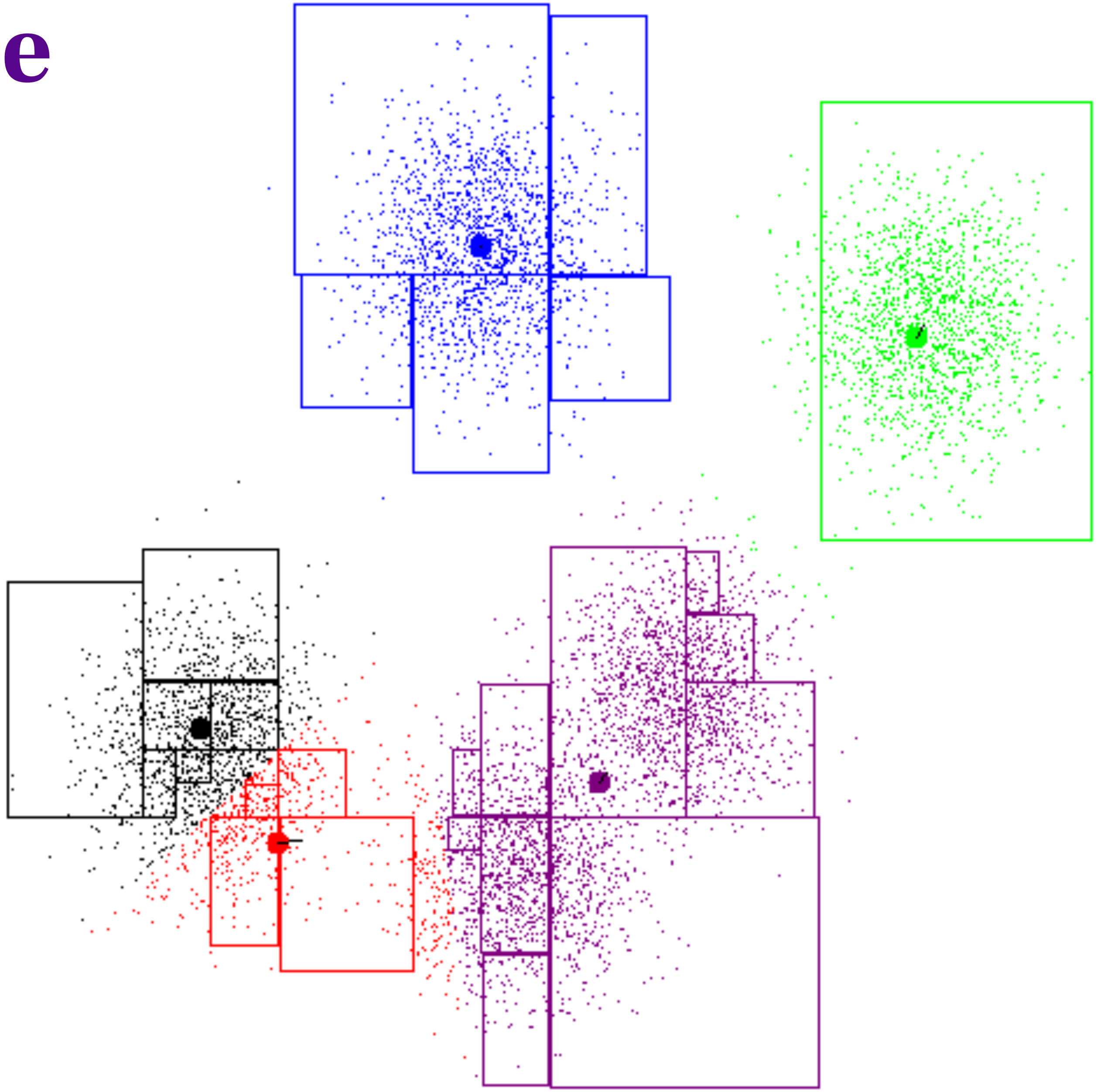

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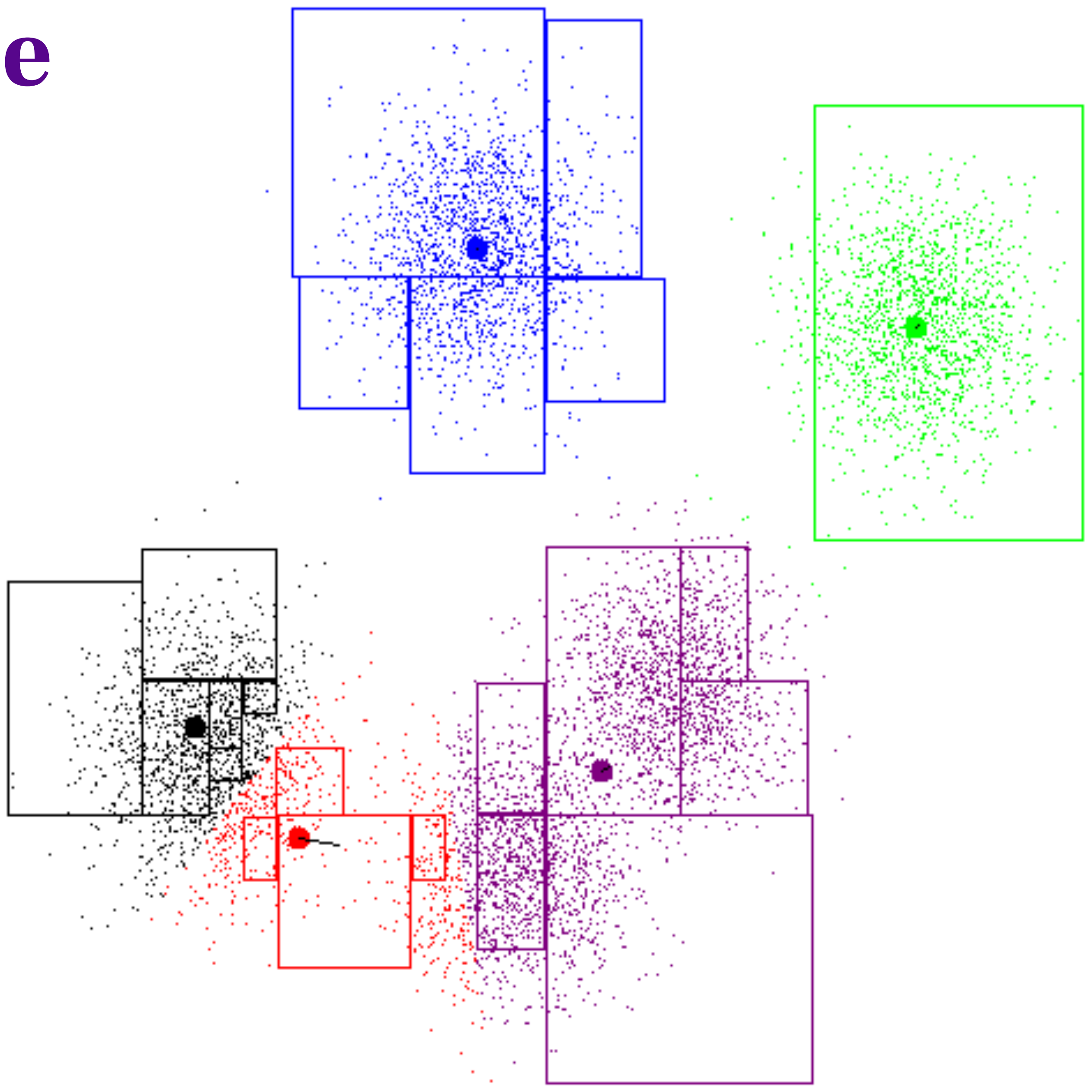

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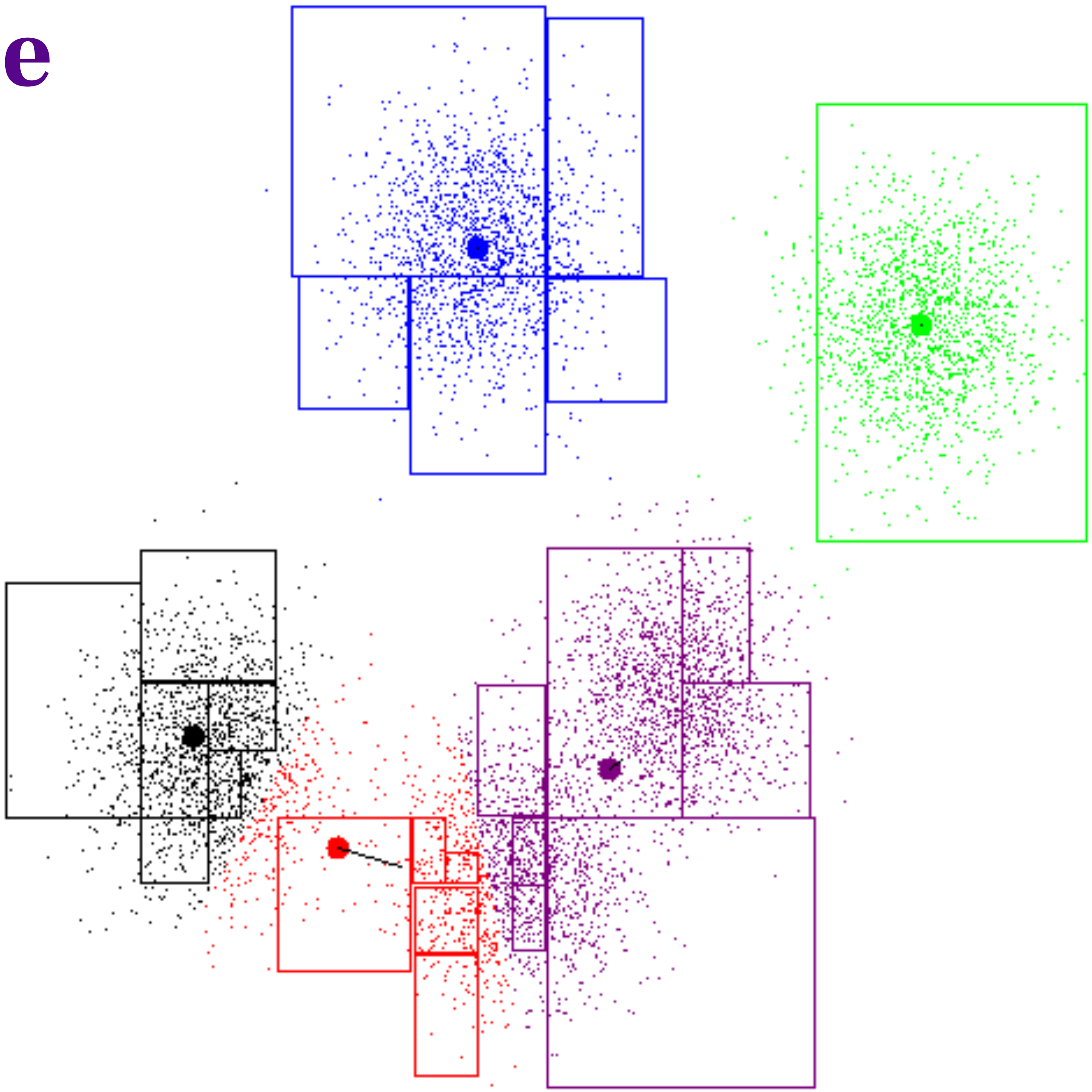

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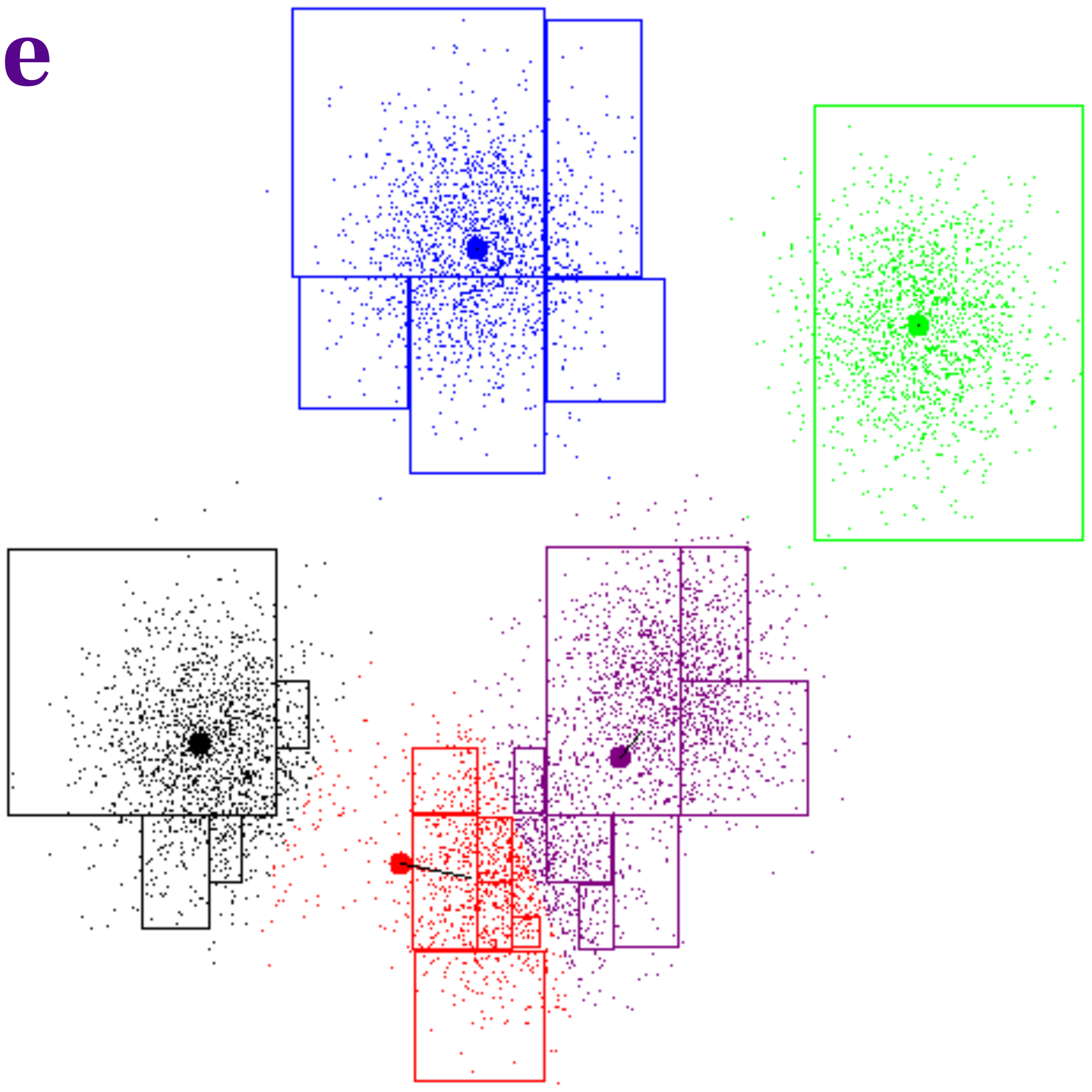

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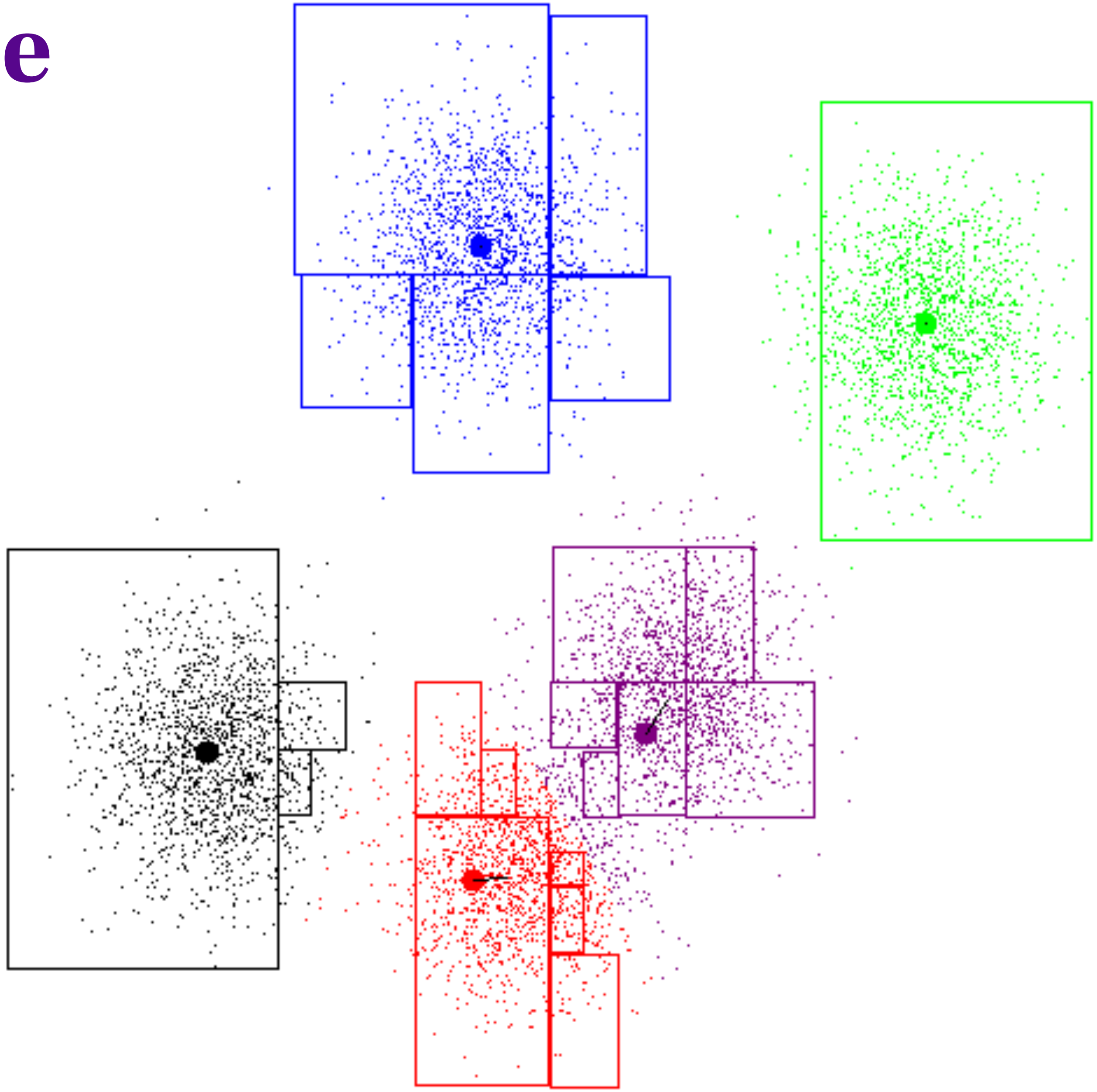

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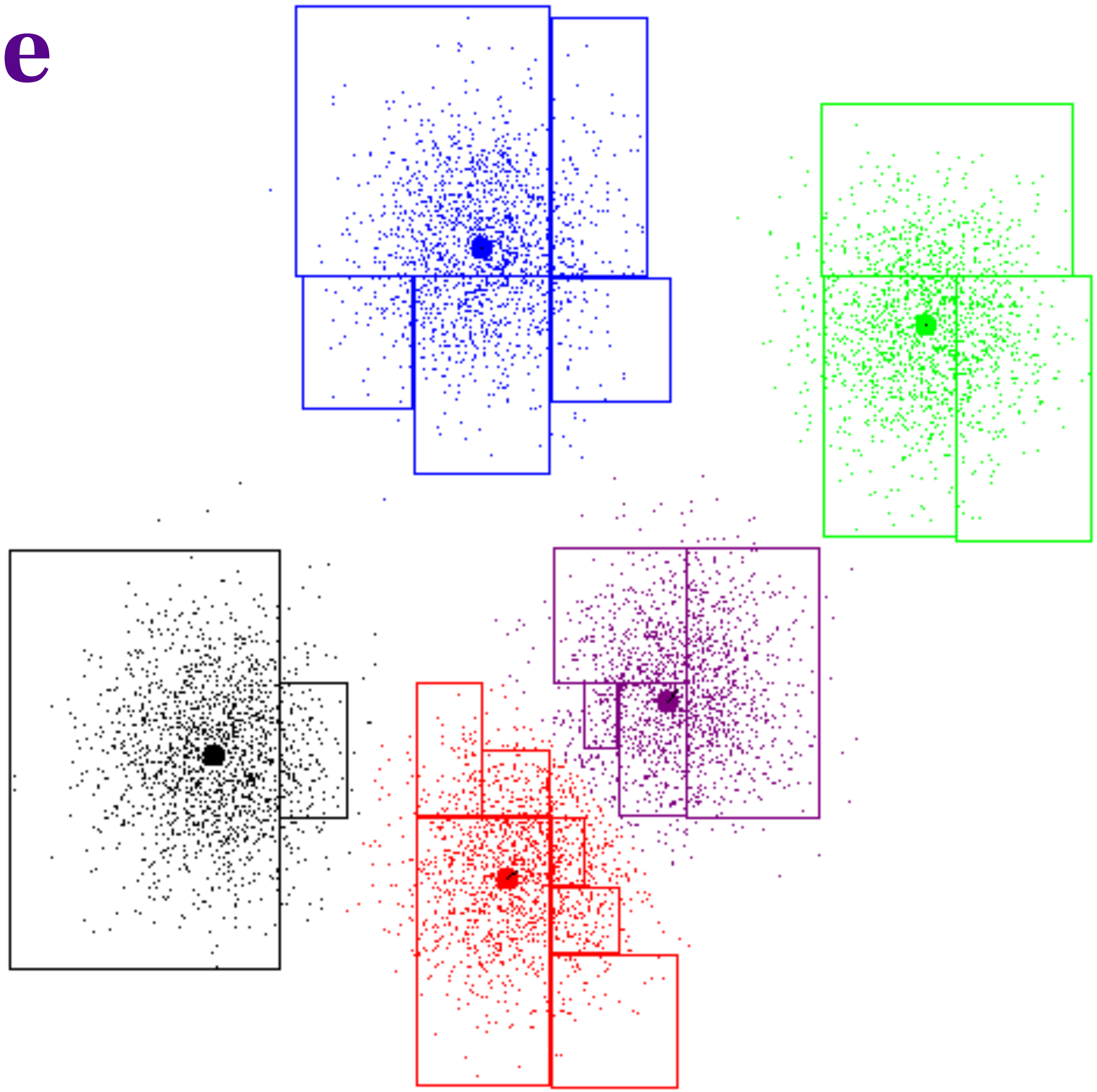
K-means real example

Here's the final result when the algorithm converges.



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K-means Clustering

Question 1: Will k-means always converge to a solution?

Yes! Distortion decreases monotonically, and it will end in a state where neither type of move will further reduce the distortion.

K-means Clustering

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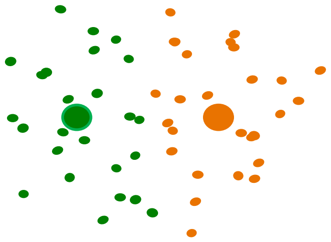
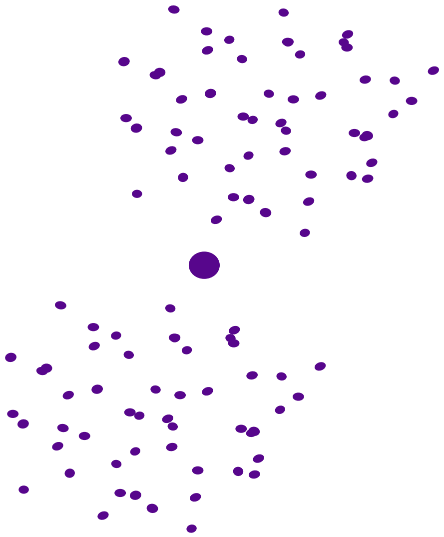
Question 2: Will k-means always find the optimal solution?

No! Here is one example where k-means converges to a locally optimal solution that does not have the global minimum distortion.





K-means Clustering

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Question 2: Will k-means always find the optimal solution?

No! Here is one example where k-means converges to a locally optimal solution that does not have the global minimum distortion.

Question 3: How can we avoid these poor local optima?

K-means is a form of hill-climbing, so we can use many of the same tricks!

1. Run multiple times with different start states and choose the best result.
2. Allow some moves that increase distortion, as in simulated annealing.
3. Choose a start state that is less likely to result in a poor local optimum.

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Center 1 = randomly chosen data point
Center 2 = data point that's farthest from center 1
Center 3 = data point that's farthest from the closest of centers 1 and 2, etc.

K-means Clustering

Question 4: How can we choose the number of centers k?

Run k-means multiple times with different values of k, and choose the k with minimum distortion?

Bad idea! Minimum distortion occurs when k = N, and each cluster contains only one point.

Better idea: choose the k that minimizes a measure of distortion with a penalty for more complex models.

Schwarz criterion: minimize (distortion + λk), where λ is a constant, proportional to (# of attributes) x log (# of records).

(Many other criteria have also been considered!)

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K-means Clustering

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Schwarz criterion: minimize (distortion + lk), where l is a constant, proportional to (# of attributes) x log (# of records).

(Many other criteria have also been considered!)

In general, we can use this criterion to pick the "best" of any set of clusterings, e.g. which links to cut for a given hierarchical clustering.

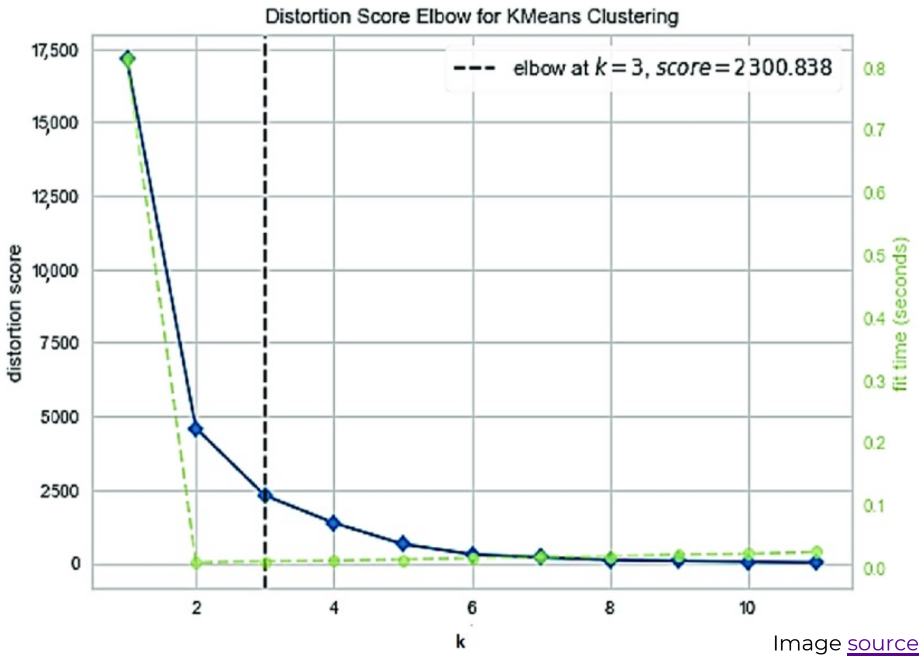


Image source

K-means vs EM

Both k-means and EM are iterative algorithms that model each cluster and assign points to clusters. How do these algorithms differ?

Assignment: k-means makes **hard** cluster assignments (each point is mapped to a single cluster), while EM makes **soft** assignments (each point is assigned a probability distribution over clusters).

Equivalence: EM reduces to k-means when covariance matrix is diagonal, and all variances are equal and very small.

Speed: k-means is much faster and consumes much less memory in practice. (the tradeoff: EM can better model the data, as measured by log-likelihood.)

Modeling: k-means models only the mean (centroid) of each cluster, while EM models the mean and **covariance matrix** (or, with naïve Bayes assumption, the **variance** of each attribute).

K-means is biased toward spherical clusters; EM+NB is biased to axis-aligned ellipses; EM with full covariance matrix can model non-axis-aligned ellipses.

Leader Clustering

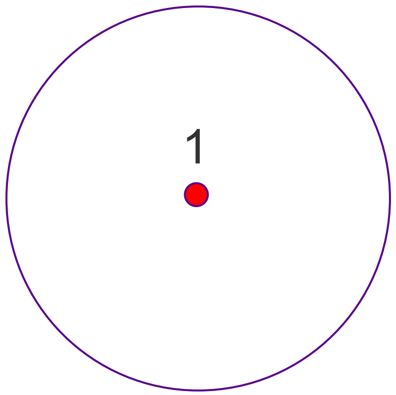
Leader Clustering

“massive streaming data”
Billions of sensor readings
for a complex system

What if the dataset is so huge that we can only look at each data point once before discarding it?

We keep only a small subset of representative points (“leaders”) and summary information about the points similar to each leader.

For each data point x_i: if x_i is within distance T of any leader, add to nearest leader’s group, otherwise make x_i a leader.



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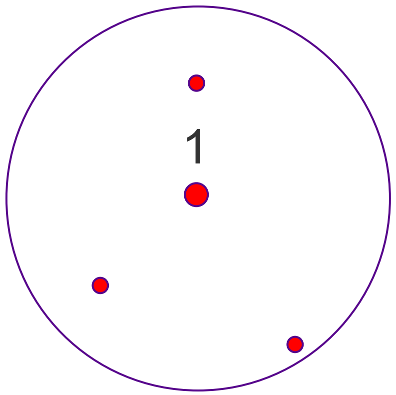

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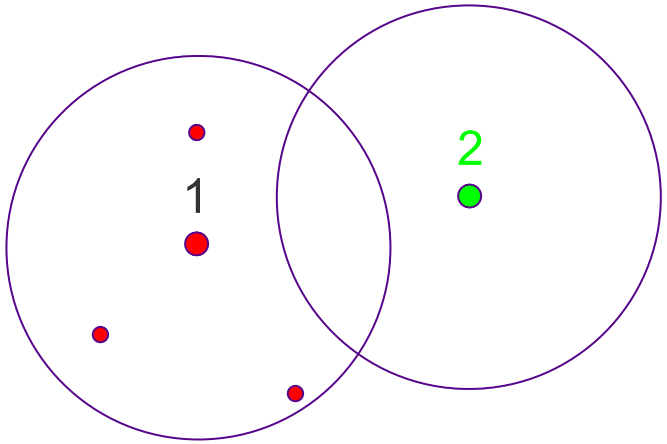

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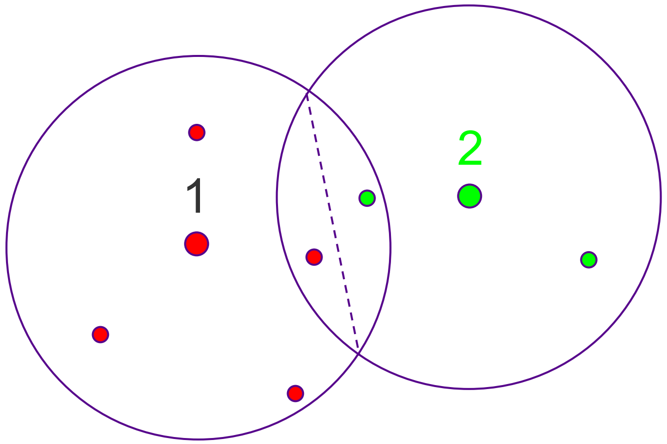

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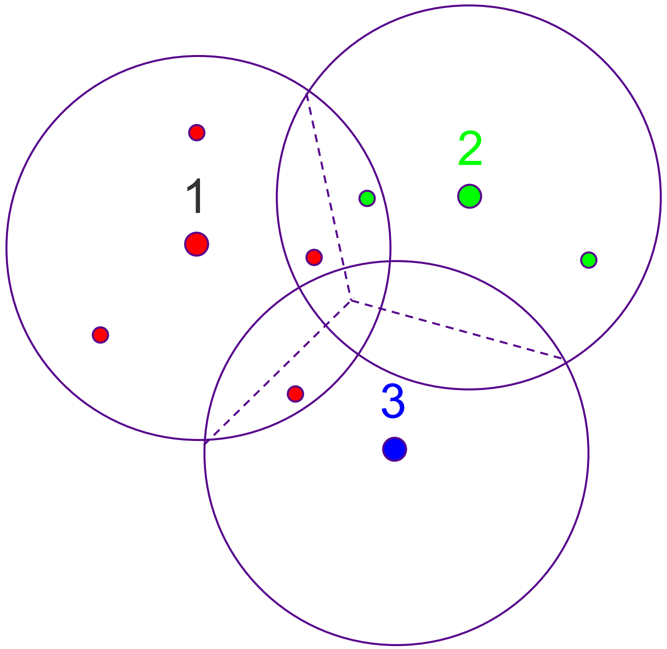

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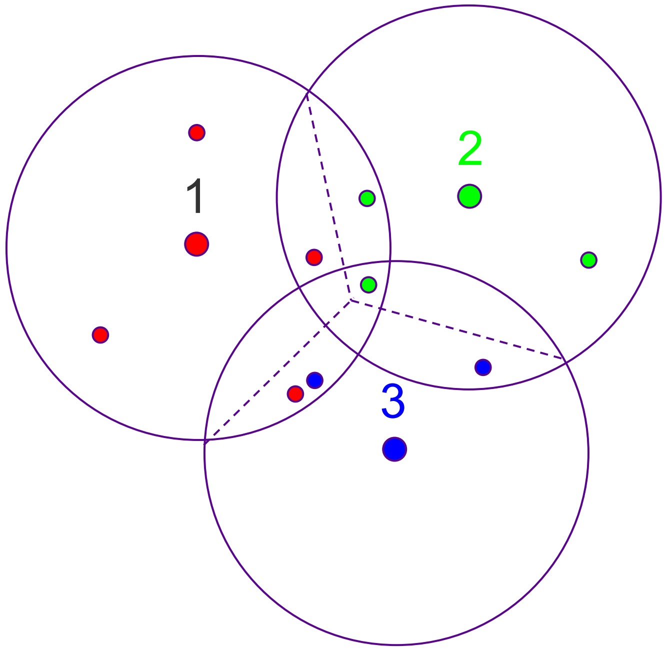

Advantages of leader clustering

1. Very fast: only need to look at leaders for each point
2. Guarantees group diameter < 2T, group leaders at least T apart

Disadvantages of leader clustering

1. Order-dependent: first point is always a leader; initial clusters tend to be larger
2. Points may not be assigned to the nearest cluster center

The Many Uses of Clustering

Clustering provides a useful **summary** of a large dataset, representing the N data records using only k << N clusters.

This can be used for **exploratory data analysis**, enabling us to understand the underlying sub-structure of the data.

Value of k?
Shape?
Size?
Hierarchy?

Important to choose correct k value

k usually small

We can often improve the performance of model-based prediction by learning separate models for each group.

We can also use clustering to detect **anomalies** by finding points that are far from any cluster center.

Choose k large as possible

We can use clustering to speed up instance-based prediction (e.g. k-NN) by reducing the training set size.

Finally, we can use clustering to handle massive streaming data by maintaining only the cluster summaries in memory.

Lab Time

For the Next Week (Week 8)

1. Prepare for the Midterm Exam (asynchronous, 2 days)
2. Assignment 2 (SVMs, Naïve Bayes, EM)
   Due: March 6, 2024 (11:59pm)

References

1. Scikit-learn clustering documentation: http://scikit-learn.org/stable/modules/clustering.html
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4. Han, J., Kamber, M., and Pei, J., 2011, "Chap. 10 Cluster Analysis: Basic Concepts and Method" in Data Mining: Concepts and Techniques, Elsevier Science.
5. Tan, P-N., Steinbach, M., Kumar, V., 2006, "Chapter 8. Cluster Analysis: Basic Concepts and Algorithms", in Introduction to Data Mining, Pearson.