What Comes After K-Means?

A Survey of Clustering

Data clustering: 50 years beyond K-means:

❖ Published by Anil K. Jain from Michigan State University in Pattern Recognition Letters 31, September 2009
❖ Emphasizes the importance of grouping data.
❖ Considers various algorithms on "tricky" clusters.
❖ Two types of algorithms:
  – Partitional: builds clusters simultaneously
  – Hierarchical: agglomerates or divides clusters.
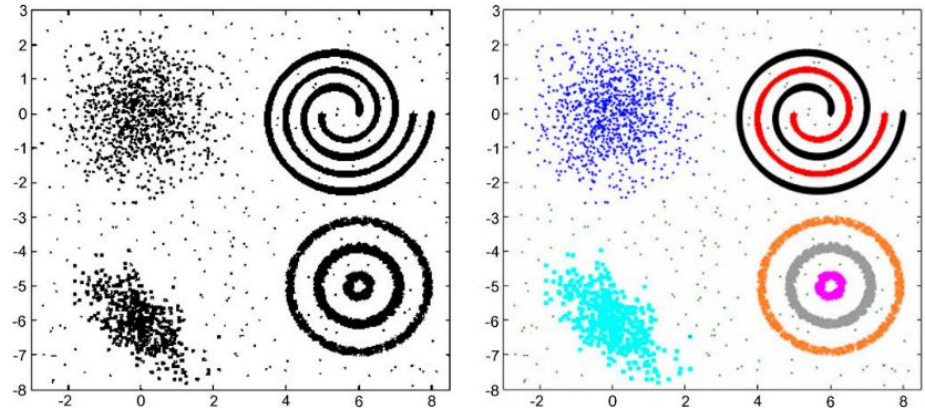

(a) Input data   (b) Desired clustering

50 years beyond K-means, cont:

❖ K-Means, 1956: partitional clustering. Strongly dependent on heuristic or analytical measures to choose an effective K.

❖ Fuzzy C-Means, 1973: extension of K-Means which assign points to clusters probabilistically rather than fixedly.

❖ DBSCAN, 1996: cluster based on region density rather than closes to some centroid. Similar to Jarvis–Patrick algorithm.

❖ CLIQUE, 1998: density based clustering that estimates density on low dimension subspace of data.

❖ Bisecting K-Means, 2000: recursively divides cluster into 2 partitions at each step.

❖ X-Means, 2000: automatically fixes K.

❖ Dirichlet Process, 1973 and 2000: later becomes DP-Means.

❖ Ensemble Methods, 2000: applying several algorithms to one dataset and collecting the results into one conclusion.
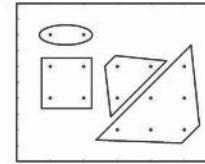
So What's Missing?

❖ Algorithms falter on sufficiently high dimension data.
❖ Datasets are getting much, much larger.
❖ The number of clusters is not always known or easily found.
❖ The "shape" of a cluster can still fool most algorithms.
❖ Fixed clustering is still the norm.
❖ "Noise" still commonly has to be cleaned out before clustering.
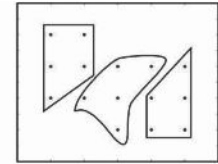❖ Streaming rather than batch methods are uncommon but would be valuable for many real world applications.
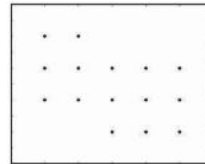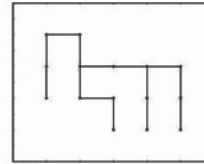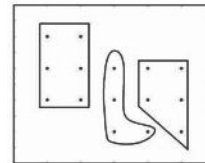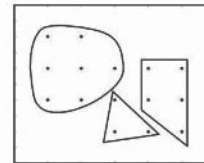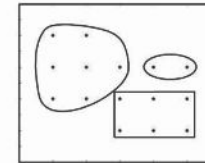

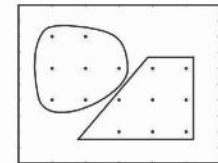(a) 15 points in 2D   (b) MST   (c) FORGY   (d) ISODATA
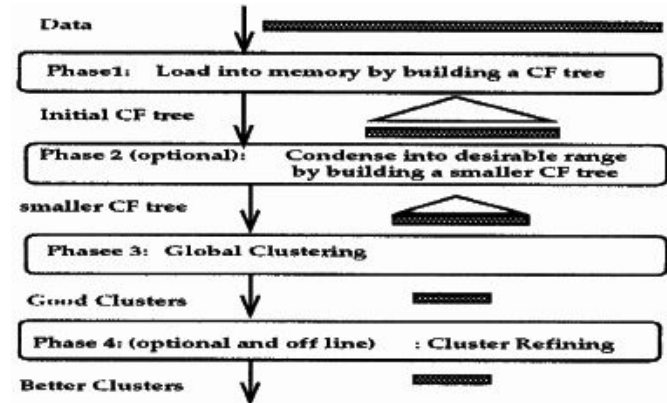(e) WISH   (f) CLUSTER   (g) Complete-link   (h) JP

BIRCH: An Efficient Data Clustering Method for Very Large Databases:

- ❖ Presented by Tian Zhang, Raghu Ramakrishnan, and Miron Livny at the ACM's SIGMOD in 1996.
- ❖ Specifically aimed to tackle big data within limited memory.
- ❖ Compares data points locally rather than globally.
- ❖ Can produce "good" results on a single scan of the data, but can optionally run for several iterations to improve the results.
- ❖ Captures the hierarchy of the dataset as a Clustering Feature Tree.

Data

Phase 1: Load into memory by building a CF tree

Initial CF tree

Phase 2 (optional): Condense into desirable range by building a smaller CF tree

smaller CF tree

Phase 3: Global Clustering

Good Clusters

Phase 4: (optional and off line) : Cluster Refining

Better Clusters

Pros and Cons of BIRCH:

❖ Built to work well in large data sets without a focus on high dimensional data.
❖ Can automatically compensate for noisy outliers without sacrificing speed.
❖ Strongly dependent on input parameters for speed and efficiency but not necessarily for producing good result.
❖ Has stayed relevant and in common usage despite being designed based on hardware which is no longer in usage.
❖ Can cluster regions of a data set based only on local data which makes the algorithm easily parallelizable.
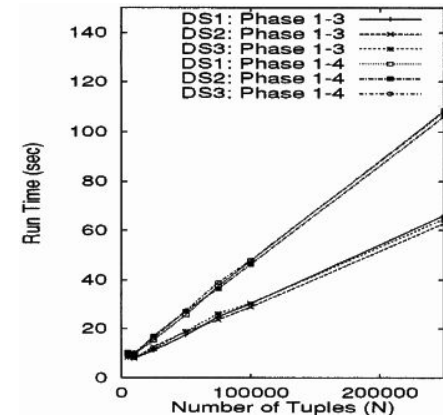
The Global Kernel K-Means Clustering Algorithm:

❖ Presented to the IEEE Joint Conference on Neural Networks in 2008 by Grigorios Tzortzis and Aristidis Likas from the University of Ioannina.

❖ Kernel K-Means attempts to distinguish clusters which are not linearly separable. Global K-Means attempts to minimize the sensitivity of K-Means to its initialization parameters. This is both.

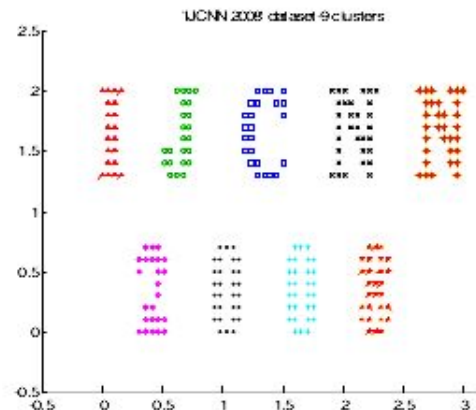❖ Comes in "fast" and "near optimal" variety.

❖ Developed on MRI images.

IJCNN 2008 dataset 9 clusters

Fig. 2. Global kernel *k*-means, fast global kernel *k*-means and kernel *k*-

Pros of GK K-Means:

- ❖ "Near optimal" variety properly identifies clusters with "tricky" shapes.
- ❖ More deterministic performance than traditional K-Means.
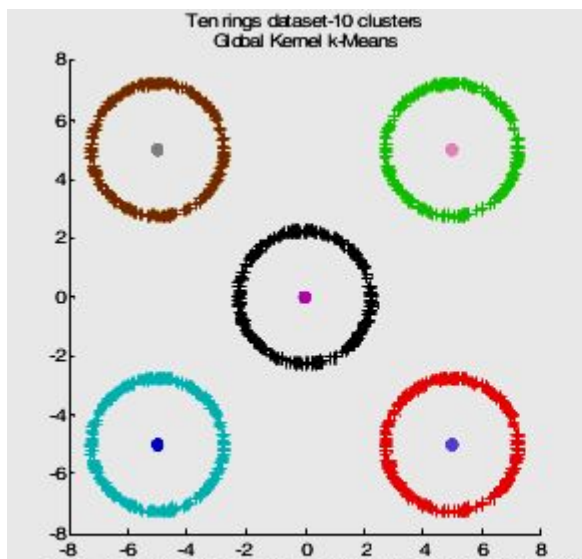- ❖ Produces solutions for cluster numbers of 1 up to K
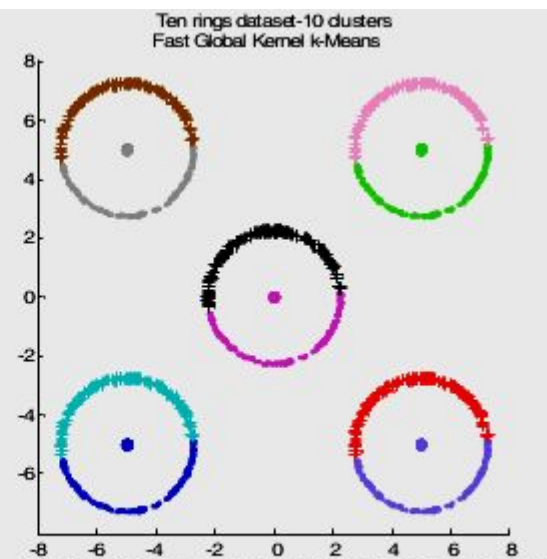

Fig. 3. Global kernel k-means on the ten rings dataset.

Fig. 4. Fast global kernel k-means on the ten rings dataset.

Cons of GK K-Means:

❖ Does not reduce or otherwise compensate for the dimensionality of the data.
❖ The testing data sets were extremely small by modern standards.
❖ The authors neglected to test their algorithm as a streaming clusterer which may have been more useful for the MRI application.
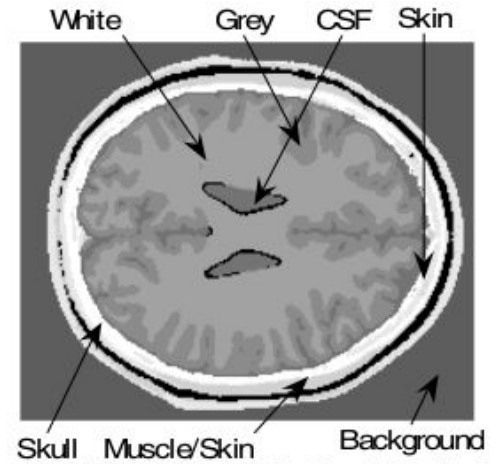❖ The implementation was written in MATLAB giving it minimal portability.

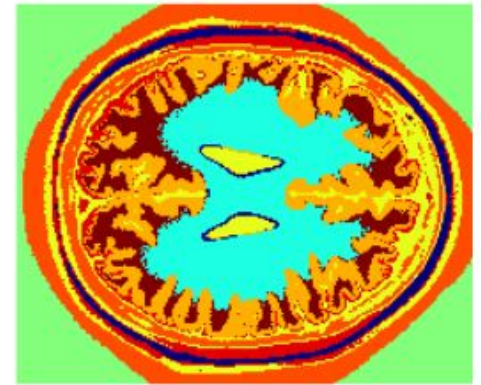Fig. 11. Ground truth for slice 100. In black are the 3 tissues we ignore in our experiments.

Fig. 14. Segmented tissues for slice 100 with fast global kernel *k*-means. In dark blue are the 3 tissues we ignore in our experiments.

TEXAS STATE UNIVERSITY

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Dynamic Clustering via Asymptotics of the Dependent Dirichlet Process Mixture:

❖ Published in Advances in Neural Information Processing Systems 26 in 2013 by Trevor Campbell, Miao Liu, Brian Kulis, Jonathan P. How, and Lawrence Carin.

❖ Based on the Dirichlet process, which is roughly a random collection of random variables.

❖ "Non-parametric": the model grows as new data is added.

❖ Tested on a dataset of aircraft trajectories.

❖ Clusters can be created, eliminated, and altered as data is added.

❖ Promises high speed for time-sensitive applications.

Pros and Cons of Dynamic Means:

❖ Scalable number of clusters.
❖ Functions as a batch or streaming algorithm.
❖ Very fast execution.
❖ Guarantees cluster validity similar to K-Means, which is part good and part bad.
❖ Demonstrated fast and effective clustering on 400-dimensional data.
❖ Focuses exclusively on fixed clustering.
❖ Despite the high dimensionality of the data set, the total size of the data was still quite small.
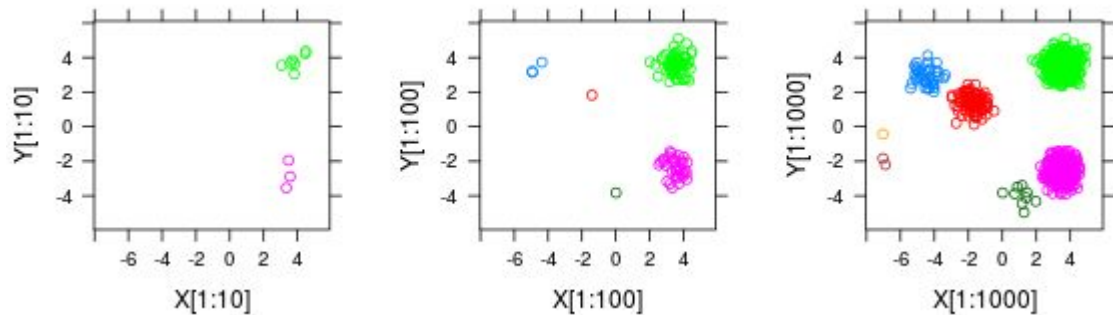
The Dirichlet Mixture Model from Victor Veitch at
https://en.wikipedia.org/wiki/Dirichlet_process#/media/File:DP_clustering_simulation.png

A Density Based Algorithm for Discovering Clusters:

❖ Presented to the Association for the Advancement of Artificial Intelligence in 1996 by Martin Ester, Hans-Peter Kriegel, Jörg Sander and Xiaowei Xu from the University of Munich.
❖ Only takes on input parameter.
❖ Clusters by density of data points rather than by placing centroids.
❖ Can define clusters of arbitrary shapes.
❖ This is a partitioning algorithm, which was unusual by this point in time.
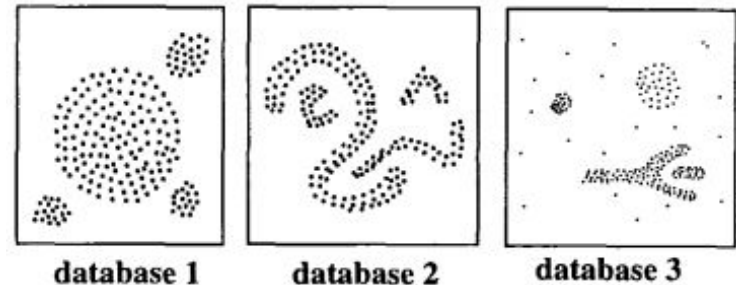

figure 1: Sample databases

Pros and Cons of DBSCAN:

❖ Near linear scaling of time requirement as the dataset grows, which is very close to BIRCH's performance.

❖ Can find clusters of absolutely any shape, rather than find clusters fitting "several" models.

❖ Compensates for noisy data, but always includes outliers in some cluster.

❖ Commonly available in Python or other languages of choice.

❖ Does not balance clusters by their number of points. Rather the algorithm focuses only on the density of the points.

❖ "Neighborhood" consideration becomes more difficult in high dimension data.

❖ Not entirely deterministic.