Clustering

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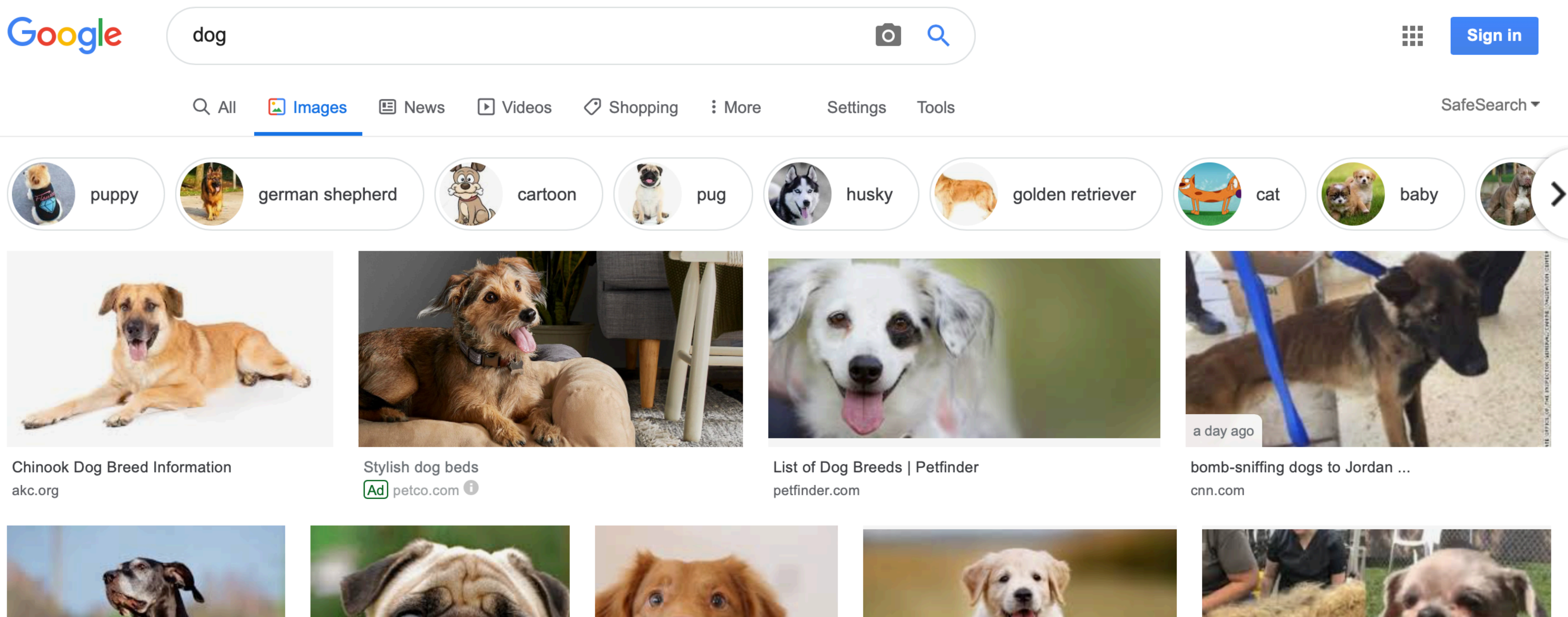
Partly based on materials by
Professors Guy Lebanon, Jeffrey Heer, John Stasko, Christos Faloutsos, Parishit Ram (GT PhD alum; IBM), Alex Gray

Clustering

The most common type of **unsupervised** learning

High-level idea: group **similar** things together

"**Unsupervised**" because clustering model is learned without any labeled examples



Applications of Clustering

- Find similar patients subgroups
  - e.g., in healthcare
- Finding groups of similar text documents (topic modeling)
- …

Clustering techniques you've got to know

K-means
Hierarchical Clustering
DBSCAN

K-means (the "simplest" technique)

Best D3 demo Polo could find: https://kkevsterrr.github.io/K-Means/

Algorithm Summary

- We tell K-means the value of **k** (#clusters we want)
- **Randomly** initialize the k cluster "means" ("centroids")
- **Assign** each item to the cluster whose mean the item is closest to (so, we need a **similarity function**)
- **Update/recompute** the new "means" of all k clusters.
- If all items' assignments do not change, **stop**.

YouTube video demo: https://youtu.be/IuRb3y8qKX4?t=3m4s

K-means What's the catch?

How to **decide k** (a hard problem)?

- A few ways; best way is to evaluate with real data

  https://www.ee.columbia.edu/~dpwe/papers/PhamDN05-kmeans.pdf
  http://nlp.stanford.edu/IR-book/html/htmledition/evaluation-of-clustering-1.html

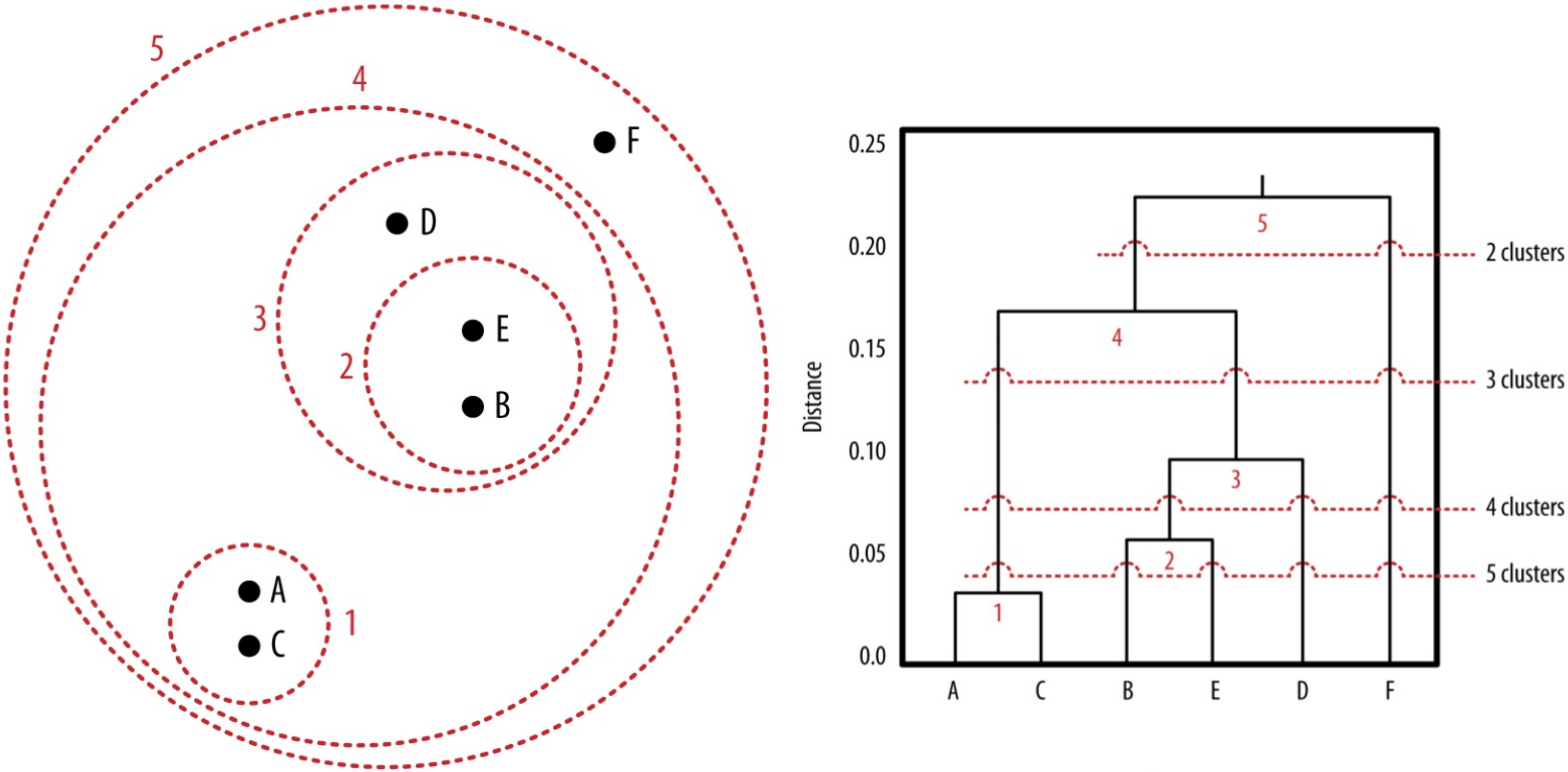
Only **locally optimal** (vs global)

- Different initialization gives different clusters
  - How to "fix" this?
- "Bad" starting points can cause algorithm to converge slowly

- Can work for **relatively large dataset**
  - Time complexity O(d n log n) per iteration
    (assumptions: n >> k, dimension d is small)
    http://www.cs.cmu.edu/~./dpelleg/download/kmeans.ps

Hierarchical clustering

High-level idea: build a tree (hierarchy) of clusters

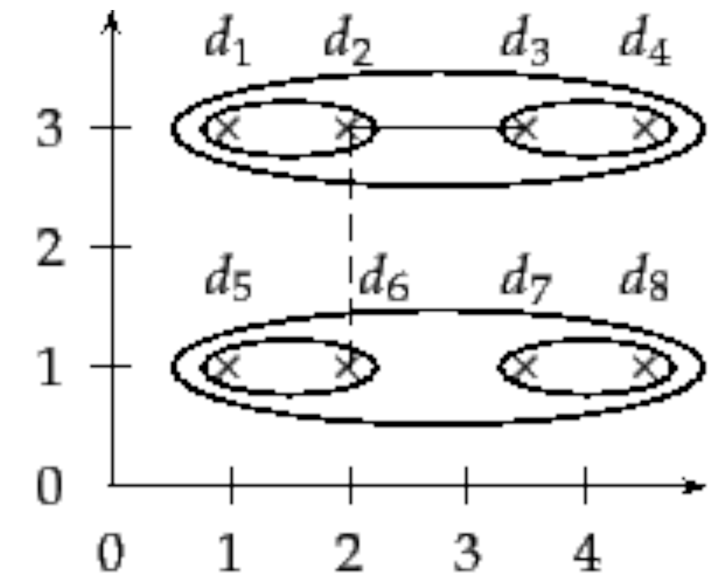


Dendrogram

Ways to calculate **distances** between two clusters

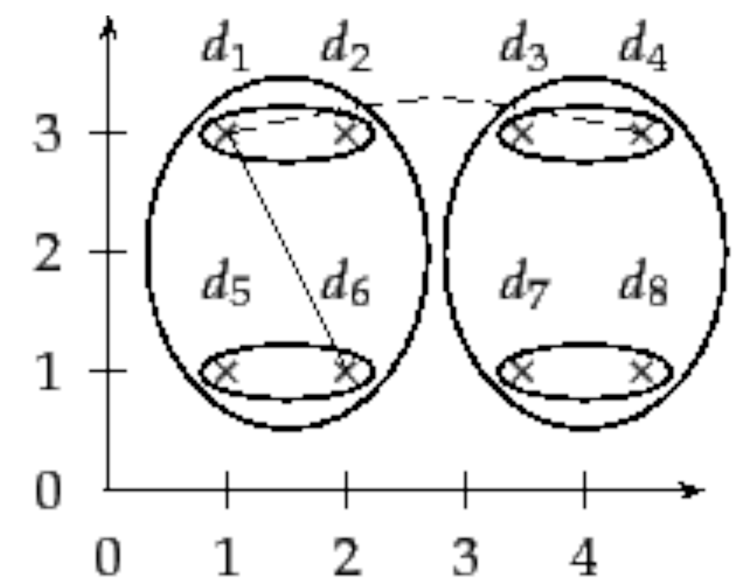
Single linkage

- minimum of distance between clusters
- similarity of two clusters = similarity of the clusters' most similar members



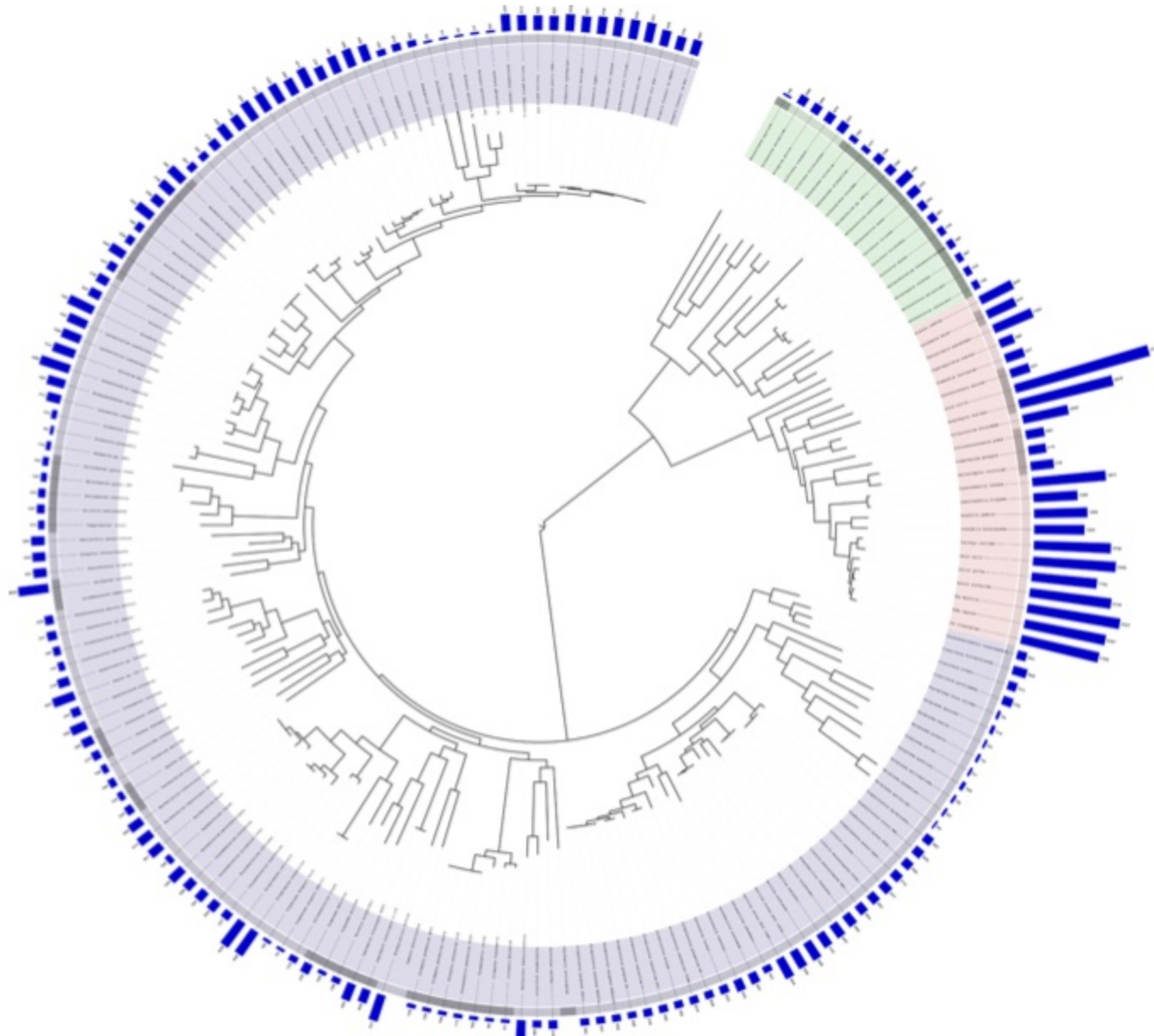
Complete linkage

- maximum of distance between clusters
- similarity of two clusters = similarity of the clusters' most dissimilar members



Average linkage

- distance between cluster centers



https://bl.ocks.org/mbostock/4063570
https://bl.ocks.org/mbostock/4339607

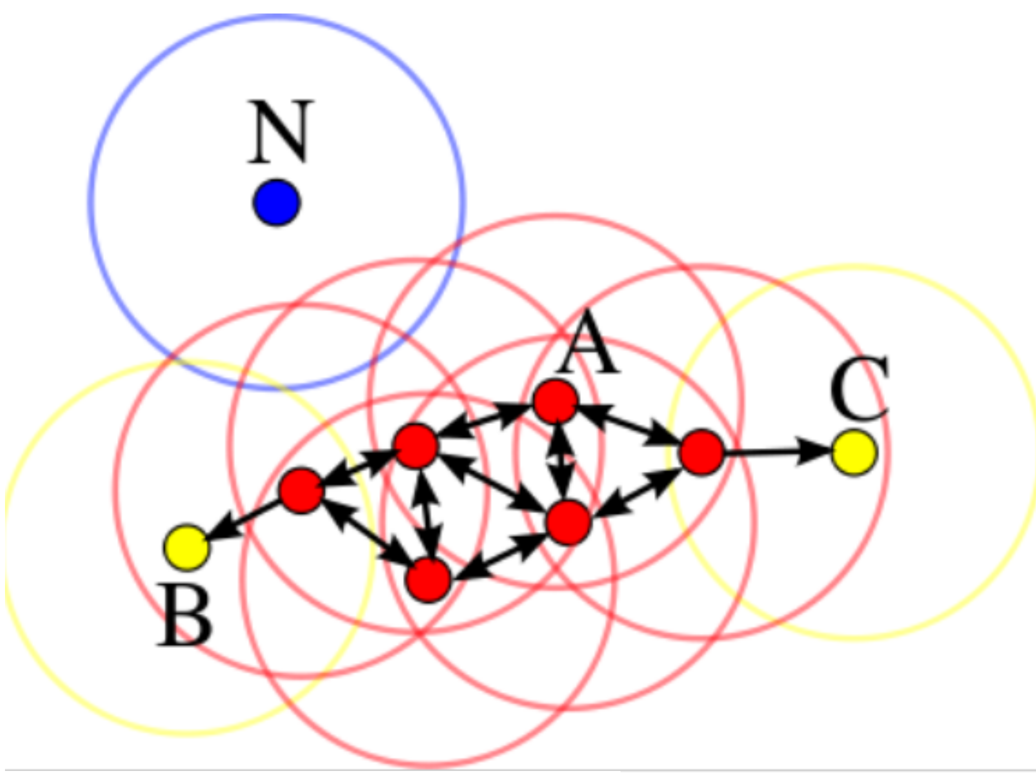
Hierarchical clustering for large datasets?

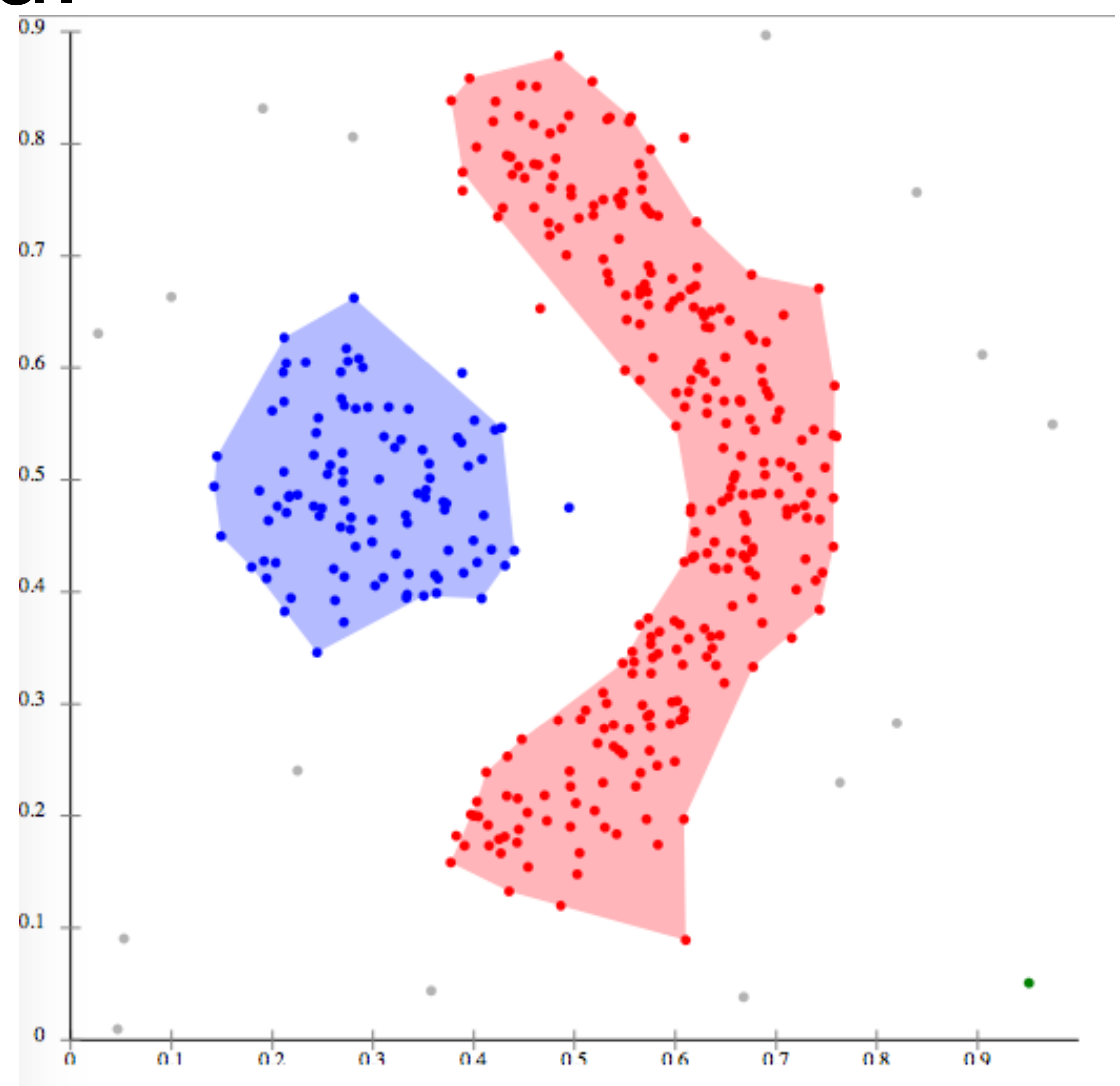
- OK for small datasets (e.g., <10K items)
  - Time complexity between $O(n^2)$ to $O(n^3)$ where n is the number of data items
  - Not good for millions of items or more
- But great for understanding concept of clustering

DBSCAN

"Density-based spatial clustering with noise"
https://en.wikipedia.org/wiki/DBSCAN

Received "test-of-time award" at KDD'14 — an extremely prestigious award.



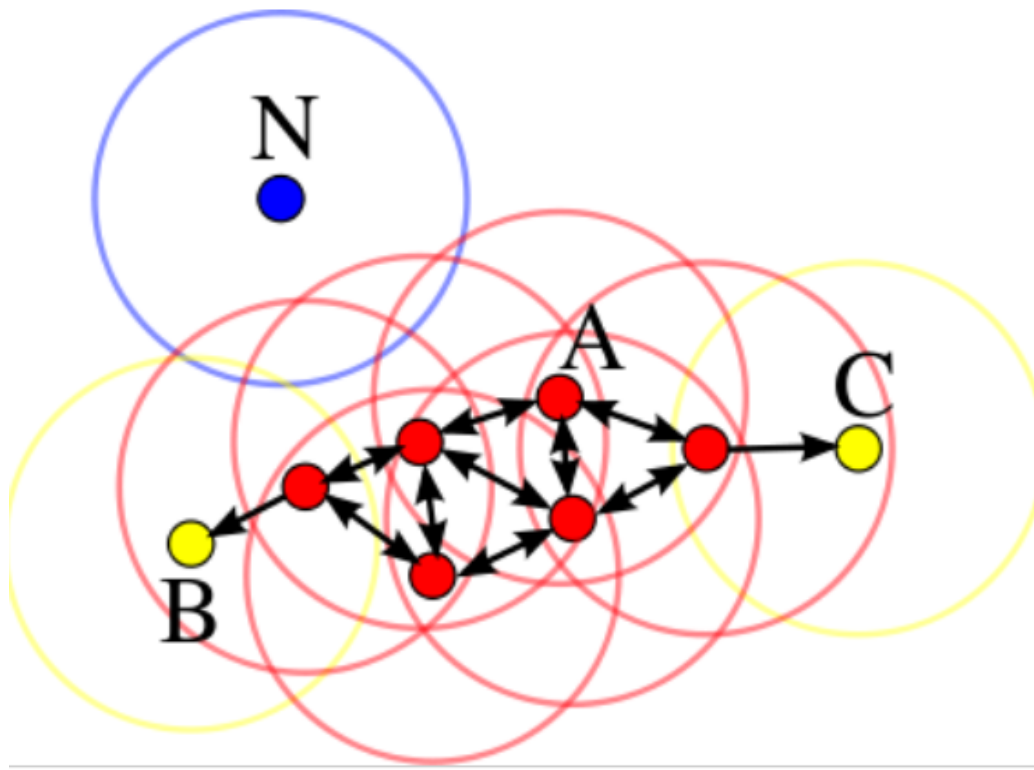


Only need two parameters:
1. "radius" epsilon
2. minimum number of points (e.g., 4) required to form a dense region

Yellow "border points" are **density-reachable** from red "core points", but not vice-versa.

Interactive DBSCAN Demo

https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/



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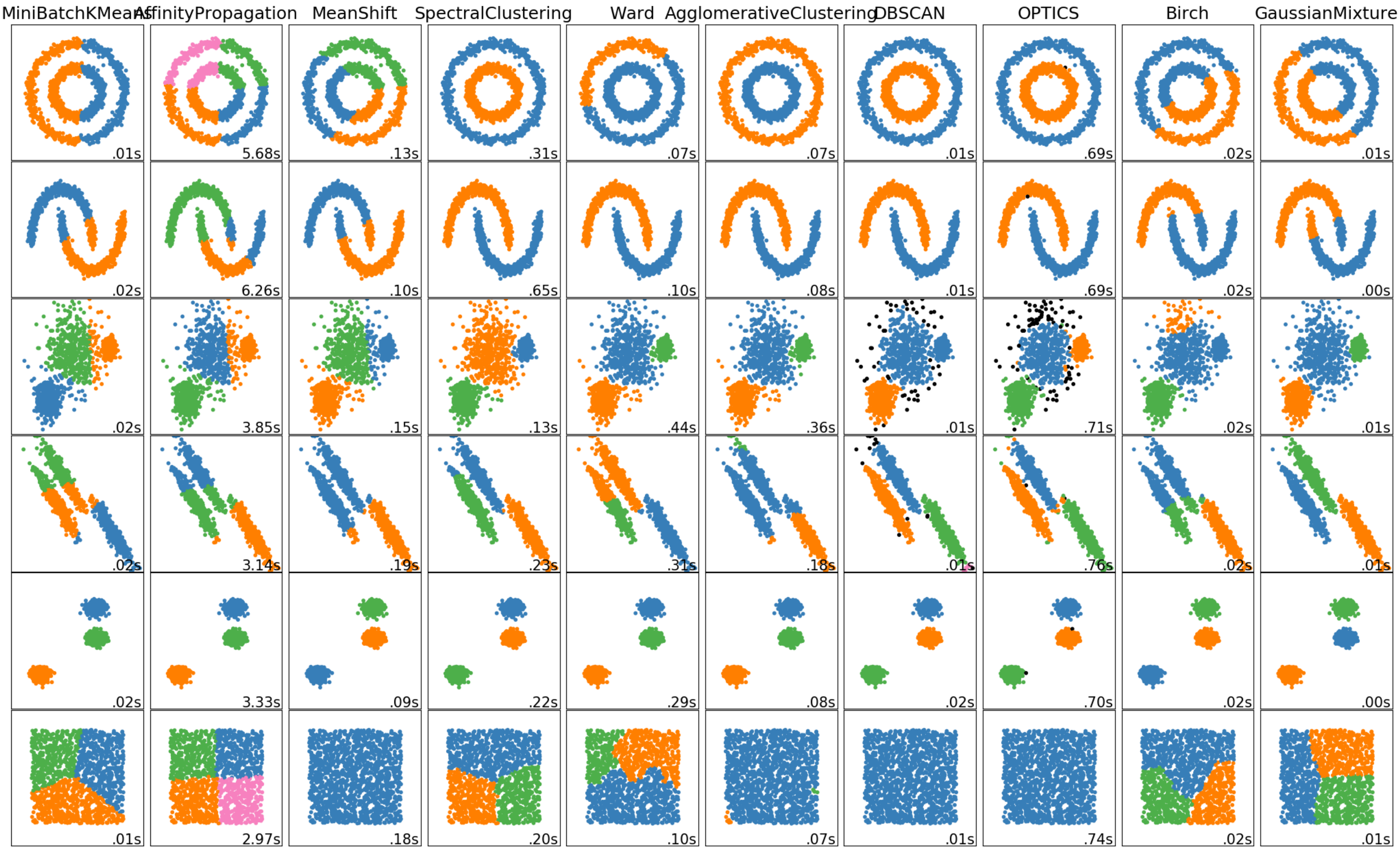
You can use DBSCAN now.

http://scikit-learn.org/stable/modules/generated/sklearn.cluster.DBSCAN.html

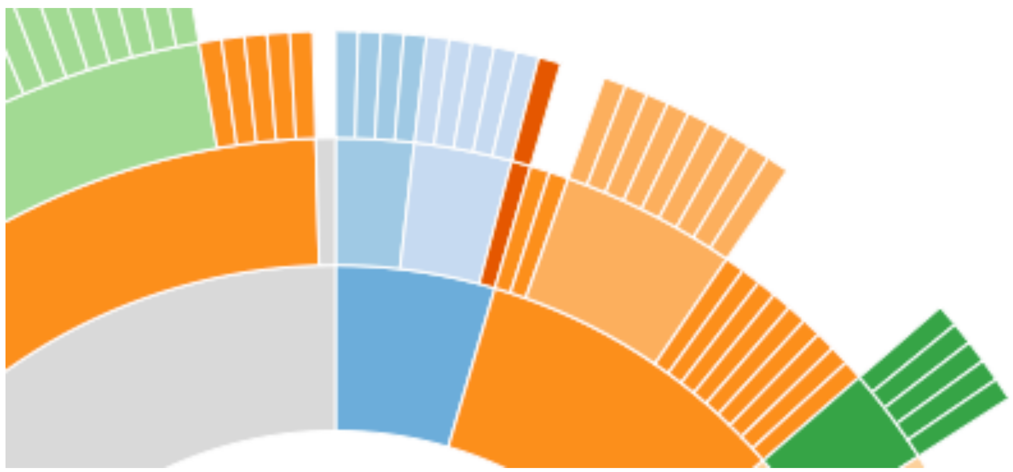


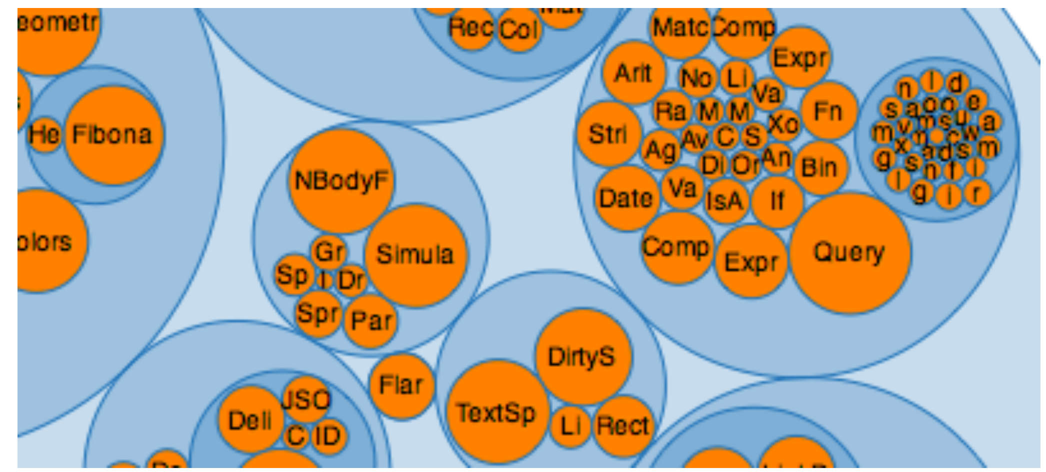
http://scikit-learn.org/dev/auto_examples/cluster/plot_cluster_comparison.html#sphx-glr-auto-examples-cluster-plot-cluster-comparison-py

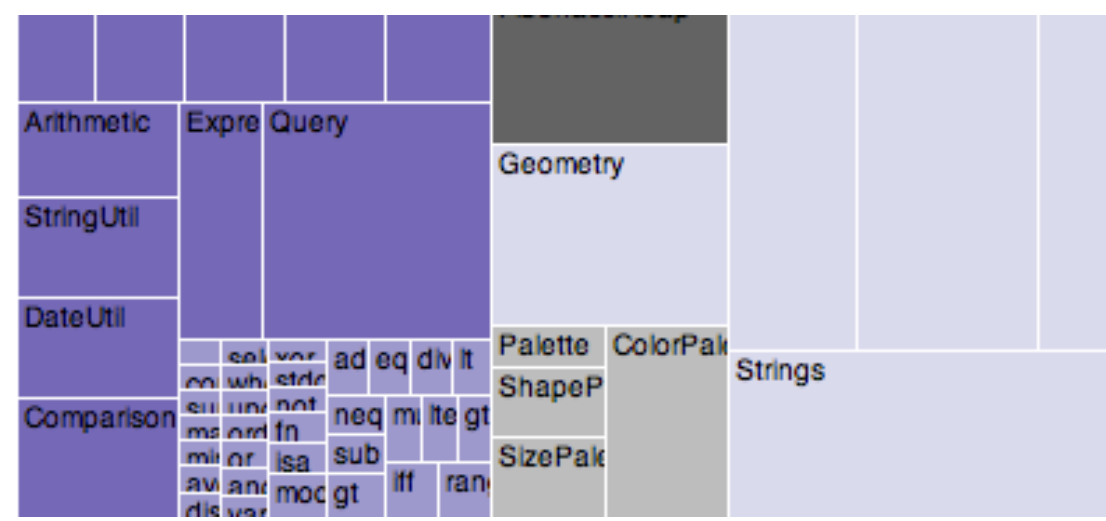
Visualizing Clusters

D3 has some built-in techniques

https://github.com/mbostock/d3/wiki/Hierarchy-Layout

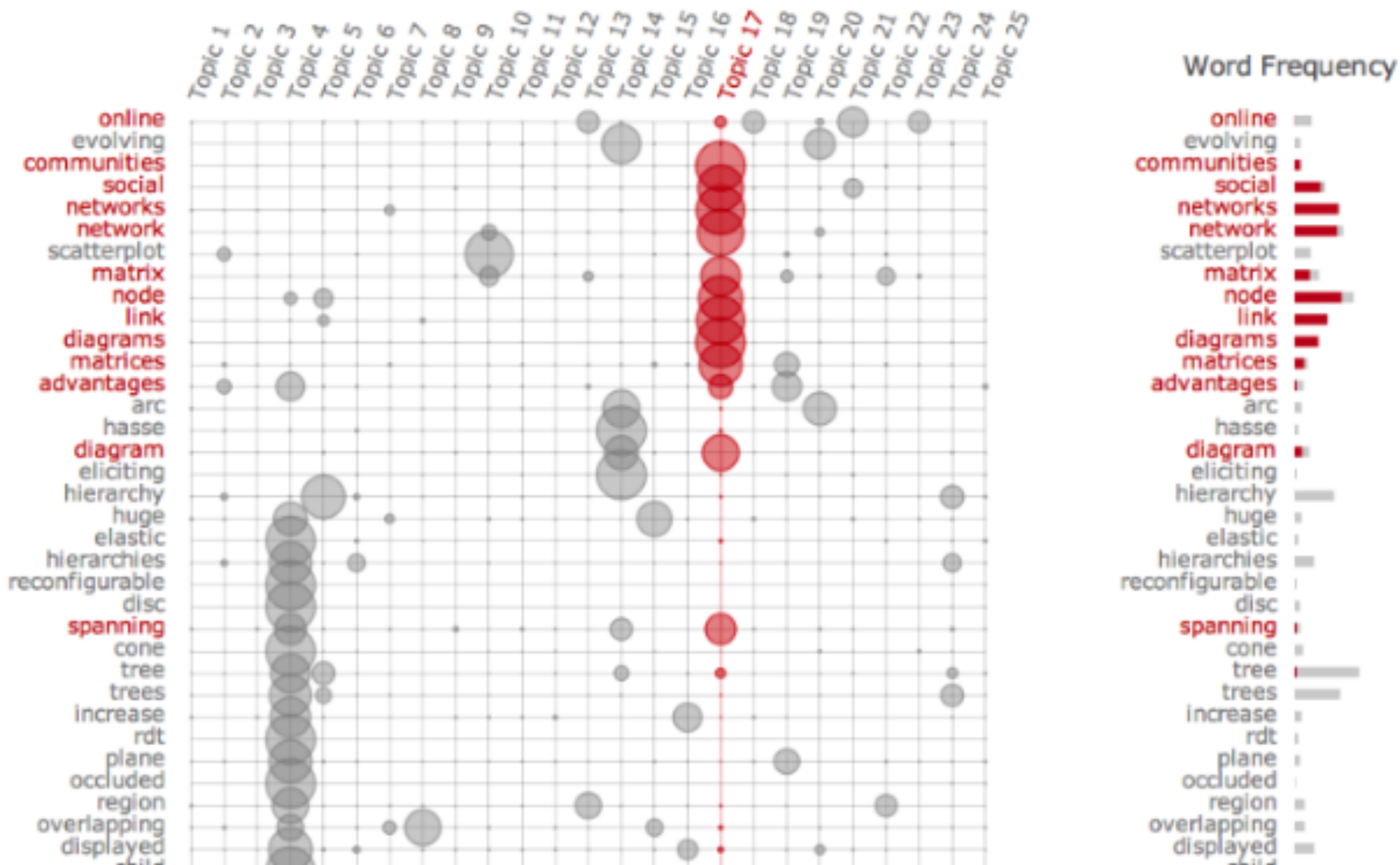






Visualizing Topics as Matrix

Termite: Visualization Techniques for Assessing Textual Topic Models
Jason Chuang, Christopher D. Manning, Jeffrey Heer. AVI 2012.
http://vis.stanford.edu/papers/termite



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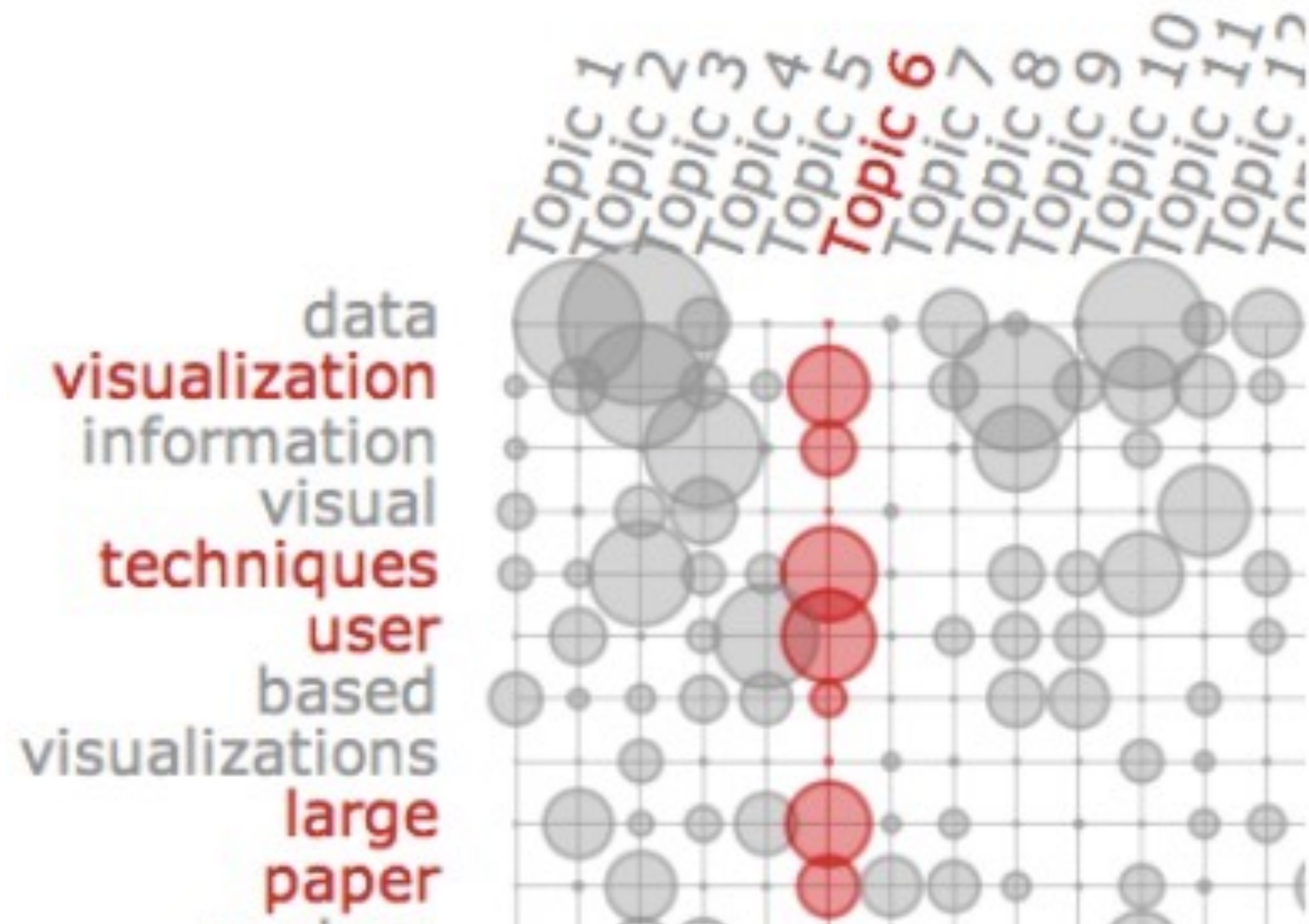
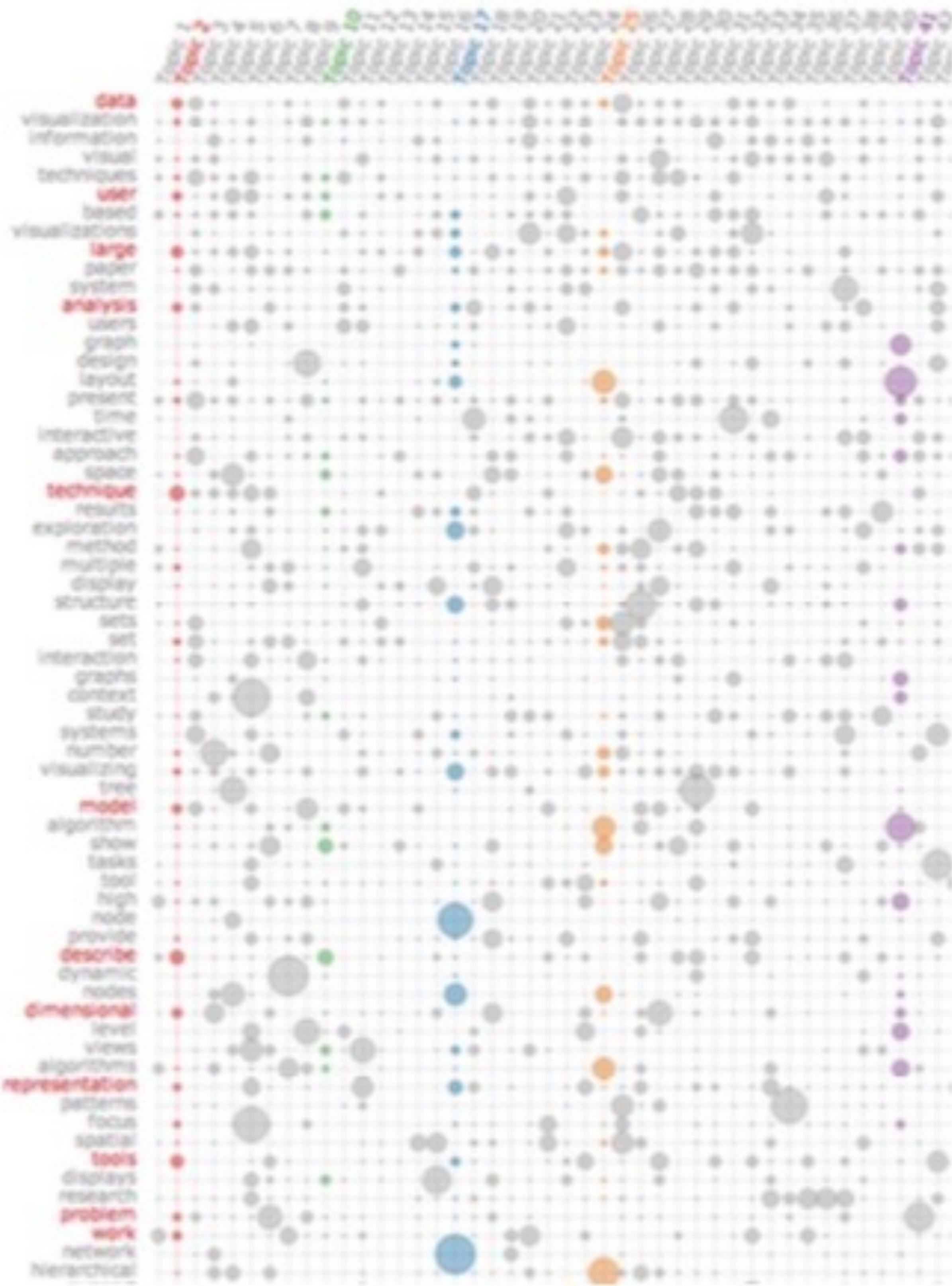
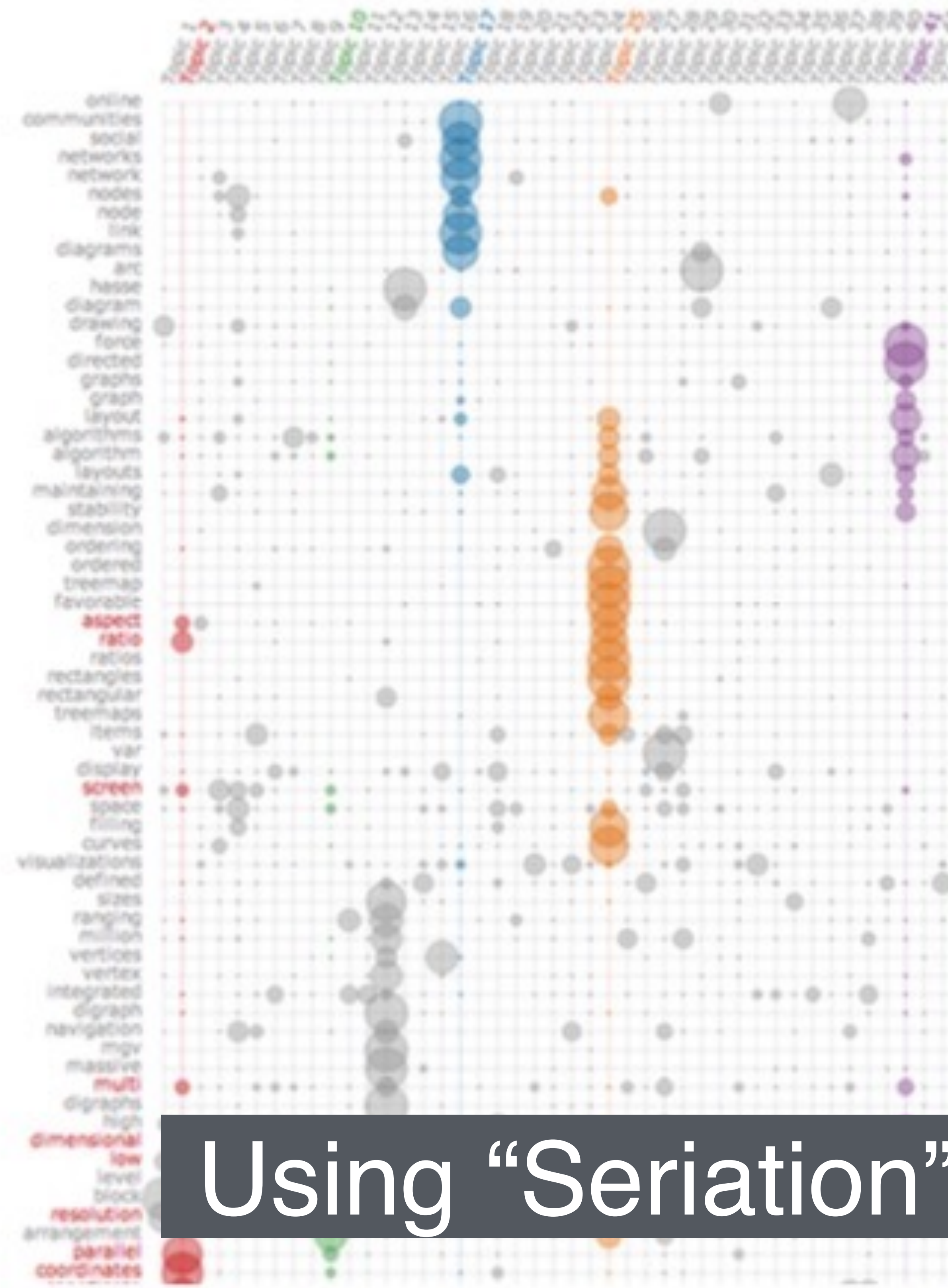


Termite: Topic Model Visualization

Analy

http://vis.stanford.edu/papers/termite

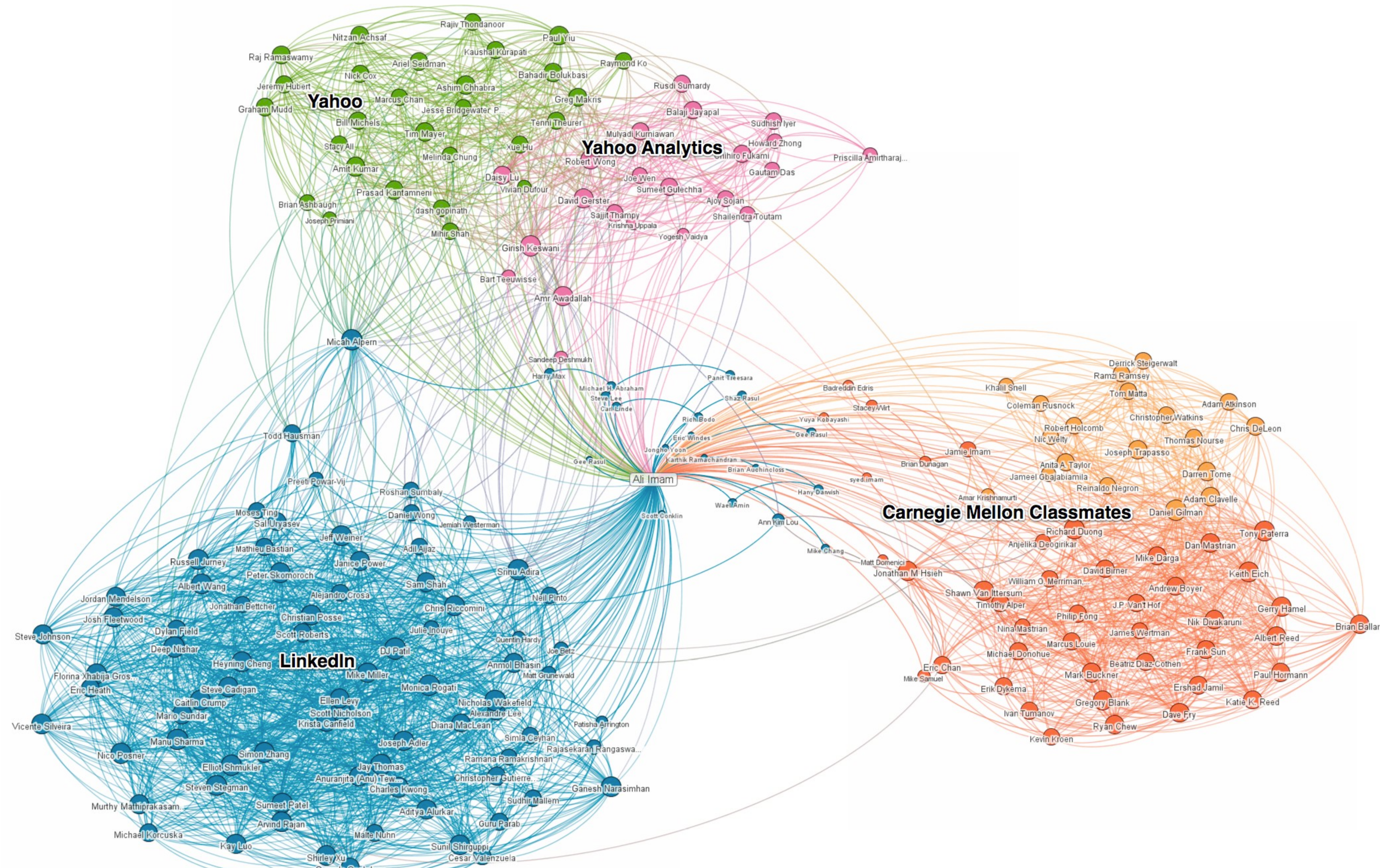




Using “Seriation”

Visualizing Graph Communities

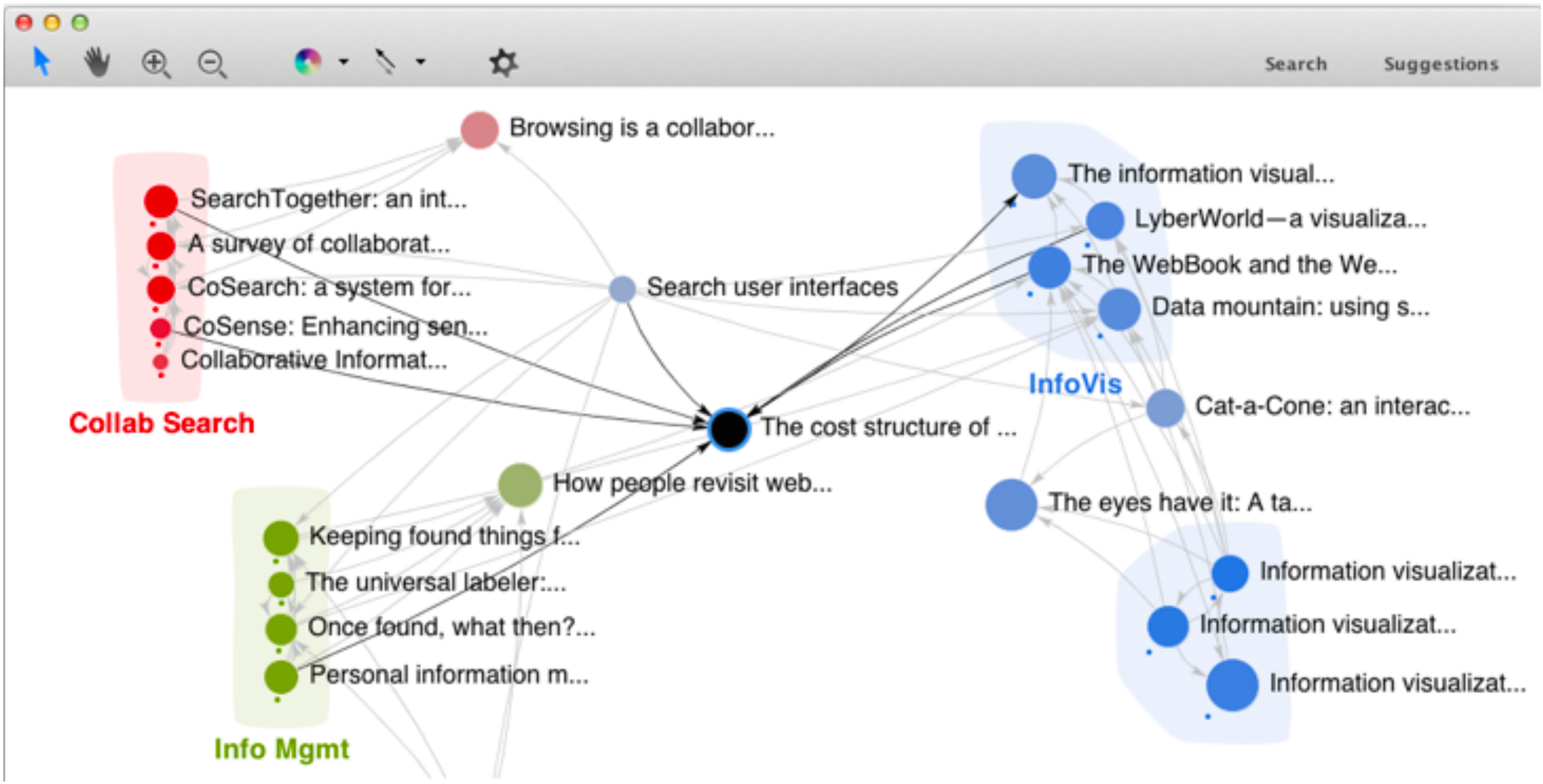
(using colors)



Visualizing Graph Communities

(using colors and convex hulls)

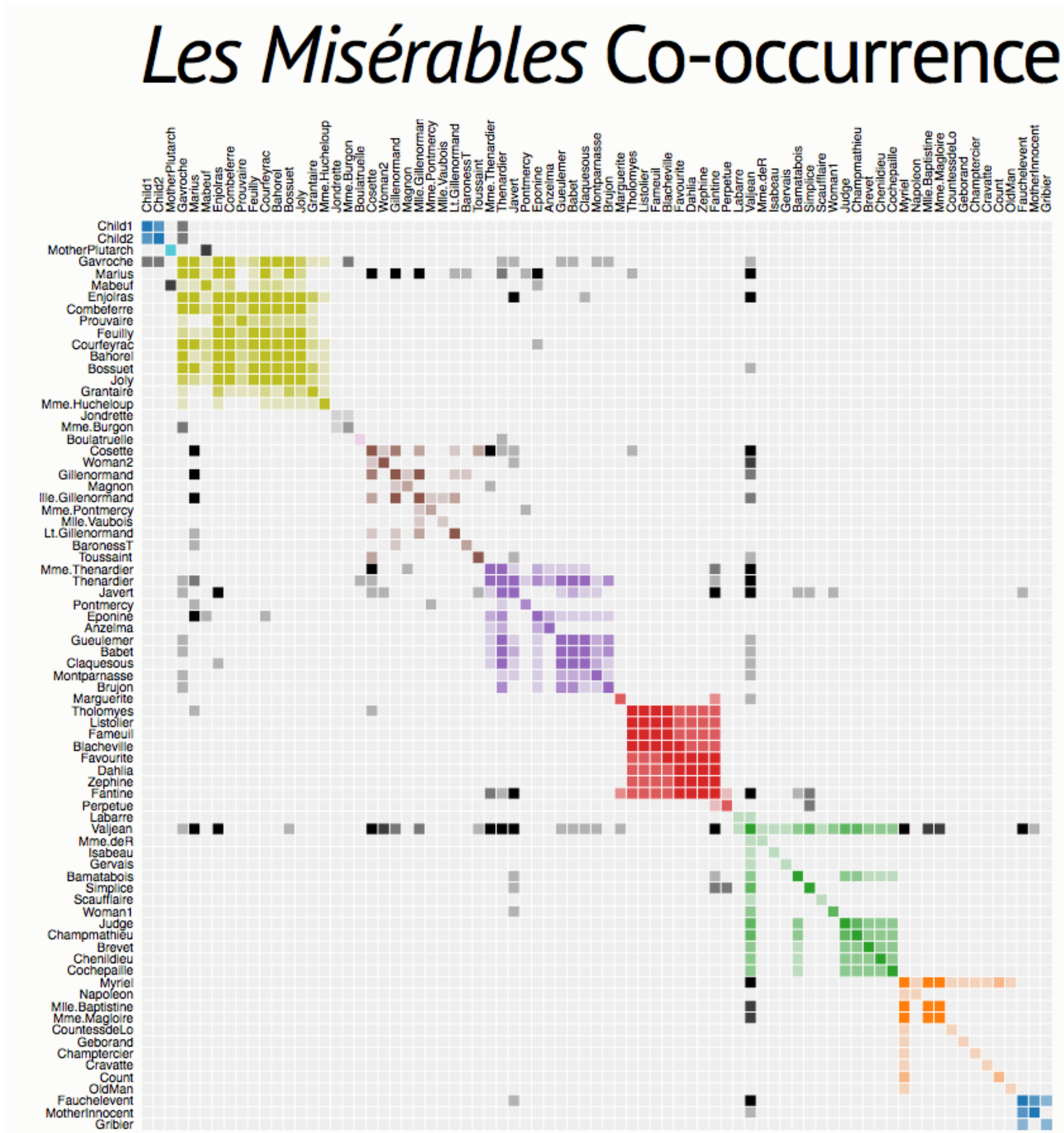
http://www.cc.gatech.edu/~dchau/papers/11-chi-apolo.pdf



Visualizing Graph Communities as Matrix

https://bost.ocks.org/mike/miserables/

Require good node ordering!



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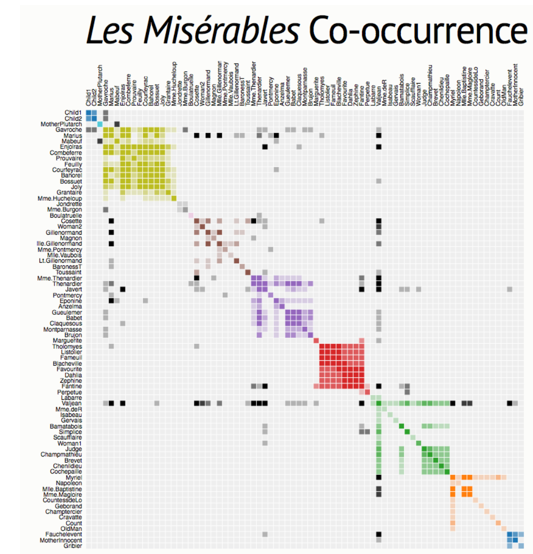
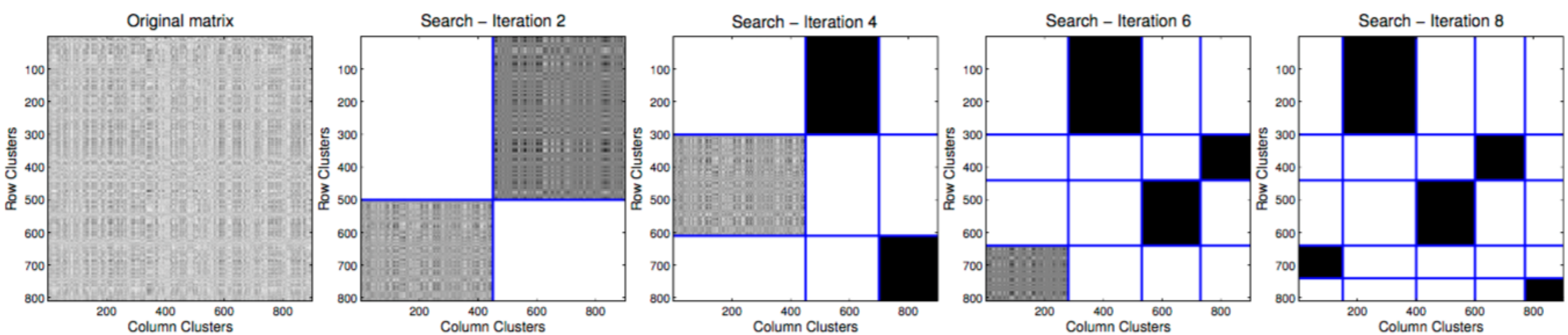


Require good node ordering!

Fully-automated way: "**Cross-associations**"

http://www.cs.cmu.edu/~christos/PUBLICATIONS/kdd04-cross-assoc.pdf



(a) Original matrix (b) Iteration pair 1 (c) Iteration pair 2 (d) Iteration pair 3 (e) Iteration pair 4

Graph Partitioning

If you know, or want to, specify #communities,
use **METIS**, the most popular graph partitioning tools

http://glaros.dtc.umn.edu/gkhome/views/metis