Lecture 14:
K-means Clustering

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Overview

Clustering

Cluster

A number of similar things that occur together (Merriam-Webster).

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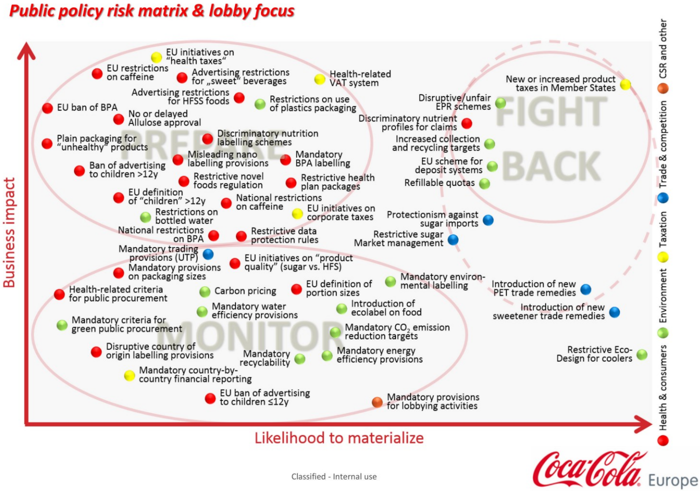
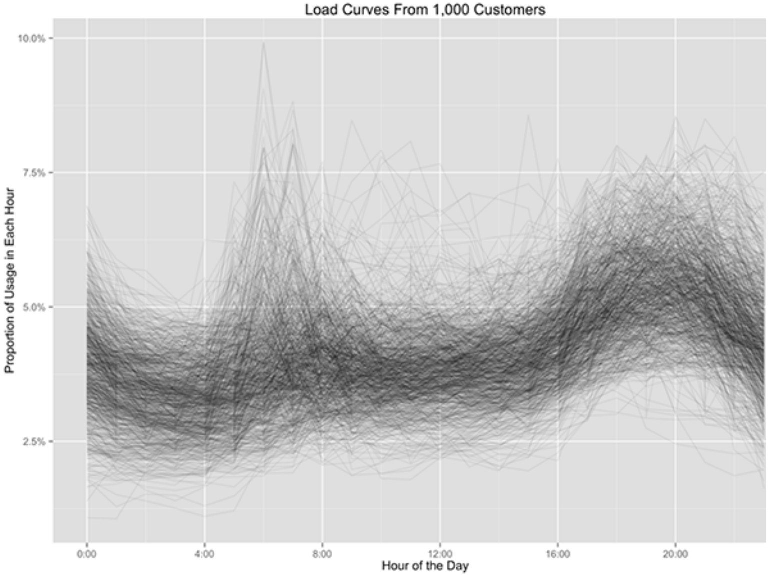
- Unsupervised learning - find patterns in unlabeled data
  - Uncover hidden structure in your dataset
  - Useful if you don't know what to look for
- Segment data into "similar" groups
  - Similarity measure is very important, but can be hard to define

Non-algorithmic Example



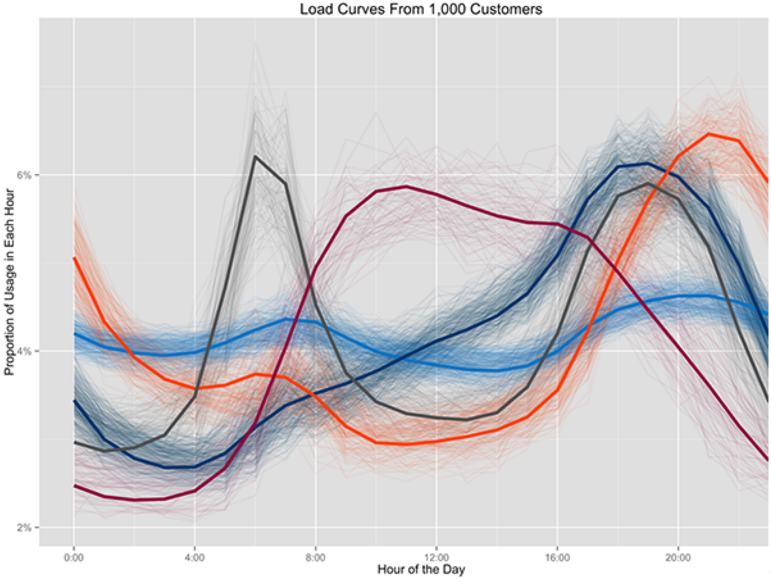
Downloaded from Ninja for Health, from leaked emails.

Time series clustering



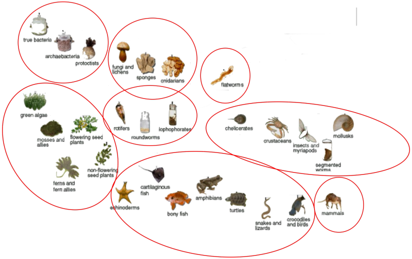
Source: Opower (2014)

Time series clustering



Clustering algorithms

Partition algorithms (flat)



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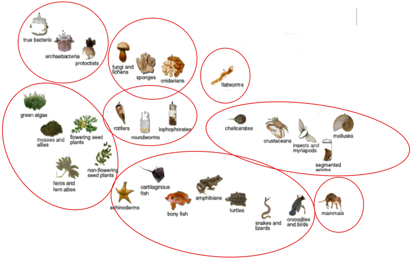
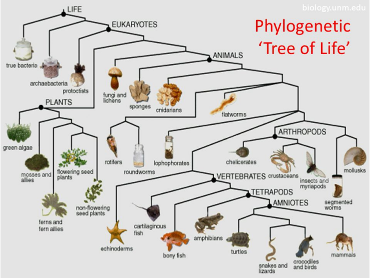
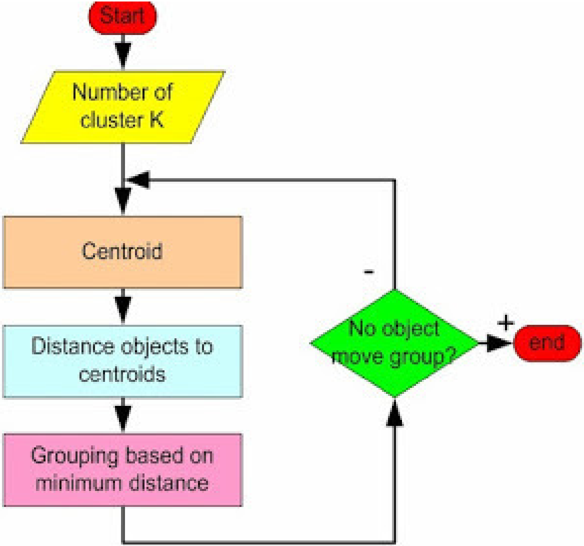


Hierarchical algorithms

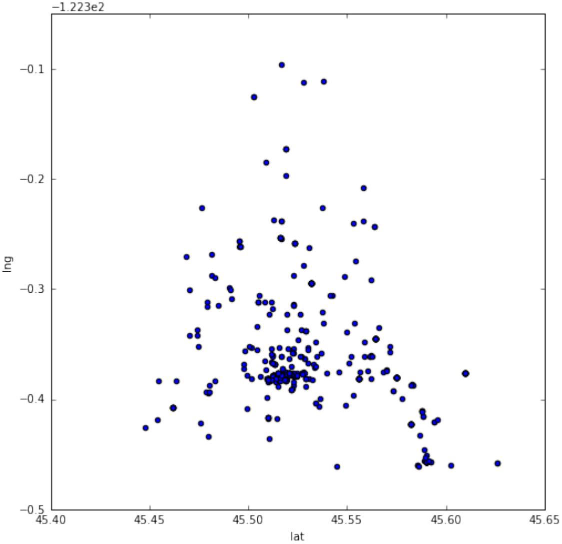


biology.unm.edu

K-means Algorithm

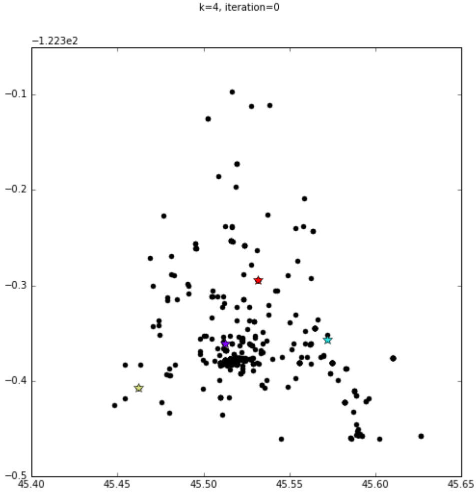


Example - Location of Public Art in Portland



Location of Public Art in Portland

Example - Location of Public Art in Portland, iterations for k=4



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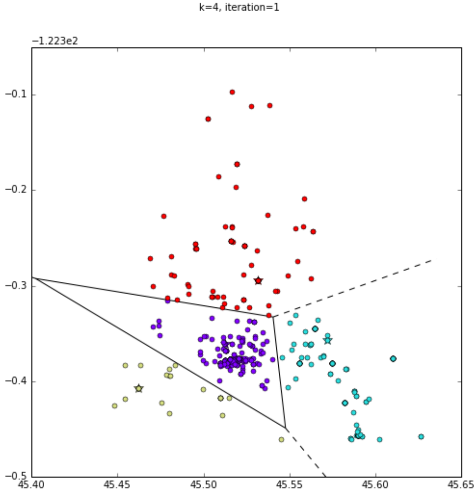

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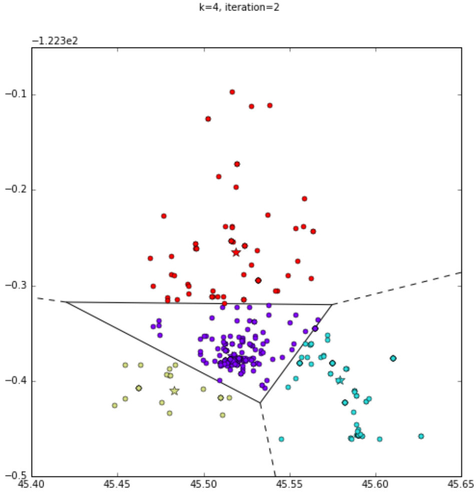

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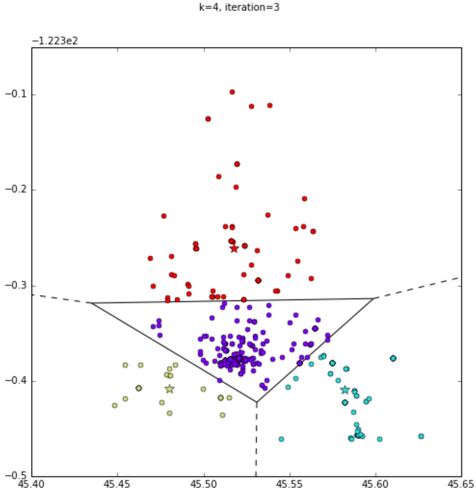

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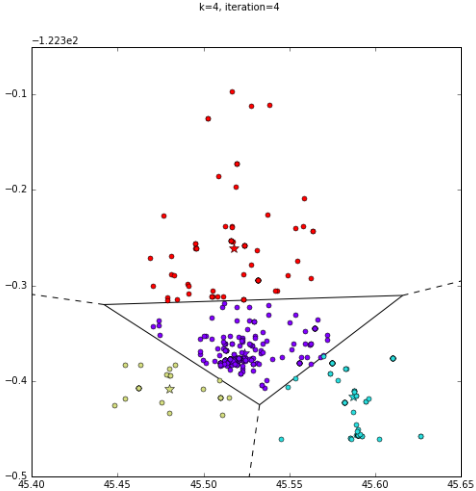

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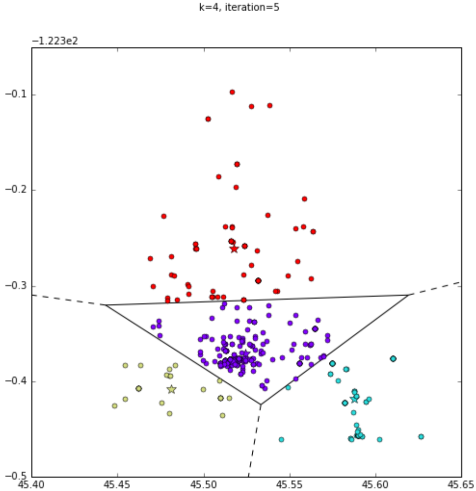

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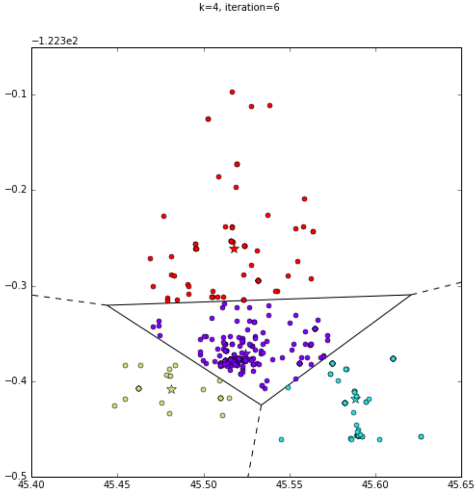
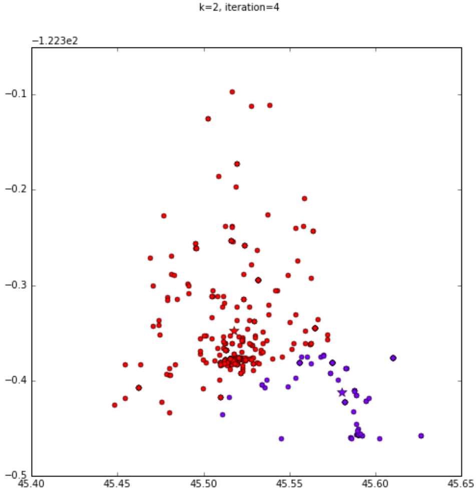


Example - Location of Public Art in Portland, various k



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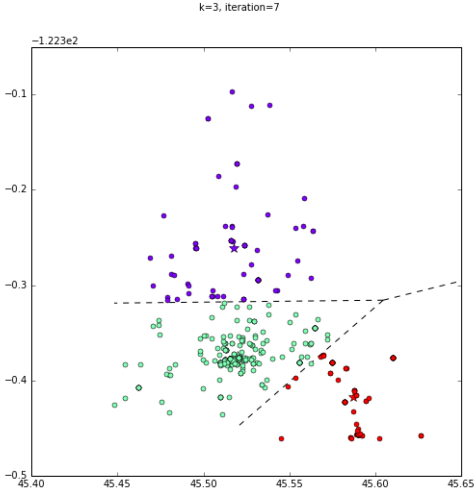

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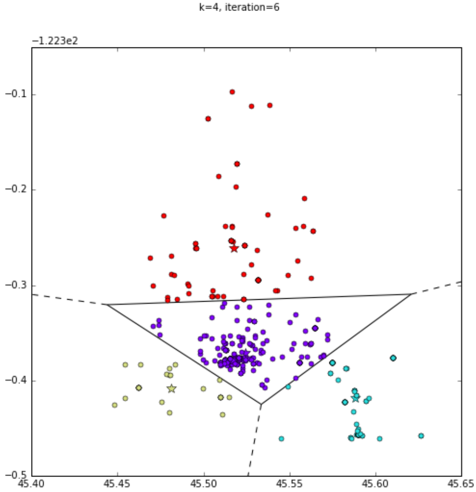

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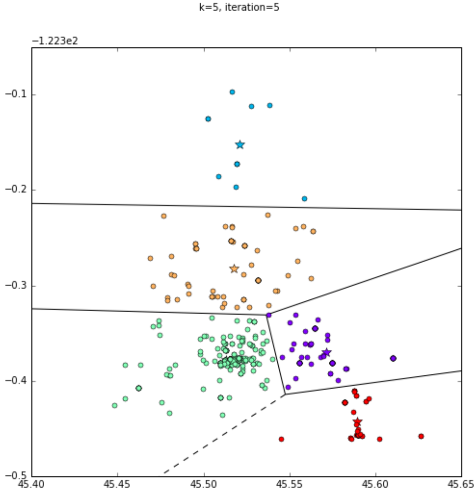

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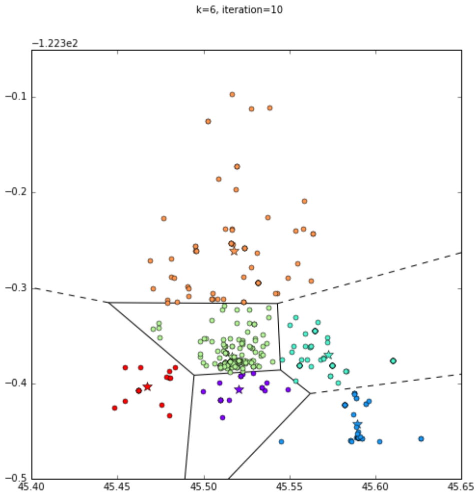

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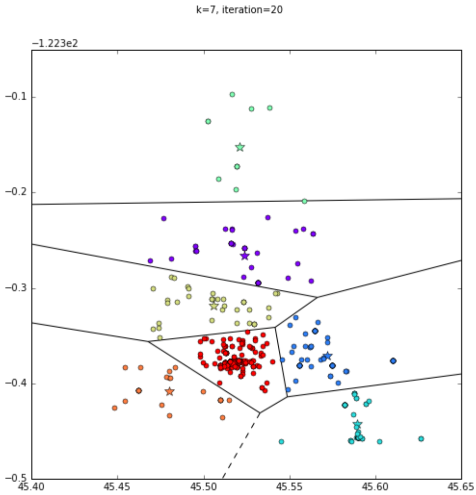

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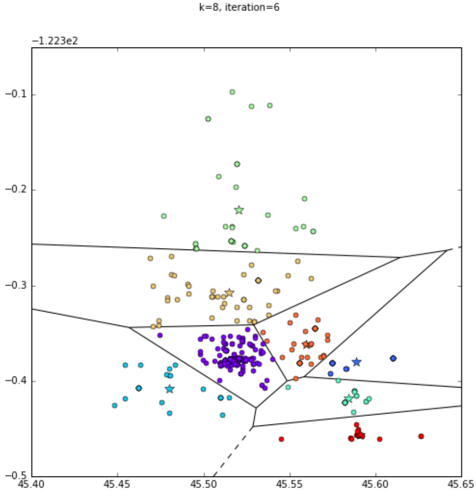

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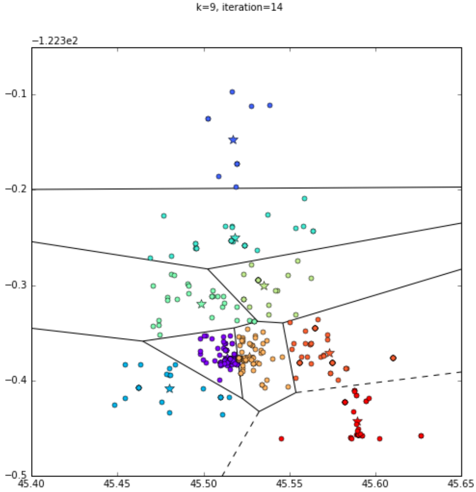

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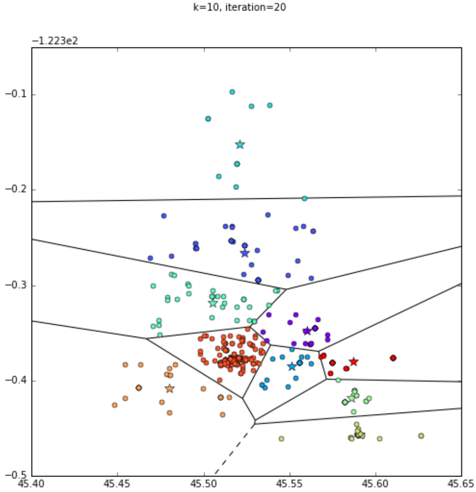

Objective Function

K-means algorithm minimizes the *residual sum of squares* of the data ($\vec{x_n}$) compared to the centroids ($\vec{\mu_k}$) of the cluster it belongs to ($r_{nk} = 1$ if $\vec{x_n}$ is in cluster k, else 0) for a given k:

$$J(\mu, r) = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} ||\vec{x_n} - \vec{(}\mu_k)||^2$$

Choosing k

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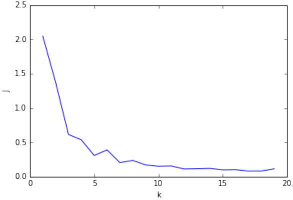
One way to choose k

Find the "elbow point" in J vs. k (shown below for the public art example):



Defining 'Similar'

Similarity is inversely related to distance.

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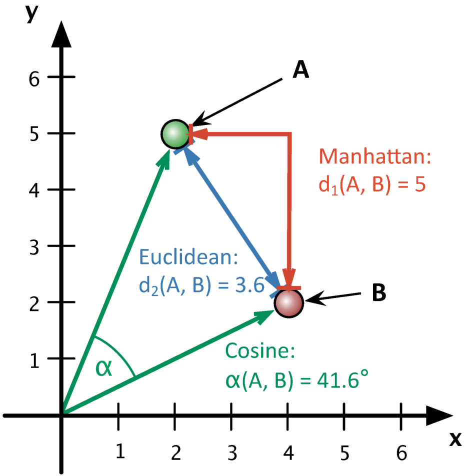
Some distance measures:



[digitalhumanities]

K-means downfalls

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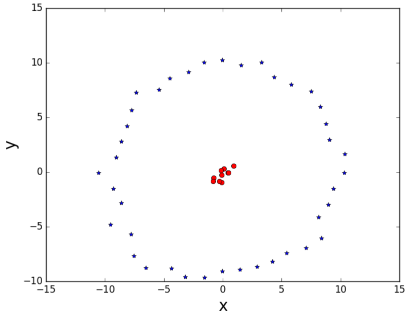
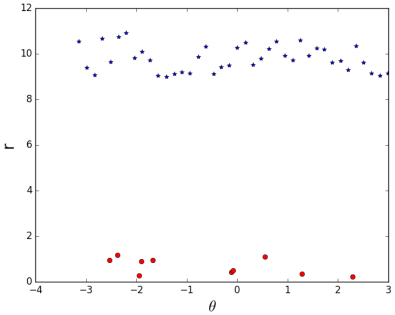
- See [Tan] pp 25-26 for examples.

Transforming can help

Some situations where k-means fails...



may be resolved with feature engineering.



K-means to reduce colors in image

Original

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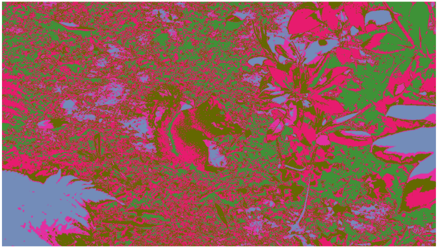
Original

Cluster colors k=5



K-means to segment image

Original

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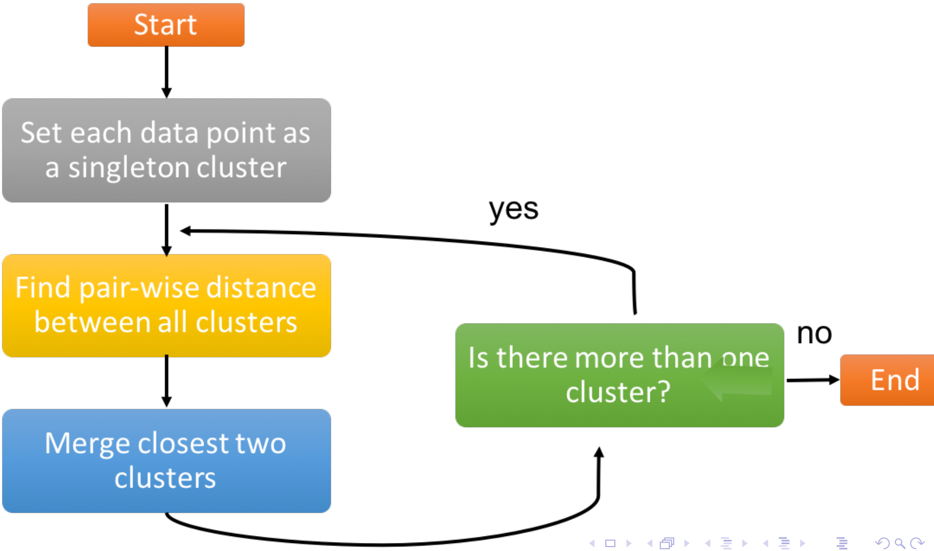
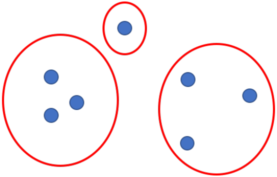
Original

Segment k=25

Agglomerative Clustering



Different choices result in different clustering behaviors.



A few of the options:

- Closest pair (single-link clustering)
- Farthest pair (complete-link clustering)
- Average of all pairs

Defining Distance Between Clusters

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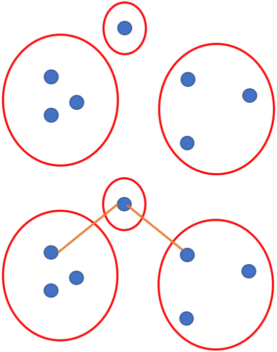

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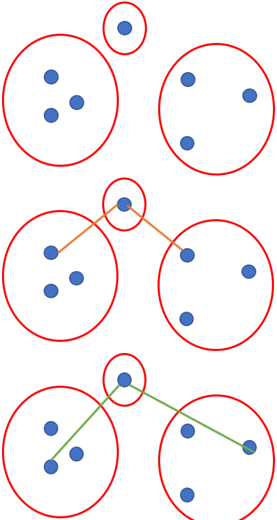

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References

- Pang-Ning Tan, Michael Steinbach, and Vipin Kumar
  Introduction to Data Mining

- Evert, S., Jannidis, F., Proisl, T., Vitt, T., Schch, C., Pielstrm, S., Reger, I. (2016). Outliers or Key Profiles? Understanding Distance Measures for Authorship Attribution. In Digital Humanities 2016: Conference Abstracts. Jagiellonian University & Pedagogical University, Krakw, pp. 188-191. Digital Humanities 2016

- Tibshirani, Robert; Walther, Guenther; and Hastie, Trevor (2001) Estimating the number of clusters in a data set via the gap statistic. J. R. Statist. Soc. B 63, Part 2, pp. 411-423. stanford.edu

Recommended Reading

Data Science from Scratch, Chapter 19

Further investigation

skikit learn Clustering

The Data Science Lab k-means clustering series