Data Clustering:
50 Years Beyond K-means

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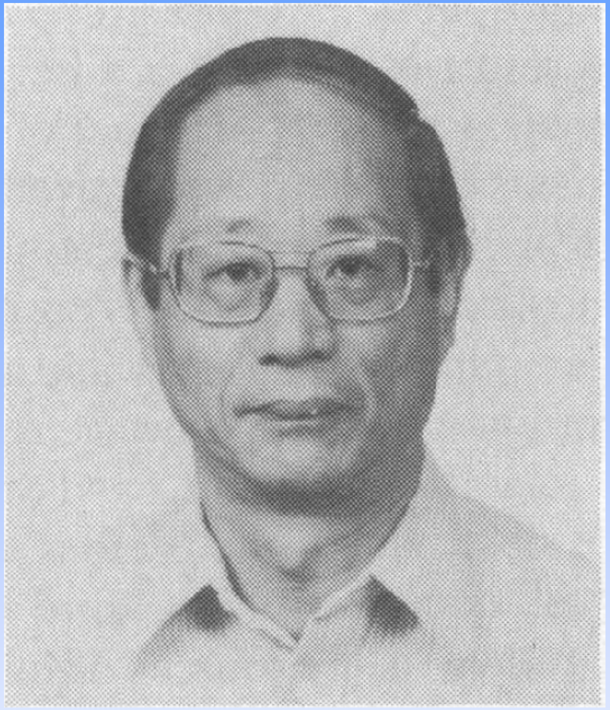
King-Sun Fu



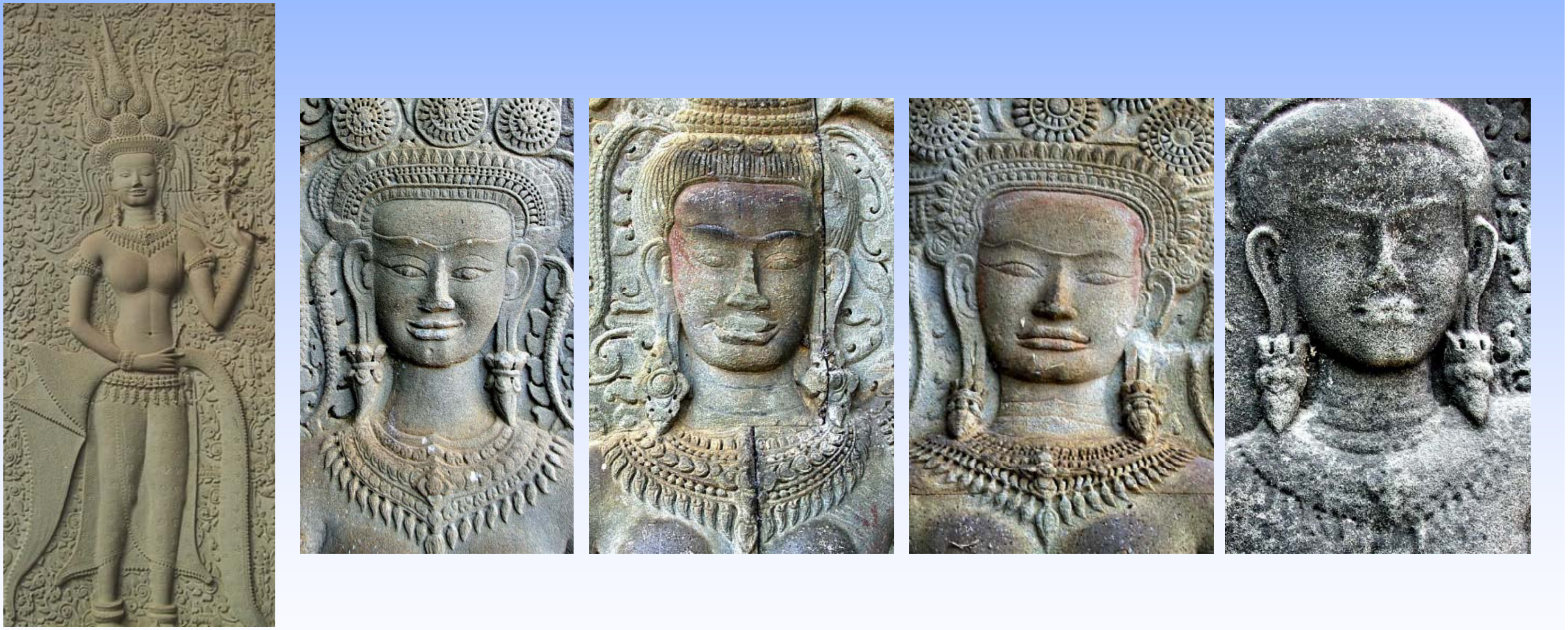
King-Sun Fu (1930-1985), a professor at Purdue was instrumental in the founding of IAPR, served as its first president, and is widely recognized for his extensive contributions to pattern recognition. *(Wikipedia)*

Angkor Wat, Siem Reap

Hindu temple built by a Khmer king ~1150 AD; Khmer kingdom declined in the 15th century; French explorers discovered the hidden ruins in 1860 (Angelina Jolie alias “Lora Croft” in *Tomb Raider* thriller)

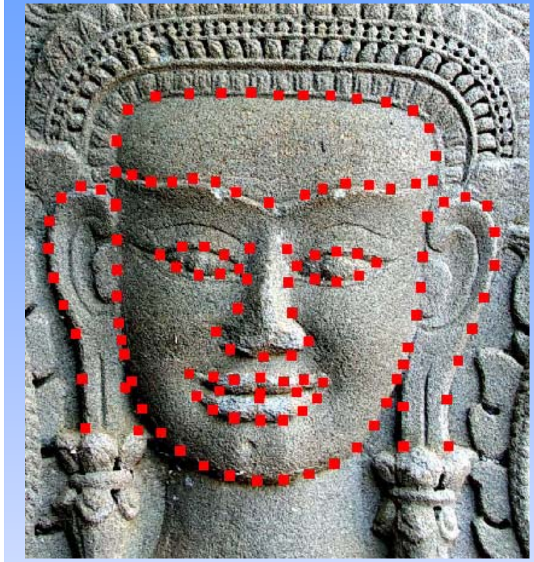
Apsaras of Angkor Wat

- Angkor Wat contains the most unique gallery of over 2,000 women depicted by detailed full body portraits
- What facial types are represented in these portraits?

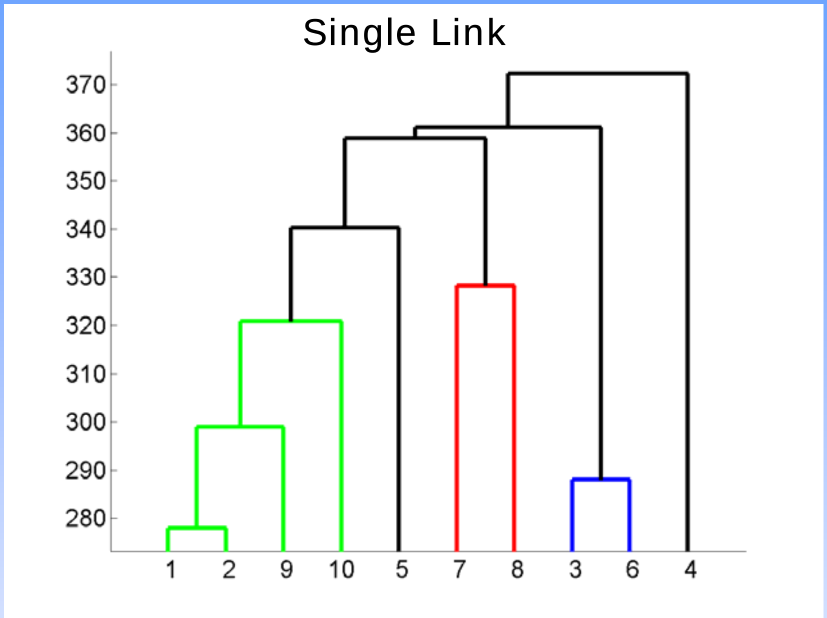


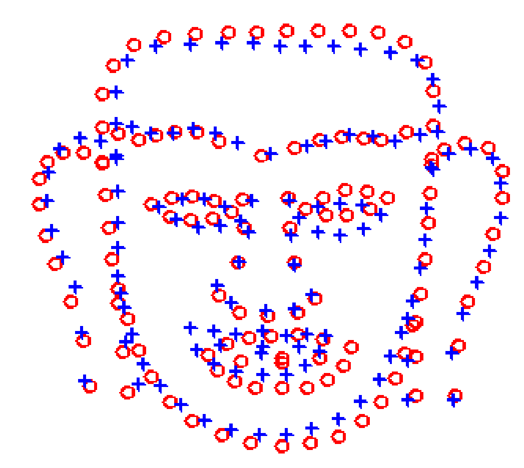
Kent Davis, Biometrics of the Godesess, DatAsia, Aug 2008
S. Marchal, Costumes et Parures Khmers: D'apres les devata D'Angkor-Vat, 1927

Clustering of Apsara Faces

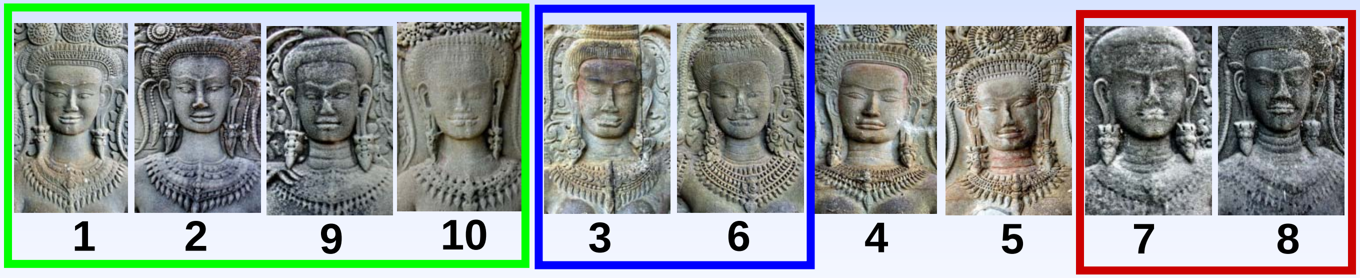


127 landmarks





Shape alignment



Single Link clusters

How do we validate the groups?

Ground Truth

Khmer Cultural Center

Data Explosion

- The digital universe was ~281 exabytes (281 billion gigabytes) in 2007; it would grow 10 times by 2011
- Images and video, captured by over one billion devices (camera phones), are the major source
- To archive and effectively use this data, we need tools for data categorization

http://eon.businesswire.com/releases/information/digital/prweb509640.htm

http://www.emc.com/collateral/analyst-reports/diverse-exploding-digital-universe.pdf

Data Clustering

- Grouping of objects into meaningful categories
- Classification vs. clustering
- Unsupervised learning, exploratory data analysis, grouping, clumping, taxonomy, typology, Q-analysis
- Given a representation of n objects, find K clusters based on a measure of similarity
- Partitional vs. hierarchical

A. K. Jain and R. C. Dubes. Algorithms for Clustering Data, Prentice Hall, 1988. (available for download at: http://dataclustering.cse.msu.edu/)

Why Clustering?

- Natural classification: degree of similarity among forms (phylogenetic relationship or taxonomy)
- Data exploration: discover underlying structure, generate hypotheses, detect anomalies
- Compression: method for organizing data
- Applications: any scientific field that collects data! Astronomy, biology, marketing, engineering,…..

Google Scholar: ~1500 clustering papers in 2007 alone!

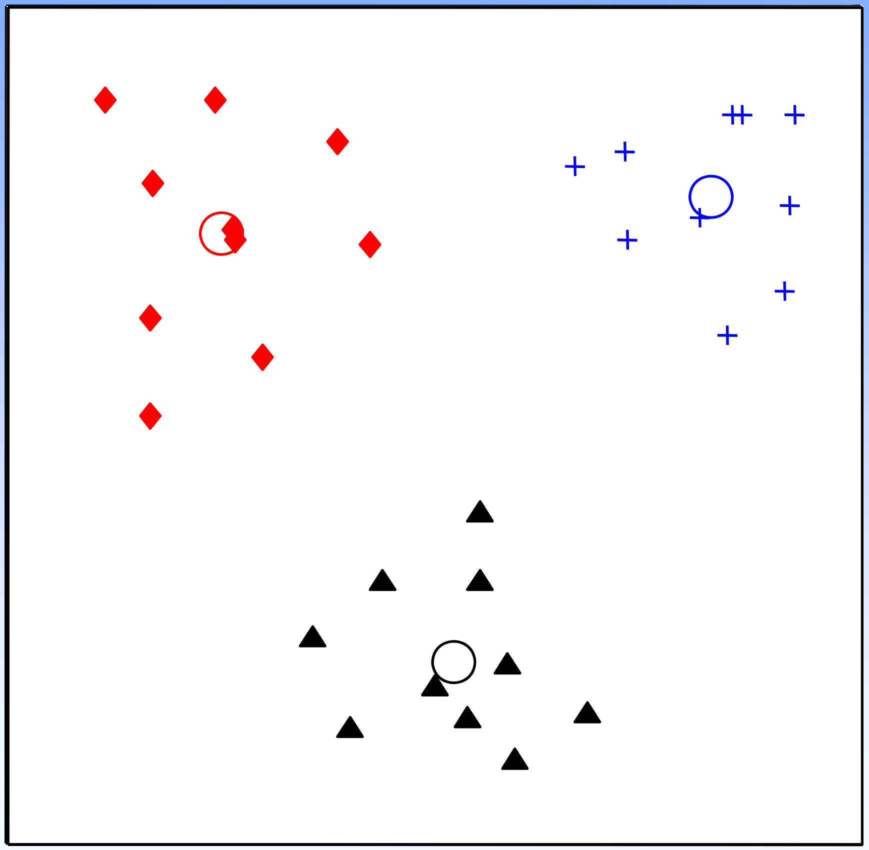
Historical Developments

- Cluster analysis first appeared in the title of a 1954 article analyzing anthropological data *(JSTOR)*
- Hierarchical Clustering: *Sneath (1957), Sorensen (1957)*
- K-Means: independently discovered *Steinhaus[1] (1956), Lloyd[2] (1957), Cox[3] (1957), Ball & Hall[4] (1967), MacQueen[5] (1967)*
- Mixture models (*Wolfe, 1970*)
- Graph-theoretic methods *(Zahn, 1971)*
- K Nearest neighbors *(Jarvis & Patrick, 1973)*
- Fuzzy clustering *(Bezdek, 1973)*
- Self Organizing Map *(Kohonen, 1982)*
- Vector Quantization *(Gersho and Gray, 1992)*

[1] Acad. Polon. Sci., [2] Bell Tel. Report, [3] JASA, [4] Behavioral Sci., [5] Berkeley Symp. Math Stat & Prob.

K-Means Algorithm

Minimize the squared error; Initialize K means; assign points to closest mean; update means; iterate



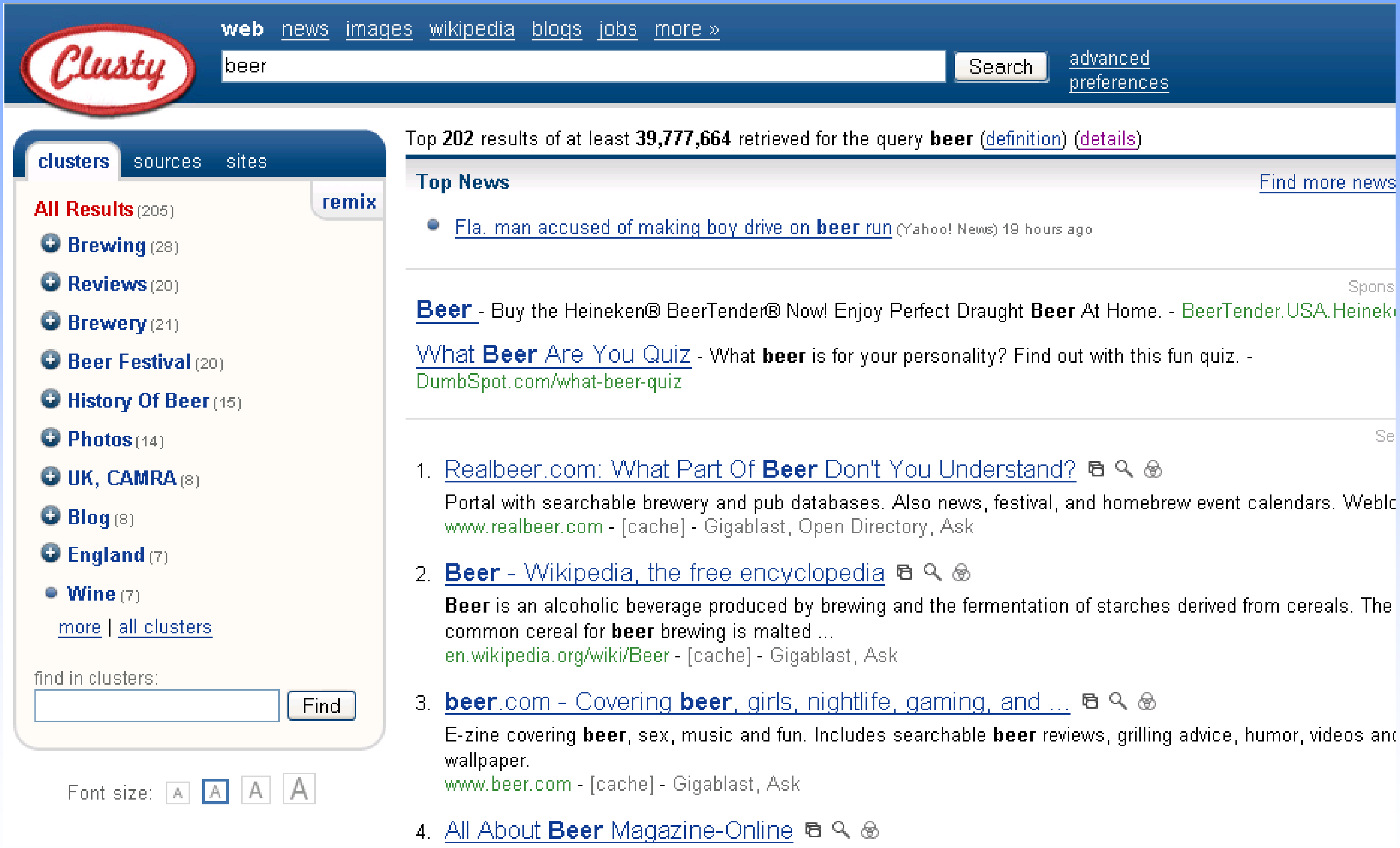
Bisecting K-means *(Karypis et al.)*; X-means *(Pelleg and Moore)*; Constrained K-means *(Davidson)*; Scalable K-means *(Bradley et al.)*

Beyond K-Means

- Developments in Data Mining and Machine Learning
  - Bayesian models, kernel methods, association rules (subspace clustering), graph mining, large scale clustering
- Choice of models, objective functions, and heuristics
- Density-based *(Ester et al., 1996)*
- Spectral *(Hagen & Kahng, 1991; Shi & Malik, 2000)*
- Information bottleneck *(Tishby et al., 1999)*
- Non-negative matrix factorization *(Lee & Seung, 1999)*
- Ensemble *(Fred & Jain, 2002; Strehl & Ghosh, 2002)*
- Semi-supervised *(Wagstaff et al., 2003; Basu et al., 2004)*

Structure Discovery

Cluster web retrieved documents



All Results (205)
- Brewing (28)
- Reviews (20)
- Brewery (21)
- Beer Festival (20)
- History Of Beer (15)
- Photos (14)
- UK, CAMRA (8)
- Blog (8)
- England (7)
- Wine (7)

more | all clusters

find in clusters:

Top **202** results of at least **39,777,664** retrieved for the query **beer** (definition) (details)

Top News Find more news

- Fla. man accused of making boy drive on **beer** run (Yahoo! News) 19 hours ago

Spons

Beer - Buy the Heineken® BeerTender® Now! Enjoy Perfect Draught **Beer** At Home. - BeerTender.USA.Heinek

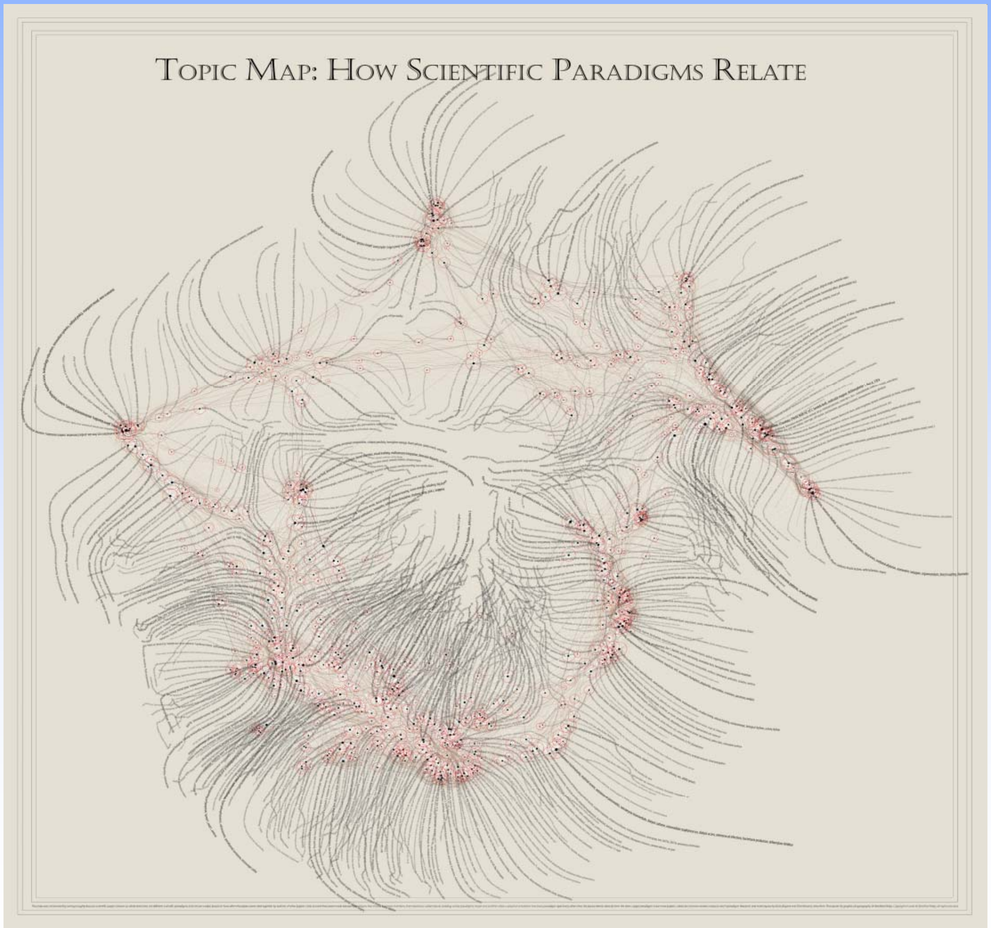
What **Beer** Are You Quiz - What **beer** is for your personality? Find out with this fun quiz. - DumbSpot.com/what-beer-quiz

Se

1. Realbeer.com: What Part Of **Beer** Don't You Understand?
   Portal with searchable brewery and pub databases. Also news, festival, and homebrew event calendars. Weblo
   www.realbeer.com - [cache] - Gigablast, Open Directory, Ask
2. **Beer** - Wikipedia, the free encyclopedia
   Beer is an alcoholic beverage produced by brewing and the fermentation of starches derived from cereals. The common cereal for **beer** brewing is malted ...
   en.wikipedia.org/wiki/Beer - [cache] - Gigablast, Ask
3. **beer**.com - Covering **beer**, girls, nightlife, gaming, and ...
   E-zine covering **beer**, sex, music and fun. Includes searchable **beer** reviews, grilling advice, humor, videos and wallpaper.
   www.beer.com - [cache] - Gigablast, Ask
4. All About **Beer** Magazine-Online

Topic Discovery

800,000 scientific papers clustered into 776 paradigms (topics) based on how often the papers were cited together by authors of other papers



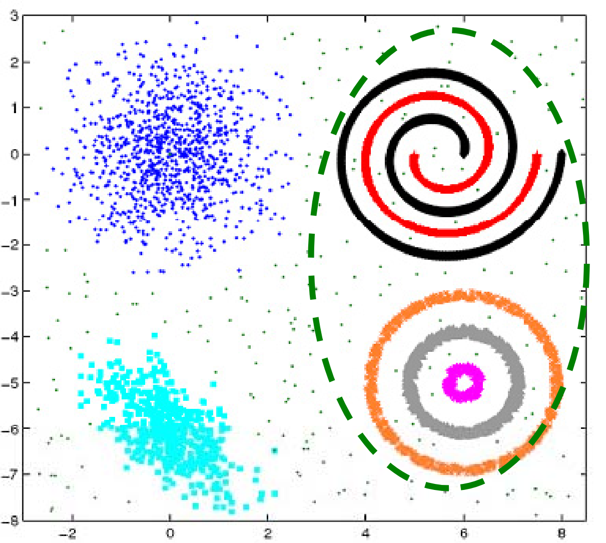
Map of Science, *Nature (2006)*

User’s Dilemma!

- What is a cluster?
- Which features and normalization scheme?
- How to define pair-wise similarity?
- How many clusters?
- Which clustering method?
- Does the data have any clustering tendency?
- Are the discovered clusters & partition valid?

R. Dubes and A.K. Jain, Clustering Techniques: User’s Dilemma, *Pattern Recognition*, 1976

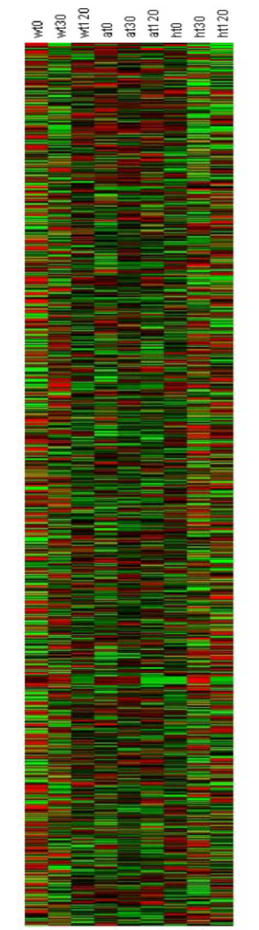
Cluster



- A set of similar entities; entities in different clusters are not alike
- How do we define similarity?
- Compact clusters
  - within-cluster distance < between-cluster distance
- Connected clusters
  - within-cluster connectivity > between-cluster connectivity
- Ideal cluster: compact and isolated

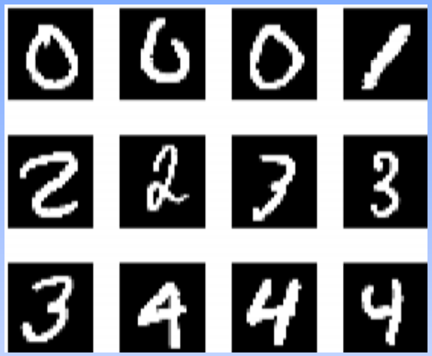
Representation

No universal representation; domain dependent

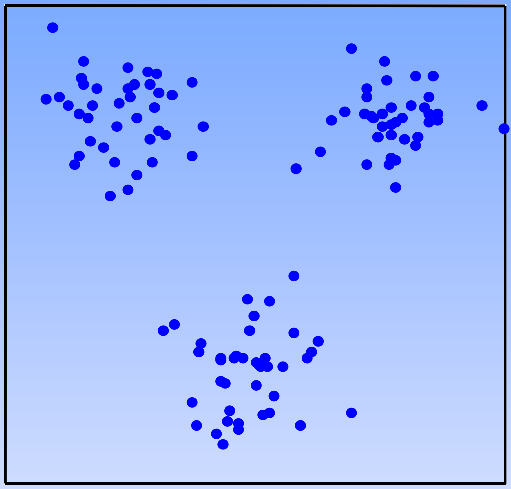


Gene Expressions

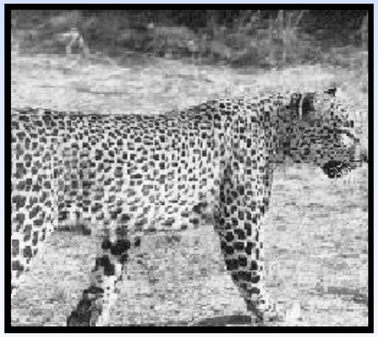
Image retrieval



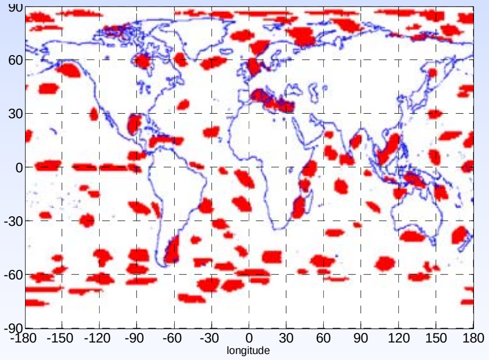
Handwritten digits



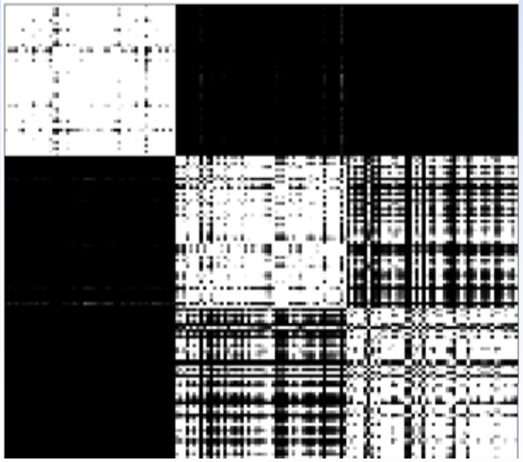
nxd pattern matrix



Segmentation



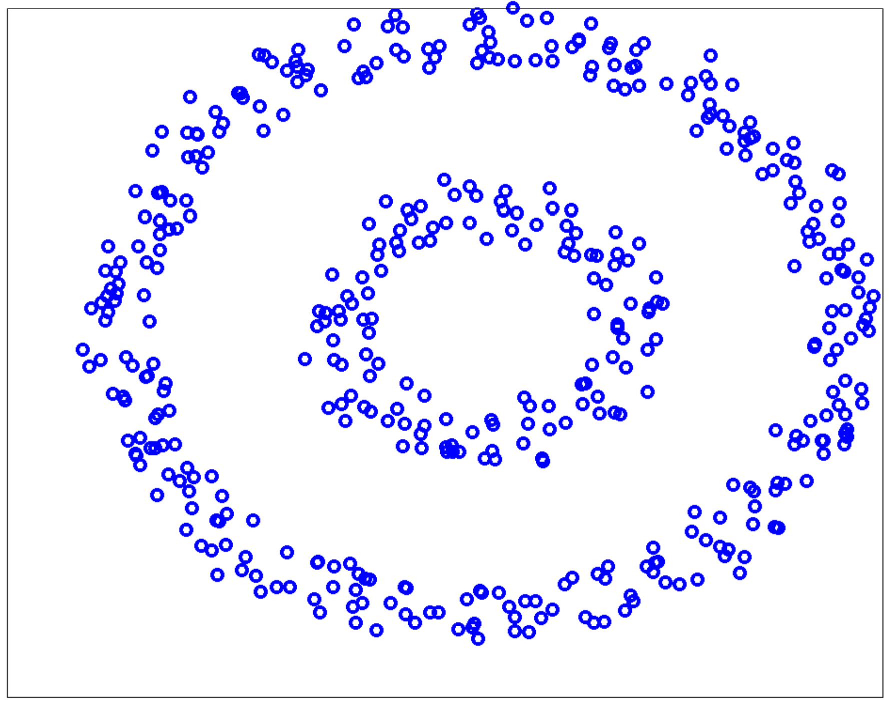
Time series (sea-surface temp)



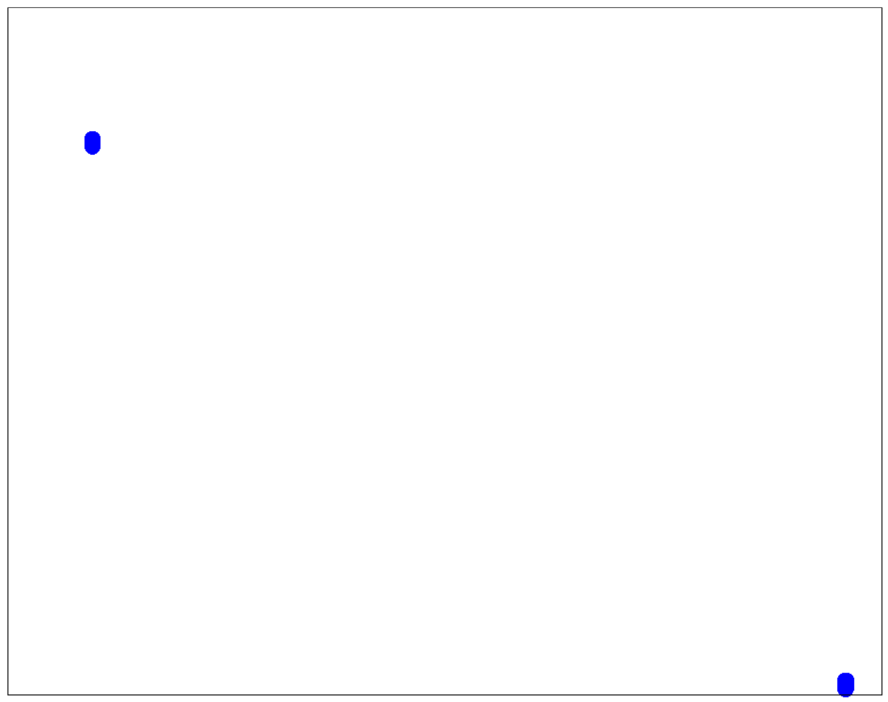
nxn similarity matrix

Good Representation

Good representation => compact & isolated clusters



Points in given 2D space



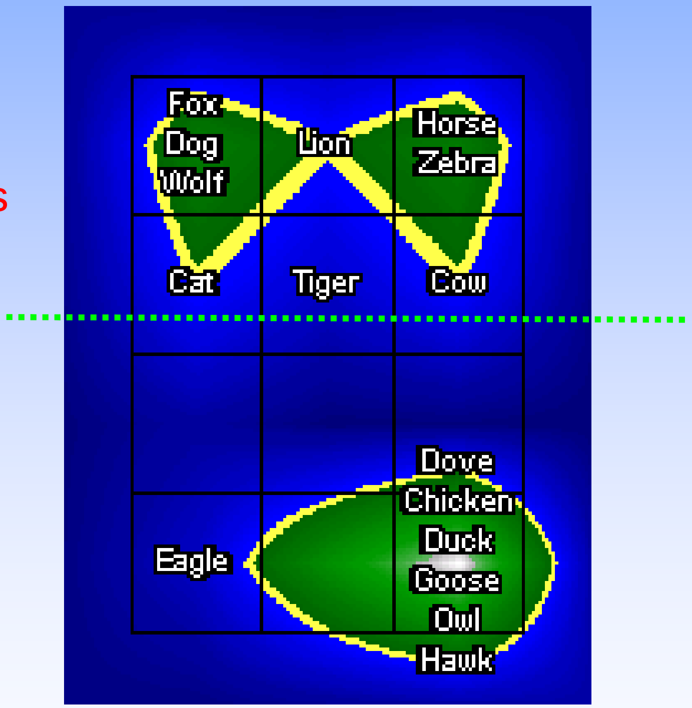
Eigenvectors of RBF kernel

Feature Weighting

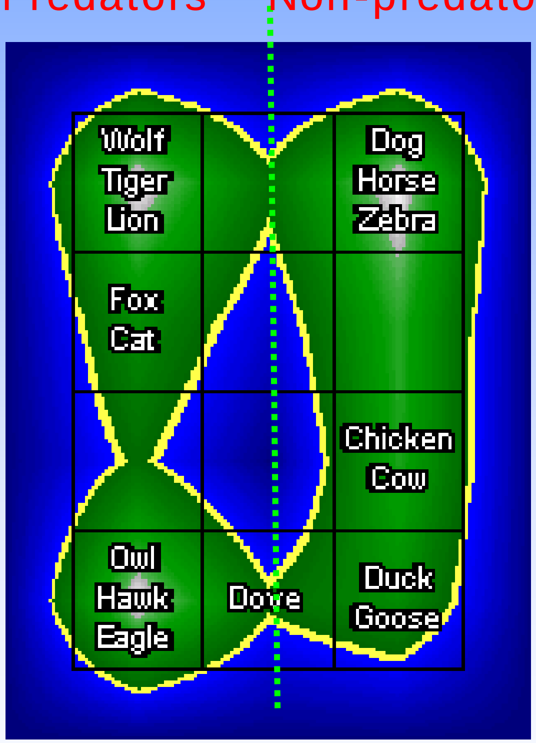
Two different meaningful groupings of 16 animals based on 13 Boolean features (appearance & activity)

Mammals

Birds



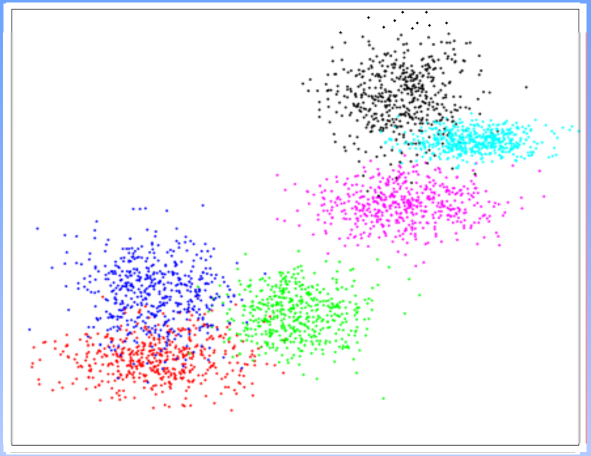
Predators Non-predators



Large weight on appearance features Large weight on activity features

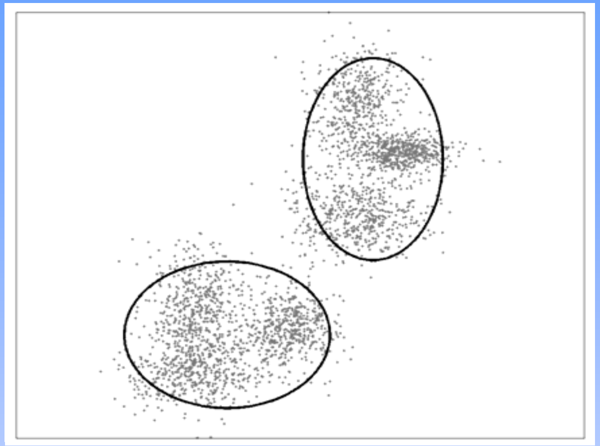
http://www.ofai.at/~elias.pampalk/kdd03/animals/

Number of Clusters

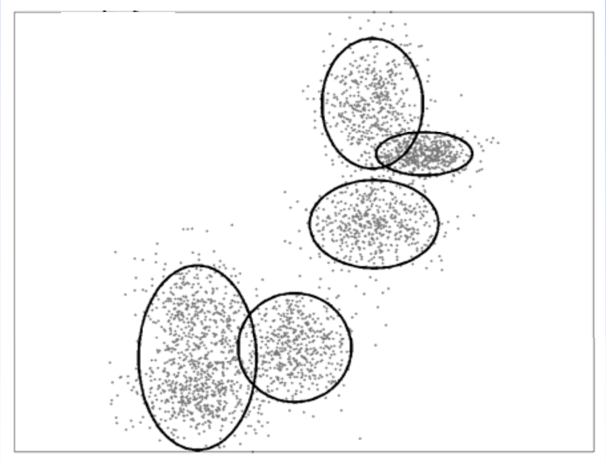


True labels, K = 6

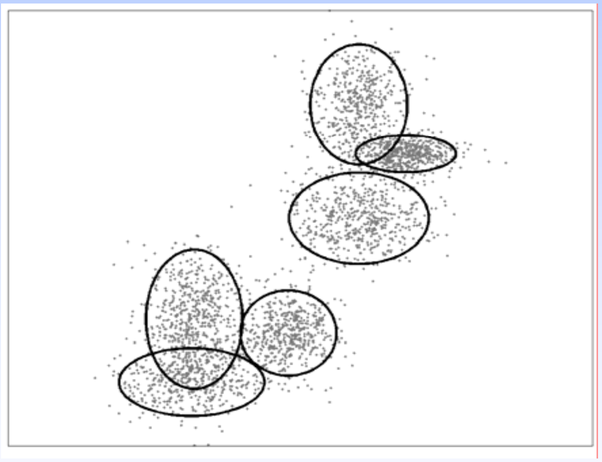
Input data



GMM (K=2)



GMM (K=5)

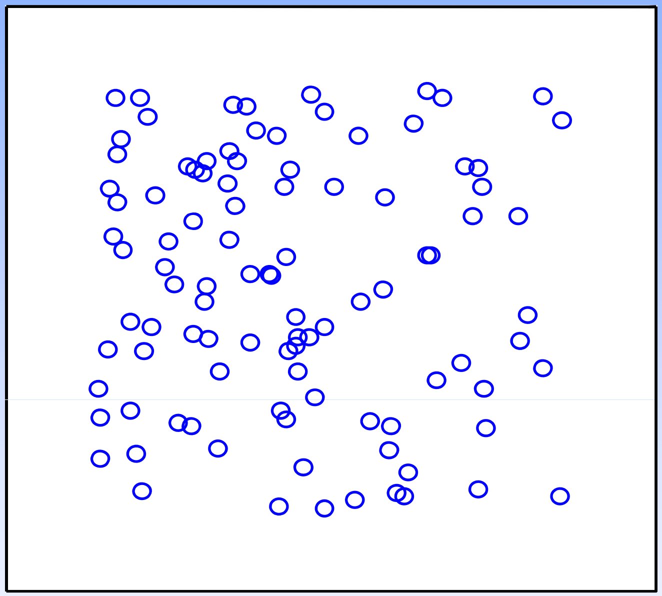


GMM (K=6)

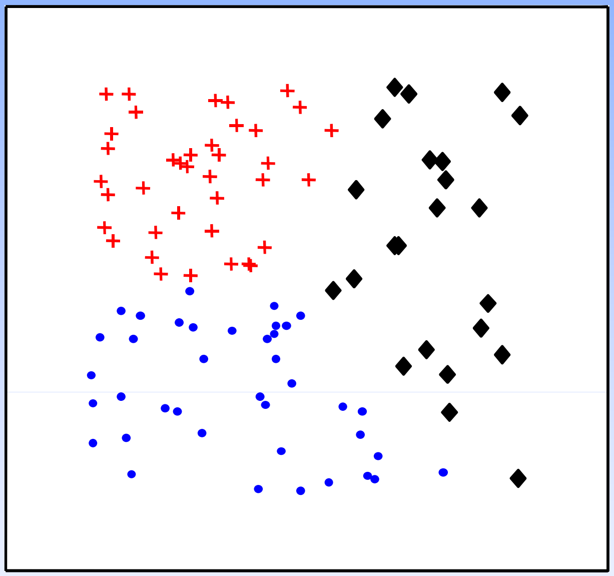
M. Figueiredo and A.K. Jain, Unsupervised Learning of Finite Mixture Models, *IEEE PAMI*, 2002

Cluster Validity

- Clustering algorithms find clusters, even if there are no natural clusters in data



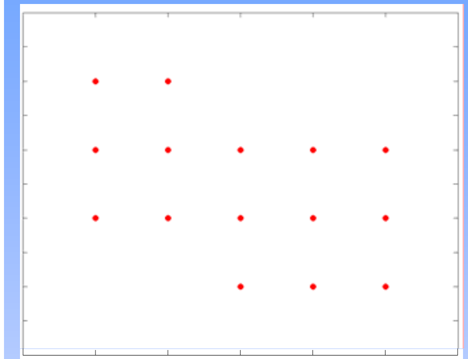
100 2D uniform data points



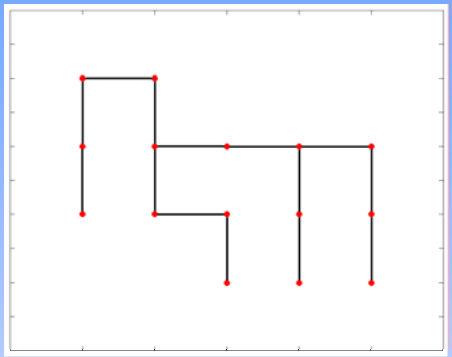
K-Means; K=3

- Easy to design new methods, difficult to validate
- Cluster stability *(Jain & Moreau, 1989; Lange et. al, 2004)*

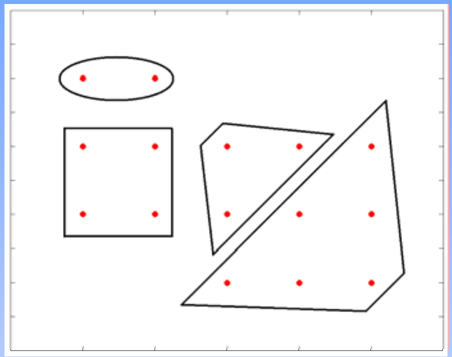
Comparing Clustering Algorithms



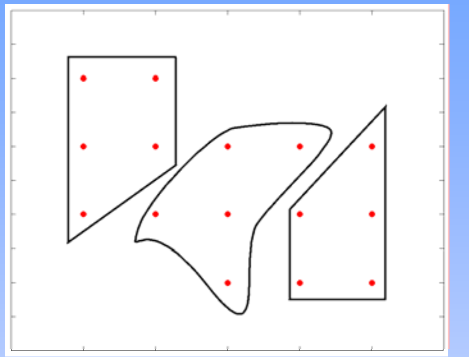
15 points in 2D



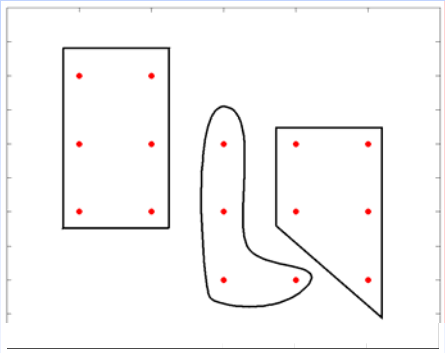
MST



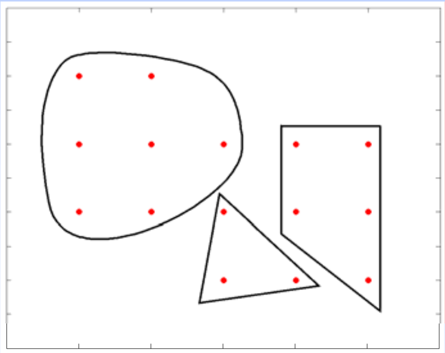
FORGY



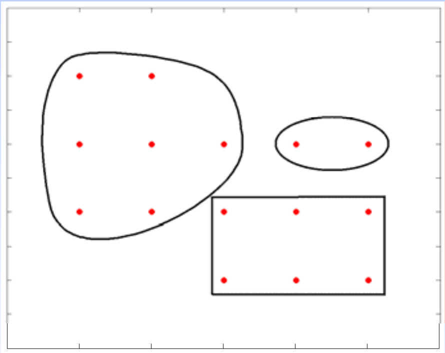
ISODATA



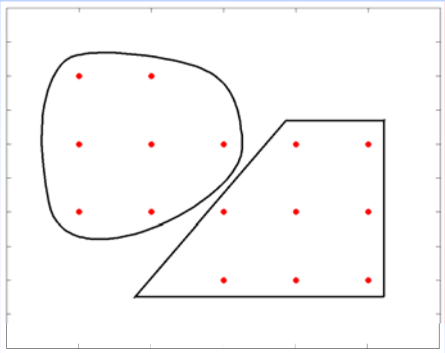
WISH



CLUSTER



Complete-link



JP

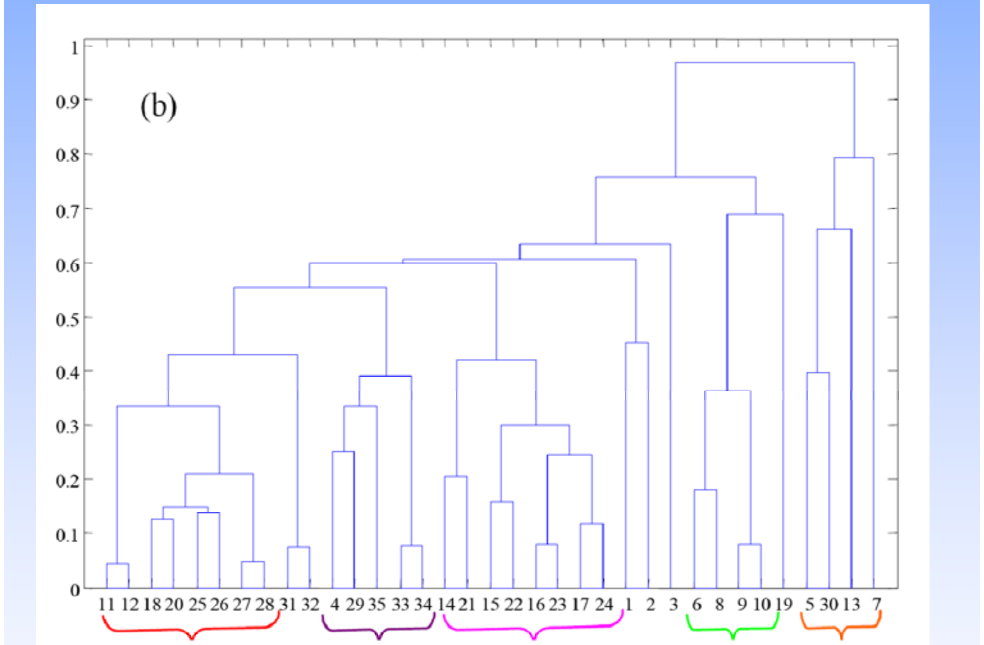
FORGY, ISODATA, WISH, CLUSTER are all MSE algorithms

R. Dubes and A.K. Jain, Clustering Techniques: User's Dilemma, *Pattern Recognition*, 1976

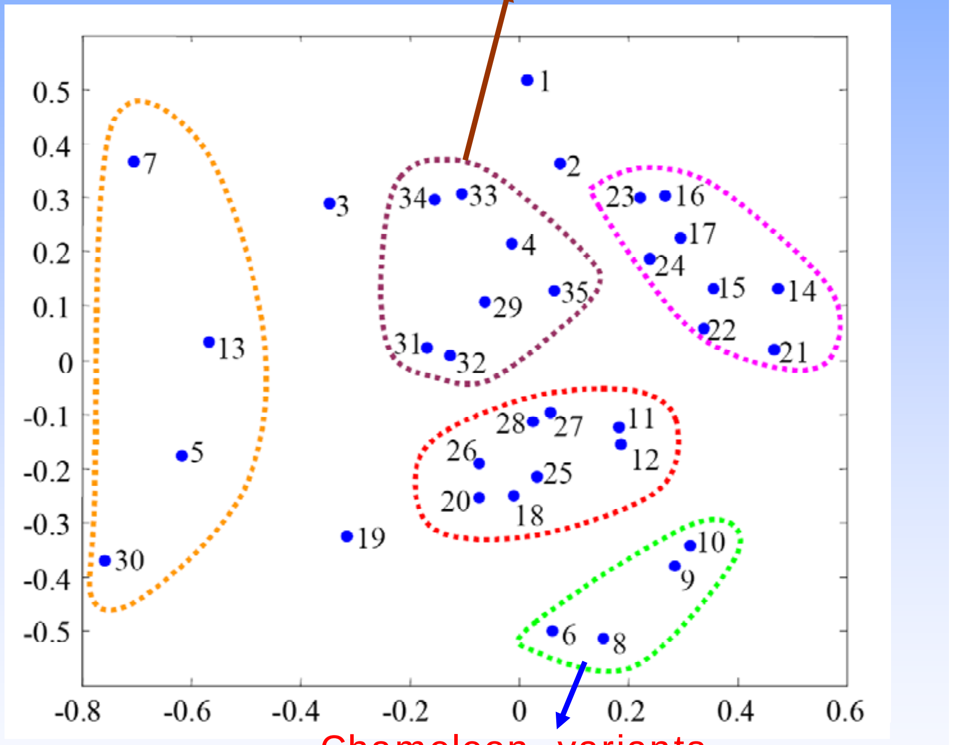
Grouping of Clustering Algorithms

Clustering method vs. clustering algorithm

K-means, Spectral, GMM, Ward’s linkage



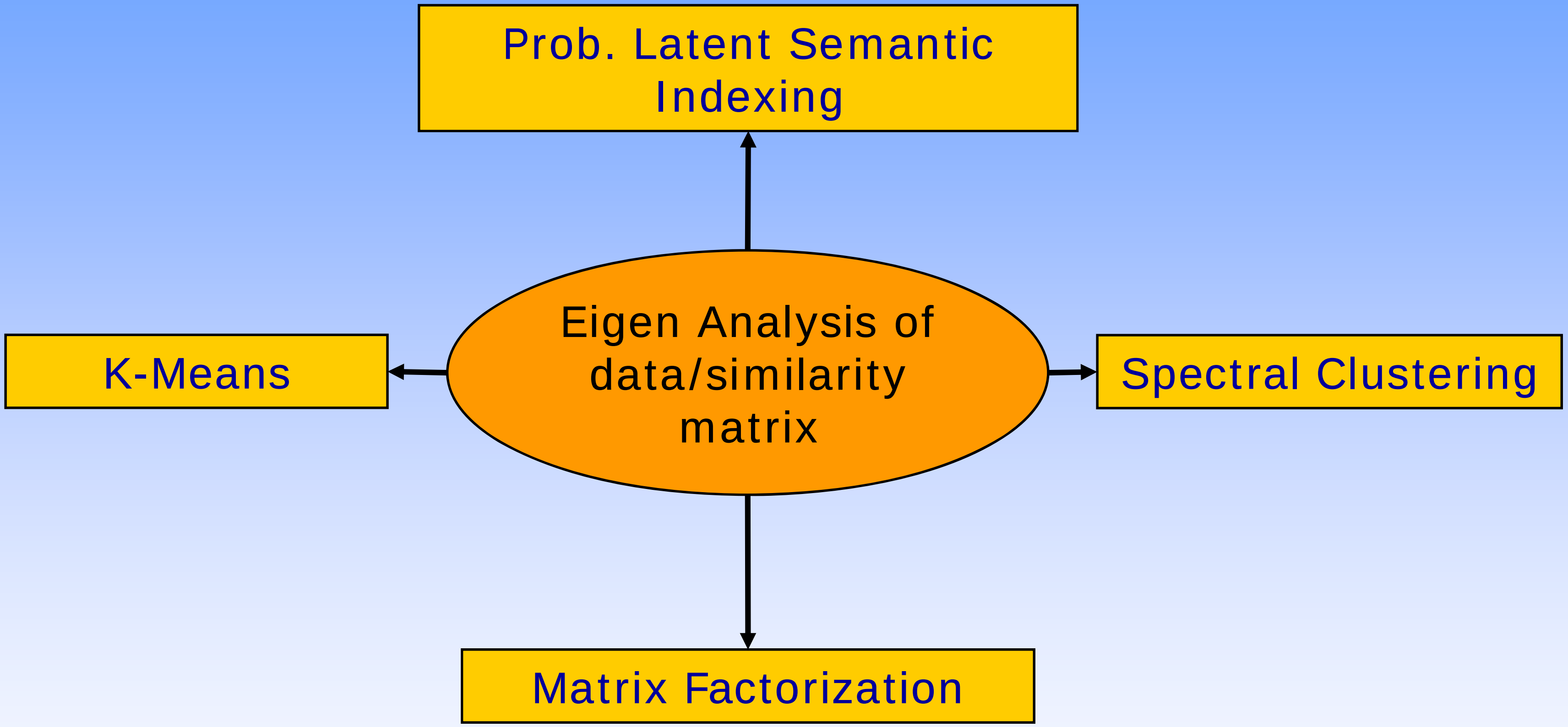
Hierarchical clustering of 35 different algorithms



Chameleon variants

A. K. Jain, A. Topchy, M. Law, J. Buhmann, Landscape of Clustering Algorithms, *ICPR*, 2004

Mathematical & Statistical Links


Prob. Latent Semantic Indexing
K-Means
Eigen Analysis of data/similarity matrix
Spectral Clustering
Matrix Factorization

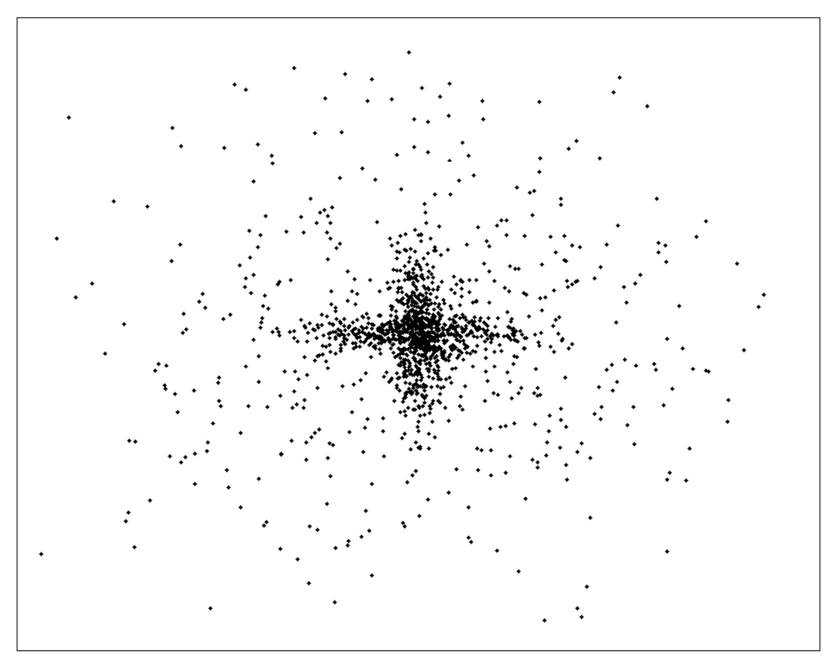
Zha et al., 2001; Dhillon et al., 2004; Gaussier et al., 2005, Ding et al., 2006; Ding et al., 2008

Admissibility Criteria

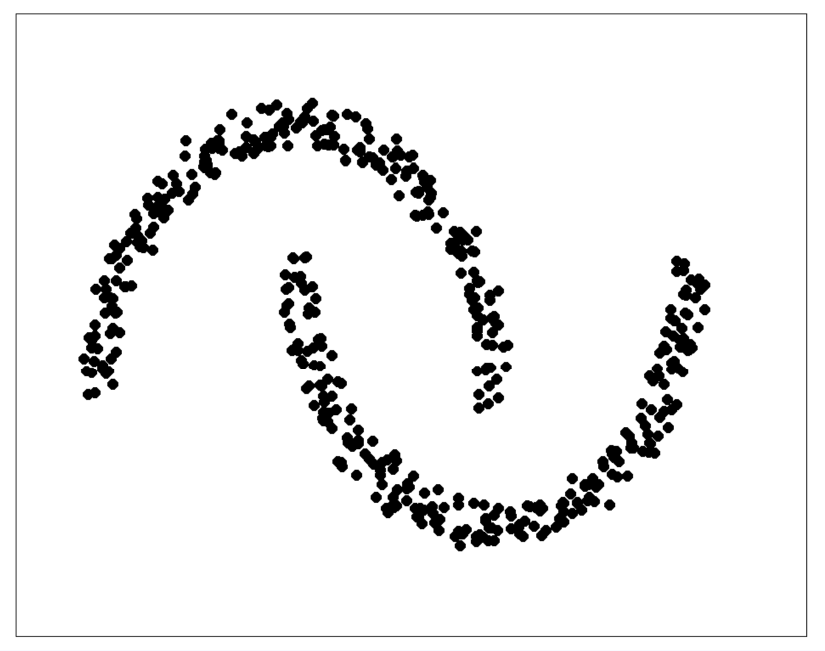
- A technique is P-admissible if it satisfies a desirable property P (*Fisher & Van Ness, Biometrika, 1971*)
- Properties that test sensitivity w.r.t. changes that do not alter the essential structure of data: point & cluster proportion, cluster omission, monotone
- Could be used to eliminate obviously bad methods
- Impossibility theorem (*Kleinberg, NIPS 2002*); no clustering function satisfies all three properties: scale invariance, richness and consistency

No Best Clustering algorithm!

- Each algorithm imposes a structure on data
- Good fit between model & data => success



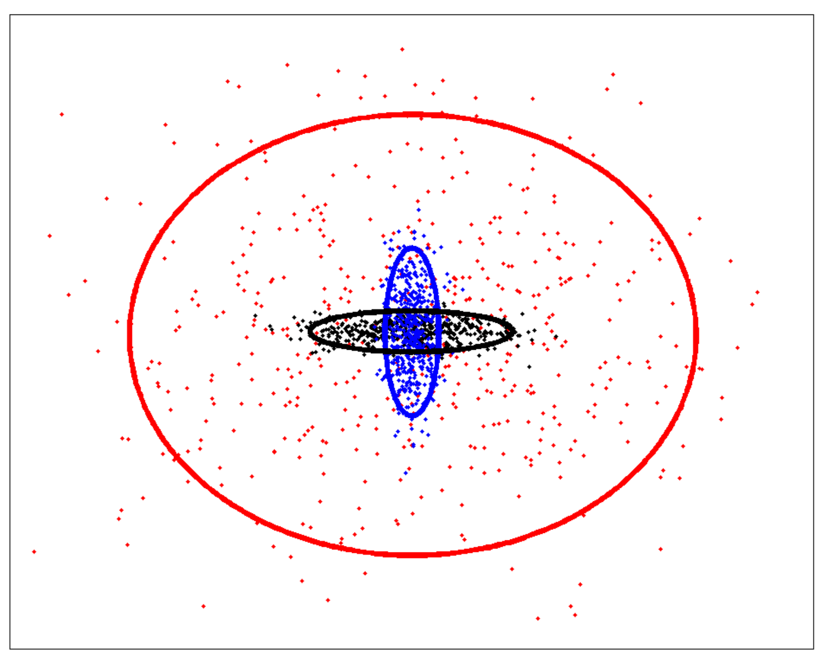
Mixture of 3 Gaussians



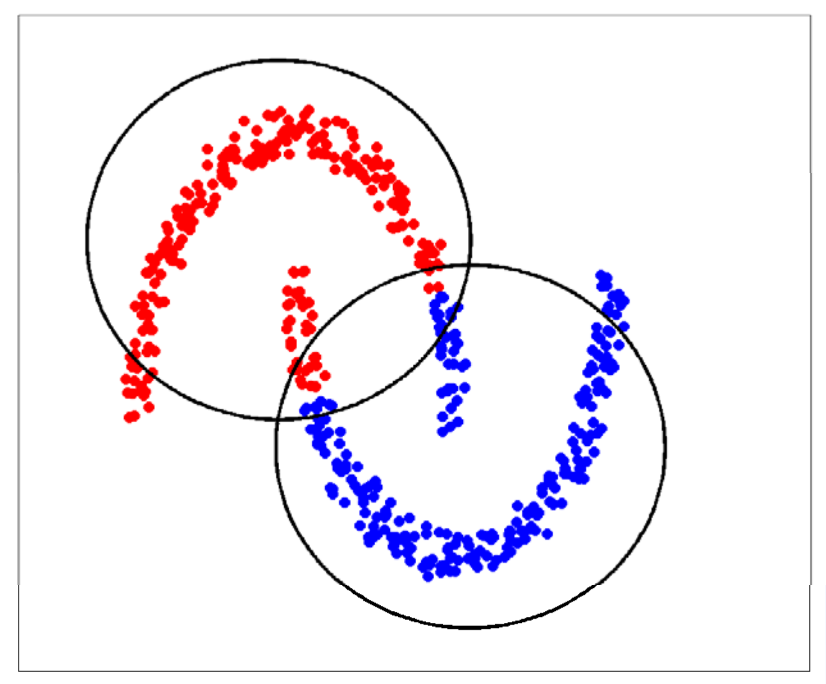
Two “half rings”

No Best Clustering algorithm!

- Each algorithm imposes a structure on data
- Good fit between model & data => success



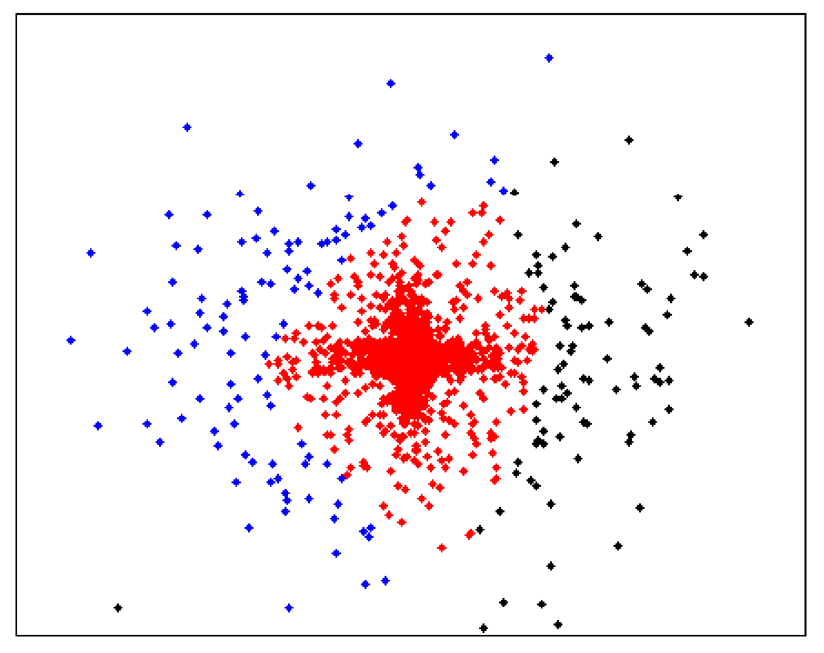
GMM; K = 3



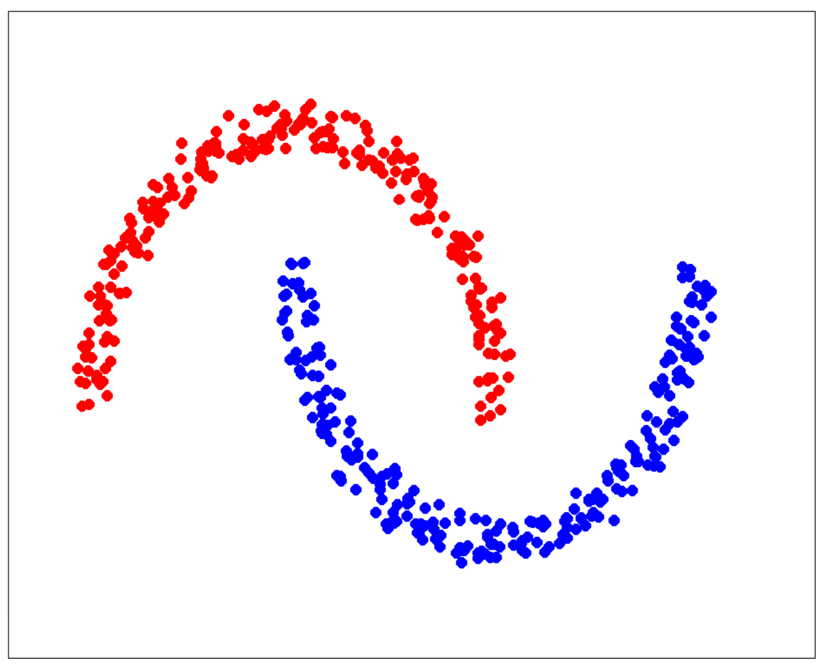
GMM; K = 2

No Best Clustering algorithm!

- Each algorithm imposes a structure on data
- Good fit between model & data => success



Spectral; K = 3



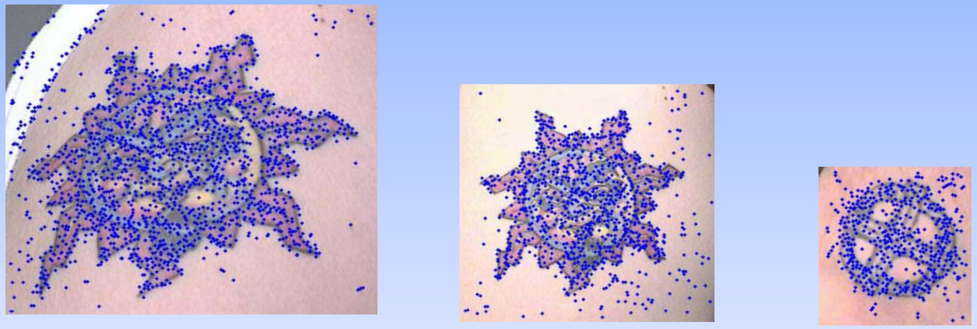
Spectral; K = 2

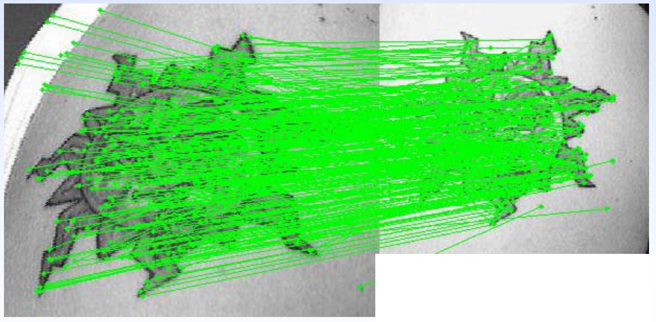
Some Trends

- Large-scale data
  - Clustering of 1.5B images into 50M clusters *(Liu et al., WACV 2007)*
- Evidence Accumulation
  - Combining multiple partitions (different algorithms, parameters, representations)
- Domain Knowledge
  - Pair-wise constraints, feature constraints (e.g., WordNet)
- Multi-way clustering
  - Simultaneously cluster documents, words and authors
- Complex Data Types
  - Dynamically evolving data (data streams)
  - Networks/graphs/tree (similarity matrix for structured data?)

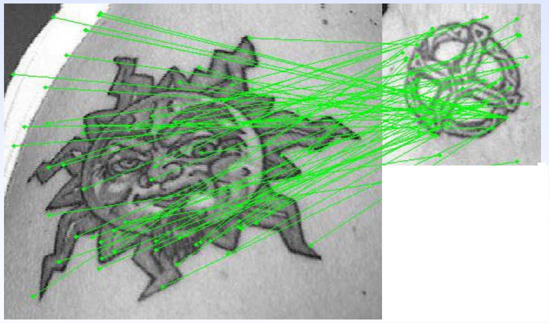
Content-based Image Retrieval

- Given a query image, retrieve visually similar images
- Key-point based CBIR: Image similarity based on the number of matching SIFT key points; ~1000 key points/image





370 matching points



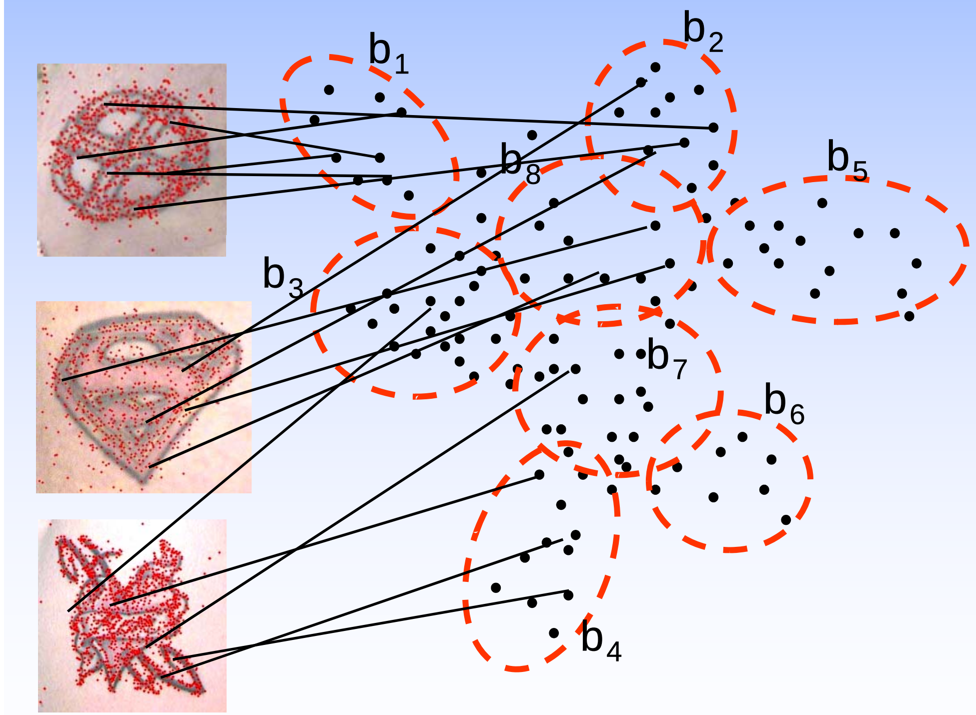
64 matching points

Large Image Database: Challenges

- A database with 10 million images
- Matching between two images ~ 10 msec.
- Linear scanning: 30 hours to answer one query!
- Text retrieval is much more efficient
  - – 0.1 sec. to search 10 billion docs in Google
- Solution: convert CBIR to text retrieval problem *(Sivic & Zisserman, ICCV 2003)*

Text Retrieval for CBIR

- Key points → visual words
  - Group key points from all the images into a number of clusters
  - Each cluster is a visual word
- Bag-of-words representation for images



Bag of key points

Visual word	b_1	b_2	b_3	b_4	b_5	...
	5	2	0	0	0	…
	0	1	3	0	0	…
	0	0	1	4	0	…
…	…	…	…	…	…	…

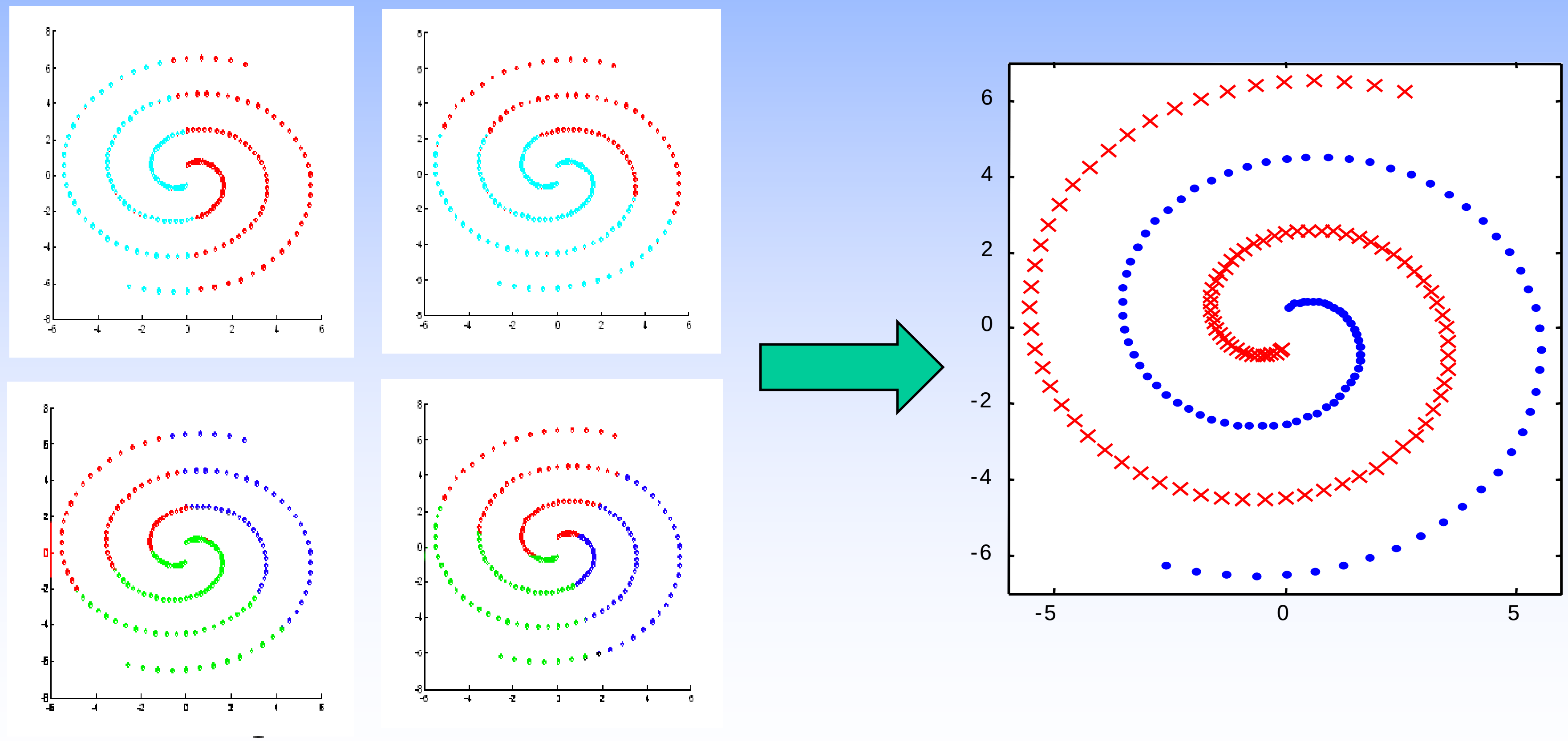
Bag of words

Large-scale Clustering

- Challenges in clustering key points
  - Very large number of key points: 10 million images x 1000 key points → 10 billion key points!
  - Very large number of clusters: 100K ~ 1 million clusters
  - Requires efficient clustering algorithms
- Efficient K-means clustering
  - Find the closest cluster center efficiently
  - Large no. of key points by KD-tree *(Moore, NIPS 1998)*
  - Large no. of clusters by KD-tree *(Philbin et al., CVPR 2007)*

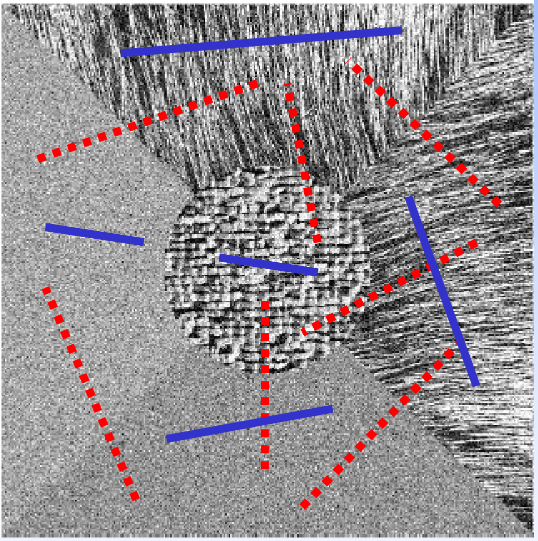
Clustering Ensemble

- Combine many “weak” partitions to generate a better partition *(Fred & Jain, 2002; Strehl & Ghosh, 2002)*
- Pairwise co-occurrences from K-Means partitions



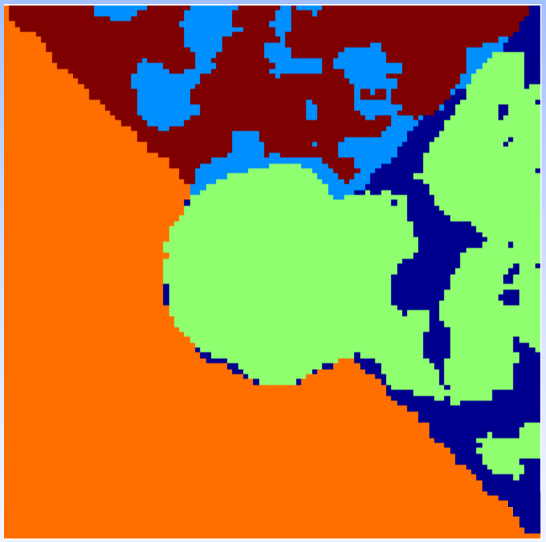
Semi-supervised Clustering

- Improve the partition given domain knowledge
- Side information: pair-wise constraints

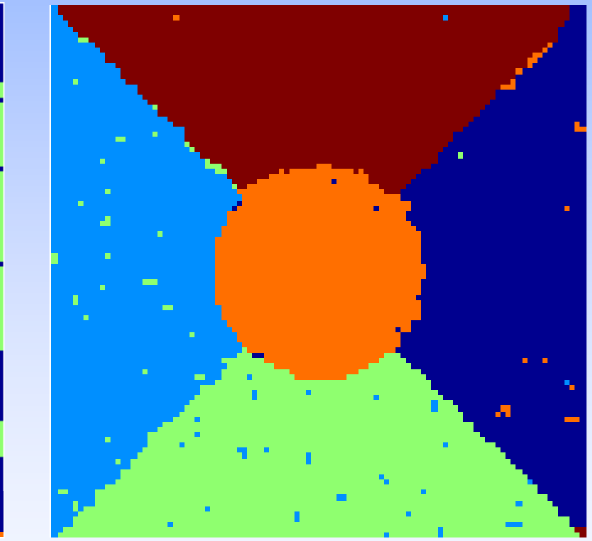


Input Image & constraints

▪▪▪▪ Must-not link ▬ Must link



No constraints

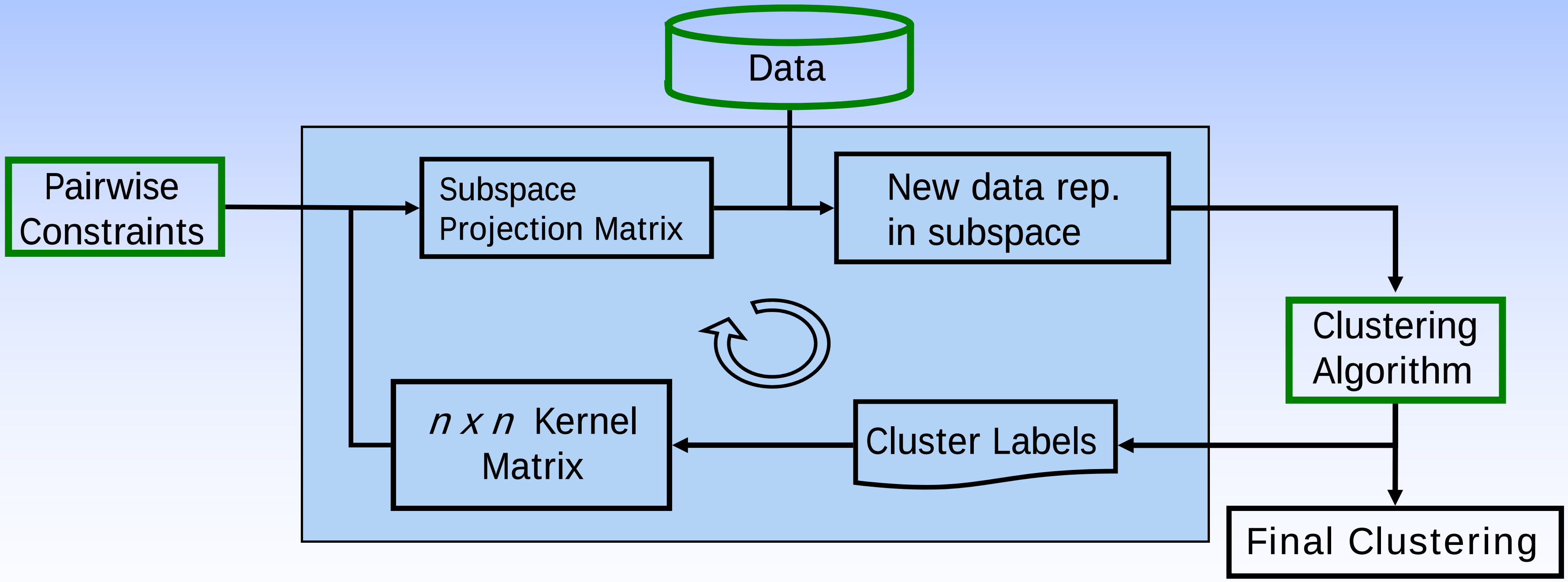


10% pixels in constraints

Lange, Law, Jain & Buhman, CVPR, 2005

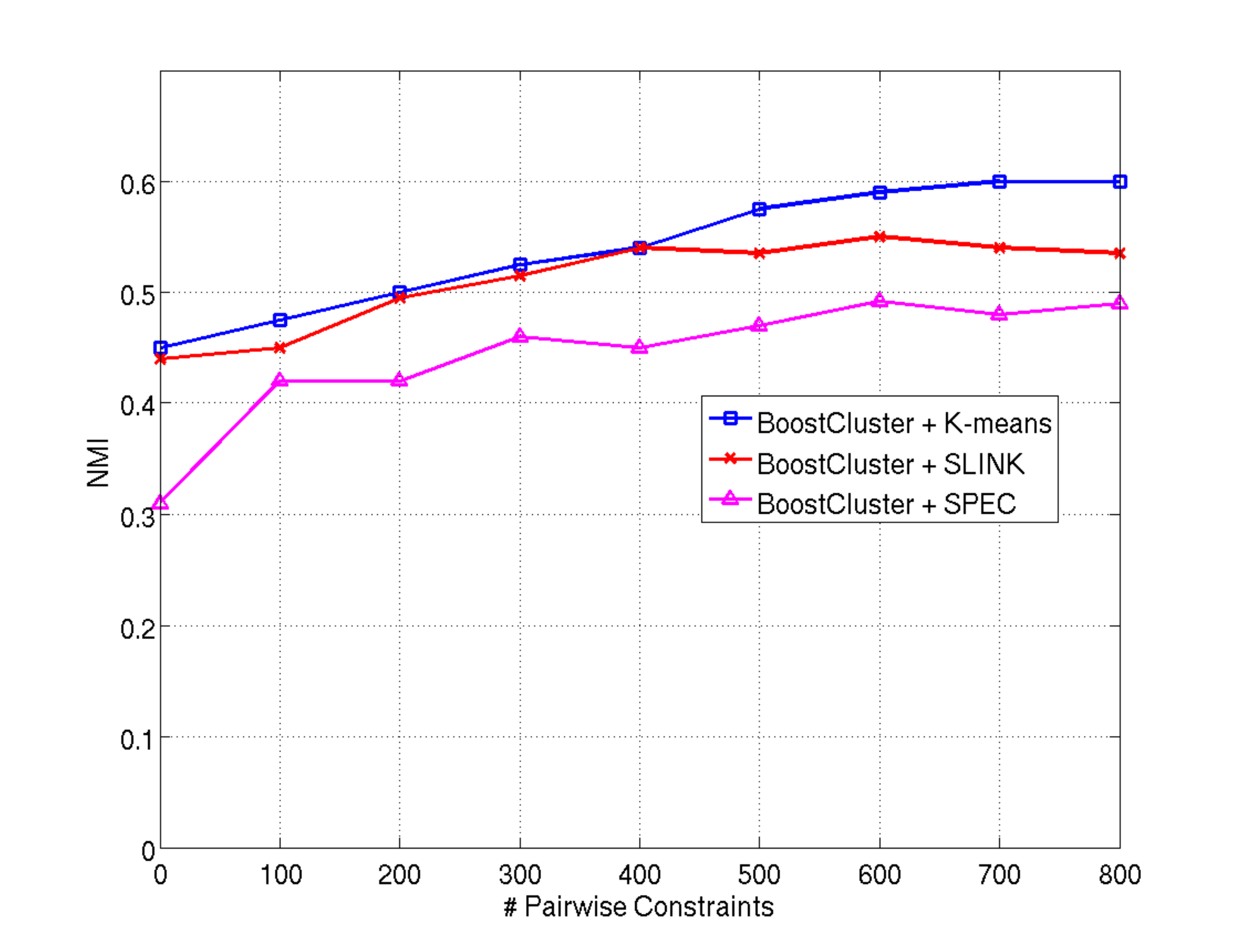
BoostCluster

- Instead of designing new objective fn. improve any given clustering algorithm
- Unsupervised boosting algorithm iteratively updates the similarity matrix input to clustering



Liu, Jin & Jain, BoostCluster: Boosting Clustering by Pairwise Constraints, *KDD*, 2007

Performance of BoostCluster



Handwritten digit (UCI); 4,000 points in 256 dimensions; 10 clusters

Summary

- Organizing data into sensible groupings arises naturally in many fields
- Cluster analysis is an exploratory tool
- Thousand of algorithms; no best algorithm
- Challenges: representation & similarity; domain knowledge; validation; rational basis for comparing methods, large databases, multiple looks at the same data
- K-means continues to be popular & admissible
- No Silver Bullet!

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