The Global Kernel *k*-Means Clustering Algorithm

Grigorios Tzortzis and Aristidis Likas

Department of Computer Science
University of Ioannina, Greece

Clustering

- Partition of a dataset into homogeneous groups

Given a dataset $X = \{x_1, x_2, \ldots, x_N\}$ of objects

we aim to partition this dataset into M disjoint clusters $C_1, C_2, \ldots, C_M$

- When the objects are data vectors, the most well-known algorithm for the above task is k-Means

k-Means

- Each cluster C_k is represented by its center $\boldsymbol{m}_k$ (mean of the cluster elements)
- Finds local minima w.r.t. the clustering error

$$E(\boldsymbol{m}_1, \ldots, \boldsymbol{m}_M) = \sum_{i=1}^{N} \sum_{k=1}^{M} I(x_i \in C_k) \|x_i - \boldsymbol{m}_k\|^2$$

  - (sum of cluster variances)
- Drawbacks
  - ✘ Highly dependent on the initial positions of the centers
  - ✘ Identifies only linearly separable clusters
- Improvements
  - √ Multiple restarts, Global *k*-Means (Likas et al. [2003])
  - √ Kernel *k*-Means

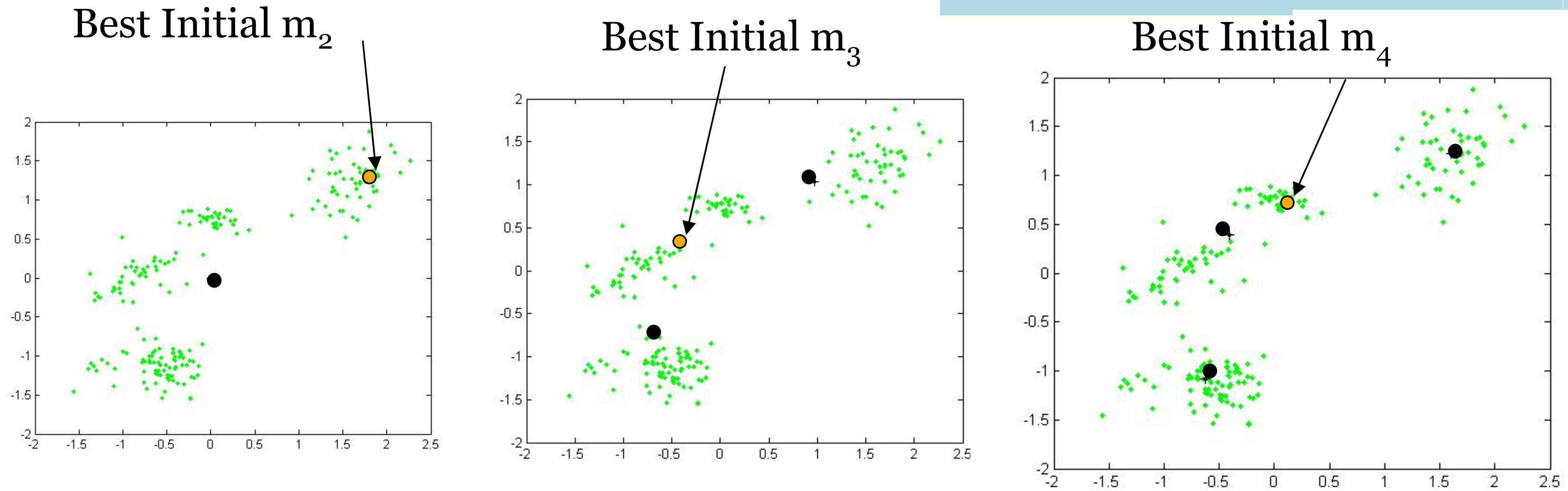
Global *k*-Means

- An incremental, deterministic clustering algorithm that runs *k*-Means several times
- Finds near-optimal solutions wrt clustering error

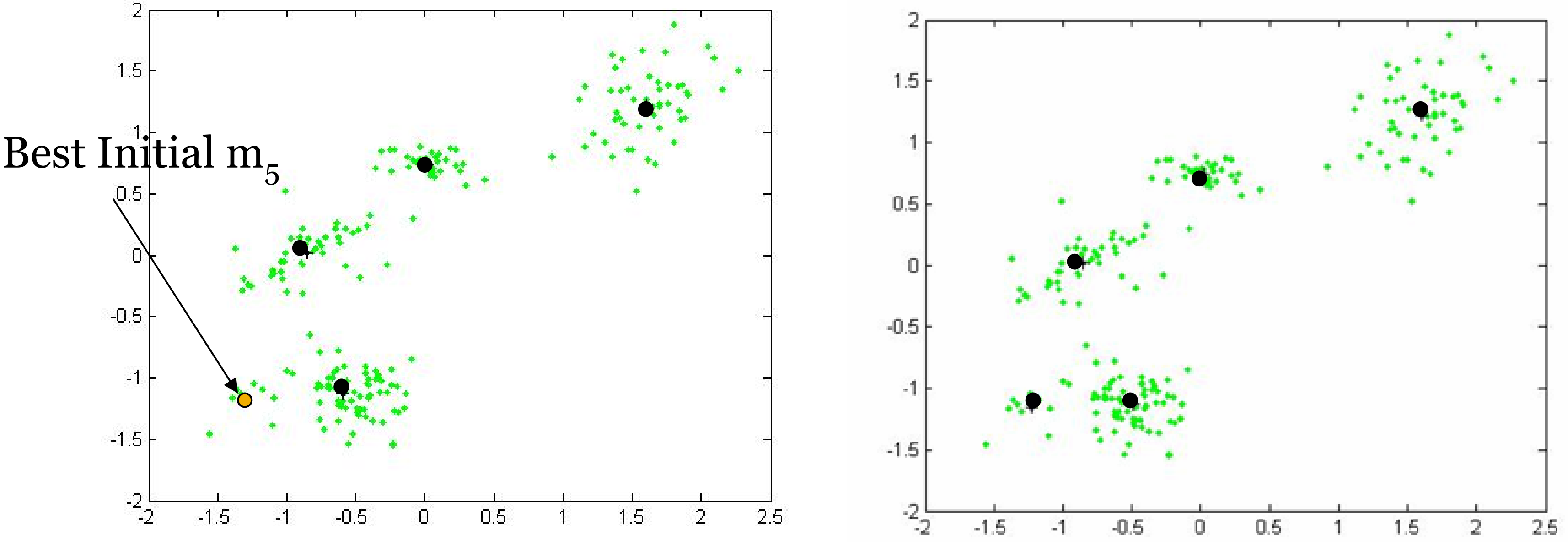
- Idea: a near-optimal solution for k clusters can be obtained by running k-means from an initial state

$$(m_1, m_2, \ldots, m_{k-1}, x_n)$$

  - the k-1 centers are initialized from a near-optimal solution of the (k-1)-clustering problem $(m_1, m_2, \ldots, m_{k-1})$
  - the k-th center is initialized at some data point $\boldsymbol{x}_n$ (which?)
- Consider all possible initializations (one for each $\boldsymbol{x}_n$)



Orange circles: optimal initial position of the cluster center to be added



Global *k*-Means - Algorithm

In order to solve the *M*-clustering problem:

1. Solve the 1-clustering problem (trivial)
2. Solve the *k*-clustering problem using the solution of the (k-1)-clustering problem $(m_1, m_2, \ldots, m_{k-1})$
   a) Execute *k*-Means *N* times, initialized as $(m_1, m_2, \ldots, m_{k-1}, x_n)$ at the *n*-th run (n=1,…,N).
   b) Keep the solution corresponding to the run with the lowest clustering error as the solution with *k* clusters $(m_1, m_2, \ldots, m_k)$
3. k:=k+1, Repeat step 2 until k=M.

✓Avoids the initialization problem of *k*-Means

✓Locates near optimal partitions w.r.t. clustering error

✓All intermediate solutions for k=1, …, *M-1* are also found: useful when searching for the number of clusters

▪Requires *MN* runs of *k*-Means to find *M* clusters

Kernel *k*-Means

- Data points are mapped from input space to a higher dimensional feature space through a transformation ϕ

Kernel *k*-Means ≡ *k*-Means in feature space

√ Identifies non-linearly separable clusters in input space

- Minimizes the clustering error in feature space

$$E(\boldsymbol{m}_1, \ldots, \boldsymbol{m}_M) = \sum_{i=1}^{N} \sum_{k=1}^{M} I(\boldsymbol{x}_i \in C_k) \| \phi(\boldsymbol{x}_i) - \boldsymbol{m}_k \|^2 \text{ where } \boldsymbol{m}_k = \frac{\sum_{i=1}^{N} I(\boldsymbol{x}_i \in C_k) \phi(\boldsymbol{x}_i)}{\sum_{i=1}^{N} I(\boldsymbol{x}_i \in C_k)}$$

Kernel *k*-Means

- Kernel trick
  - A kernel function corresponds to the inner products in feature space i.e. $K_{ij} = \phi^T(\mathbf{x}_i)\phi(\mathbf{x}_j),\ \|\phi(\mathbf{x}_i) - \phi(\mathbf{x}_j)\|^2 = K_{ii} + K_{jj} - 2K_{ij}$
  - Computation of distances from centers in feature space:

$$\|\phi(\boldsymbol{x}_i) - \boldsymbol{m}_k\|^2 = K_{ii} - \frac{2\sum_{j=1}^{N} I(\boldsymbol{x}_j \in C_k) K_{ij}}{\sum_{j=1}^{N} I(\boldsymbol{x}_j \in C_k)} + \frac{\sum_{j=1}^{N}\sum_{l=1}^{N} I(\boldsymbol{x}_j \in C_k) I(\boldsymbol{x}_l \in C_k) K_{jl}}{\sum_{j=1}^{N}\sum_{l=1}^{N} I(\boldsymbol{x}_j \in C_k) I(\boldsymbol{x}_l \in C_k)}$$

  - No need to explicitly define transformation ϕ
- Difference from k-means
  - The cluster centers are not explicitly defined
  - Each cluster C_k is described by its training data

- Finds local minima - Strong dependence on initialization

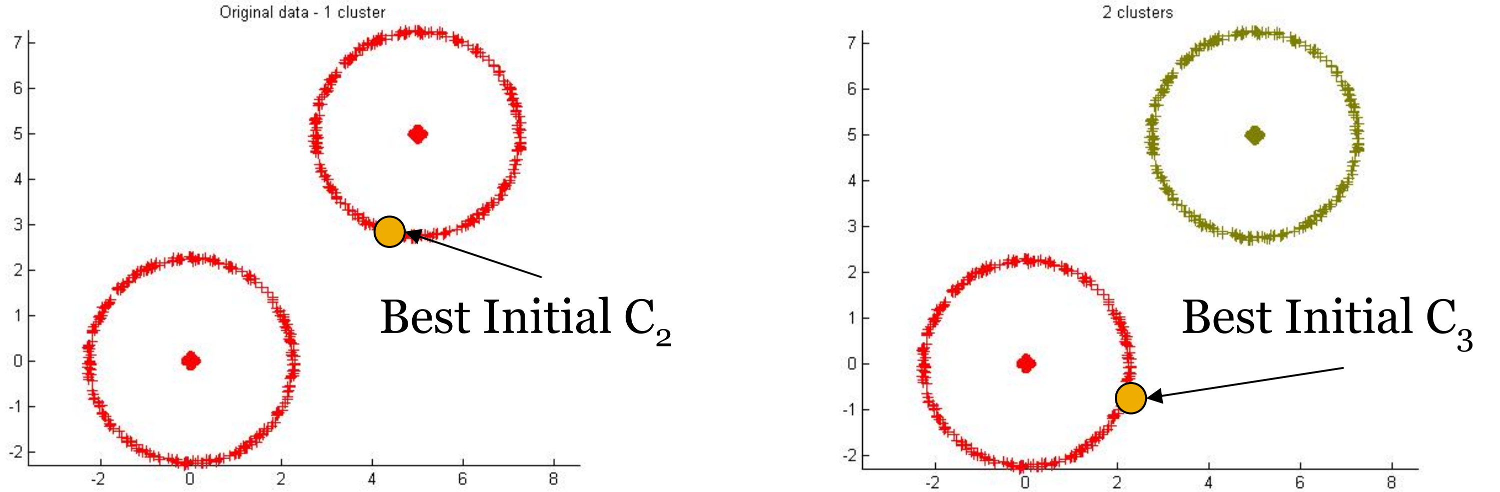
Global Kernel *k*-Means

Based on the ideas of the Global *k*-Means and Kernel *k*-Means algorithms we propose the Global Kernel *k*-Means algorithm

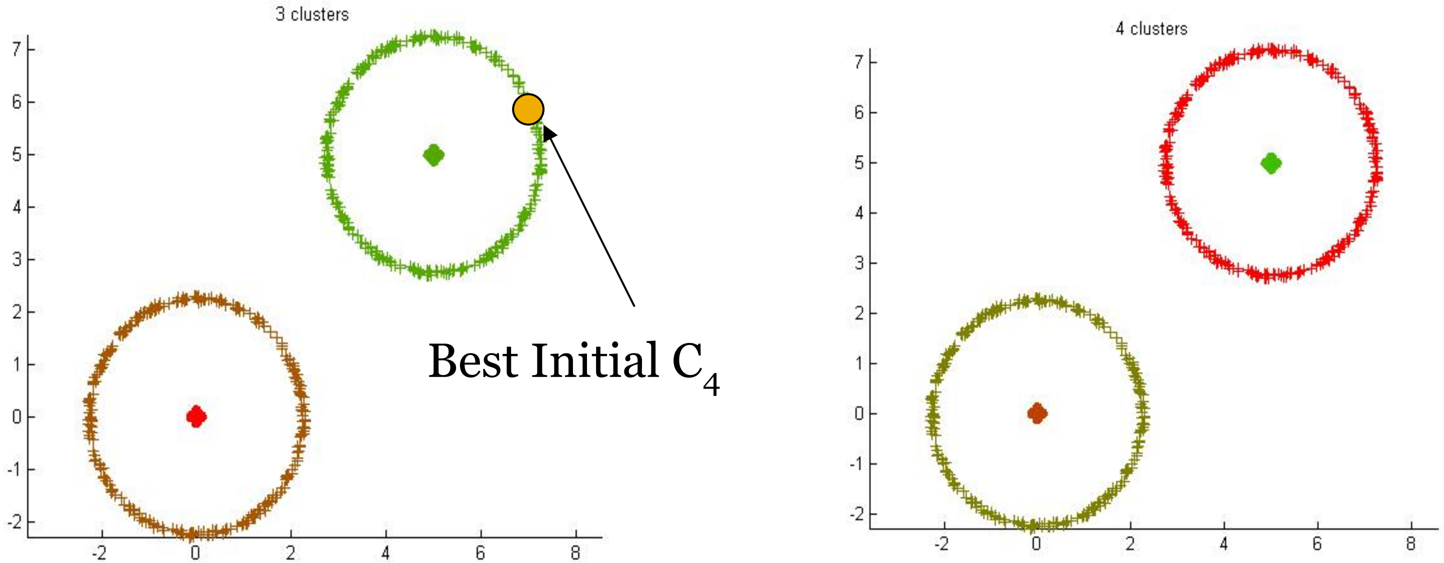
- An incremental deterministic algorithm that employs Kernel *k*-Means as a local search procedure
  - At each stage of the algorithm a new cluster is added as in Global *k*-Means
- Main idea
  - Given a near-optimal solution $(C_1, C_2, \ldots, C_{k-1})$ with k-1 clusters:
    - A near-optimal solution with *k* clusters can be obtained by running kernel k-means from an initial state

$$(C_1, \ldots, C_l := C_l - \{\mathbf{x}_n\}, \ldots, C_{k-1}, C_k = \{\mathbf{x}_n\}) \quad \mathbf{x}_n \in C_l$$

  - Which $\mathbf{x}_n$? Check all possible initializations (one for each $\mathbf{x}_n$)



Orange circles: optimal initialization of the cluster to be added



Global Kernel *k*-Means - Algorithm

In order to solve the *M*-clustering problem:

1. Solve the 1-clustering problem with Kernel *k*-Means (trivial solution)
2. Solve the *k*-clustering problem using the solution to the (k-1)-clustering problem
   a) Let $(C_1, C_2, \ldots, C_{k-1})$ denote the solution to the (*k*-1)-clustering problem
   b) Execute Kernel *k*-Means *N* times, initialized during the *n*-th run as

$$(C_1, \ldots, C_l := C_l - \{\mathbf{x}_n\}, \ldots., C_{k-1}, C_k = \{\mathbf{x}_n\}) \quad \mathbf{x}_n \in C_l$$

   c) Keep the run with the lowest clustering error as the solution with *k* clusters $(C_1, C_2, \ldots, C_k)$
   d) k := k+1

3. Repeat step 2 until k=M.

Global Kernel *k*-Means

- Advantages
  - √ Initialization independent
  - √ Finds near optimal solutions w.r.t the clustering error in feature space.
  - √ Identifies non-linear separable clusters in input space

- When solving the M-clustering problem the solutions with 1, …, M clusters are also found

- Increased Complexity
  - To solve for M clusters we must run Kernel k-Means MN times

Fast Global Kernel *k*-Means

Global Kernel *k*-Means complexity is high for large datasets ⟶ we propose a speeding up scheme: <u>Fast Global Kernel *k*-Means</u>

- How is the complexity reduced?
  - To add a new cluster *k* given the solution for the (*k*-1)-clustering problem, instead of executing Kernel *k*-Means *N* times, it is executed only once from state

$$(C_1,\ldots,C_l := C_l - \{\mathbf{x}_{n^*}\},\ldots,C_{k-1},C_k = \{\mathbf{x}_{n^*}\}) \quad \mathbf{x}_{n^*} \in C_l$$

  - $\mathbf{x}_{n^*}$ provides the greatest reduction in clustering error in the first iteration of kernel k-means

Fast Global Kernel *k*-Means - Details

- $C_k = \{\mathbf{x}_n\}, \quad \mathbf{m}_k = \phi(\mathbf{x}_n)$
- C_k allocates all points $\mathbf{x}_i$ that are closer (in feature space) to $\mathbf{x}_n$ than to their cluster center (in the solution with (*k*-1) clusters): $\|\phi(\mathbf{x}_i) - \phi(\mathbf{x}_n)\|^2 < d_i$
- d_i is the distance in feature space between $\mathbf{x}_i$ and its cluster center in the (*k*-1)-clustering solution
- The reduction in clustering error due to the reallocation is

$$b_n = \sum_{i=1}^{N} \max(d_i - \|\phi(\mathbf{x}_n) - \phi(\mathbf{x}_i)\|^2, 0)$$

- $$n^* = \arg\max b_n$$
- Run Kernel *k*-Means <u>once</u> from initial partition

$$(C_1, \ldots, C_l := C_l - \{\mathbf{x}_{n^*}\}, \ldots, C_{k-1}, C_k = \{\mathbf{x}_{n^*}\}) \quad \mathbf{x}_{n^*} \in C_l$$

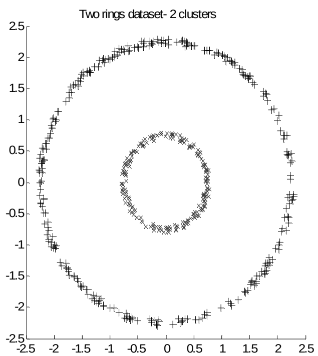
Experimental Evaluation

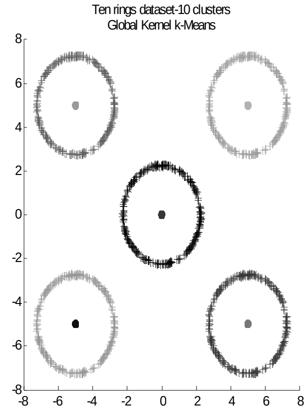
- We compared Global Kernel *k*-Means, Fast Global Kernel *k*-Means and Kernel *k*-Means with multiple restarts
  - On artificial data
  - On MRI segmentation

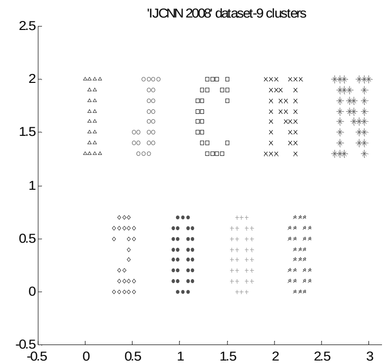
- Global Kernel *k*-Means and the fast version were run once
- Kernel *k*-Means was restarted 100 times
- We compared the algorithms in terms of clustering error

Artificial Datasets

- We created three datasets
  - i) Two rings dataset (2 clusters), ii) five copies of two rings (10 clusters), iii) ‘IJCNN 2008’ logo (9 clusters)



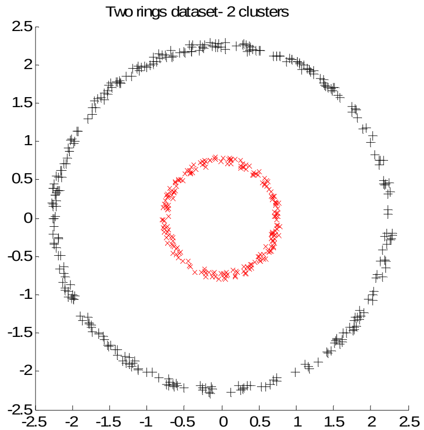




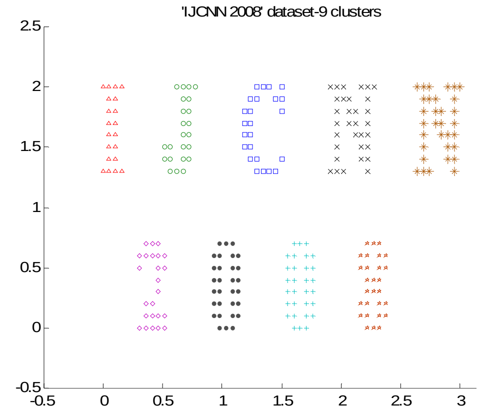
- In all the experiments we used a Gaussian kernel

$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 /(2\sigma^2)\right)$$

Artificial Datasets - Results



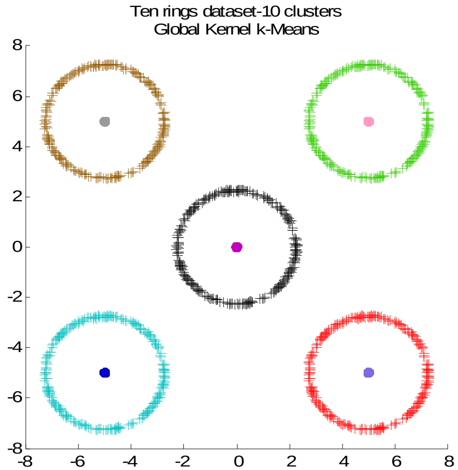
Method/Dataset		Two Rings $\sigma = 1$	Ten Rings $\sigma = 1.8$	'IJCNN 2008' $\sigma = 0.7$
Global kernel *k*-means		**320.17**	**966.87**	**27.97**
Fast global kernel *k*-means		**320.17**	1073.18	**27.97**
Kernel *k*-means (100 runs)	**Mean**	334.4	1107.97	37.72
	Std	6.4	177.24	6.16
	Min	**320.17**	981.53	**27.97**
	Max	351.05	1765.29	63.03



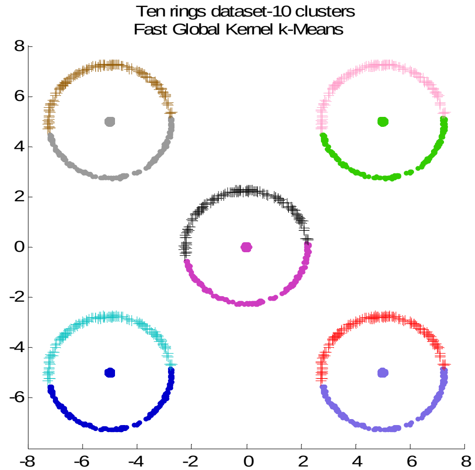
Global Kernel *k*-Means
Fast Global Kernel *k*-Means
Kernel *k*-Means (12/100 runs)

Global Kernel *k*-Means
Fast Global Kernel *k*-Means
Kernel *k*-Means (5/100 runs)

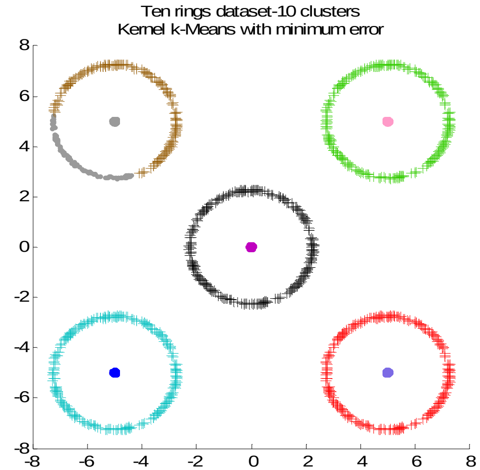
Global Kernel *k*-Means



Fast Global Kernel *k*-Means



Kernel *k*-Means Best run



Artificial Datasets - Conclusions

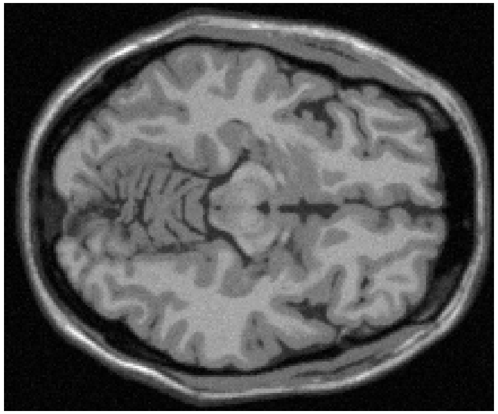
- Global Kernel *k*-Means in all cases finds the solution with the lowest clustering error and identifies the structures present in the dataset
  - This algorithm identifies near optimal solutions

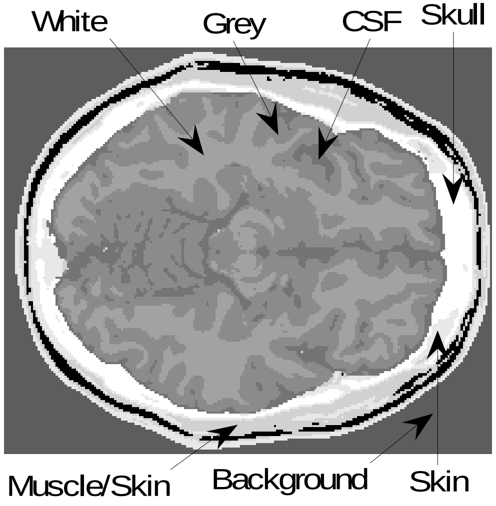
- Performance of fast Global Kernel *k*-Means is very close to the original algorithm except for the second dataset

- Kernel *k*-Means is very sensitive to initializations
  - For the second dataset it never solves the 10 rings
  - During the restarts near optimal but also very bad solutions are found
  - <u>Number of restarts? We are never sure if they suffice</u>

MRI Segmentation

- We used MRI images downloaded from the BrainWeb site (www.bic.mni.mcgill.ca/brainweb/)
  - We segmented slices of a 3-d brain image
  - In those slices seven classes prevail: background, CSF, grey matter, white matter, muscle/skin, skin and skull
  - We performed clustering into 7 clusters
  - The ground truth is also available (class for each pixel)
  - Large datasets: 181 x 217 = 39277 pixels





MRI Segmentation – Kernel Definition

  - Typical approaches cluster each pixel based on its intensity
  - The use of kernel k-means enables the use of additional information: pixel intensity + local histogram

- We used a composite kernel for MRI segmentation:

$$K_{ij} = \exp\left(\frac{-\|I(i) - I(j)\|^2}{2\sigma^2}\right)\left[\sum_{z=1}^{Bins}\sqrt{P_z(i)P_z(j)}\right]$$

Intensity of the i-th pixel

Probability of the z-th bin of pixel's i histogram

-Global Kernel *k*-Means is slow (large dataset)

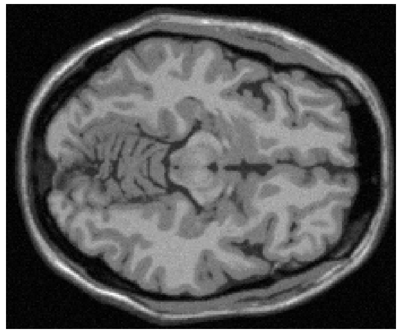
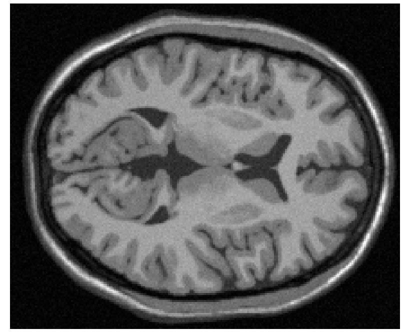
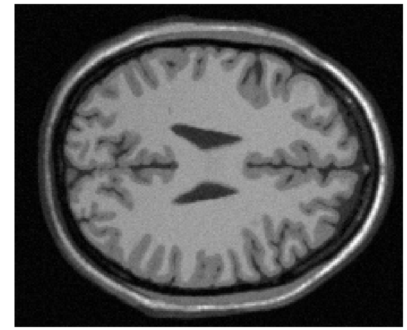
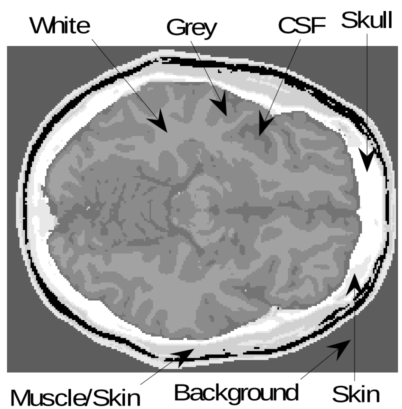
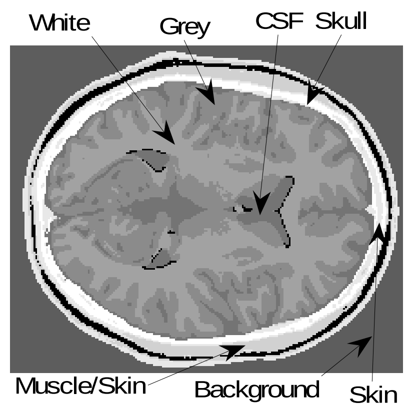
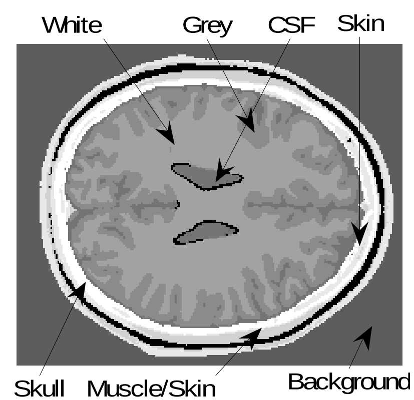
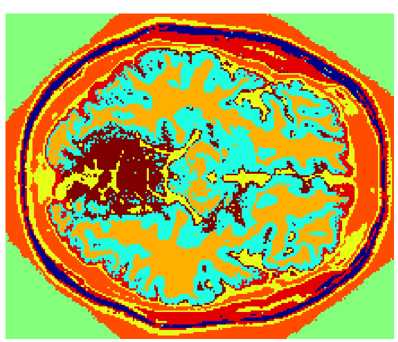
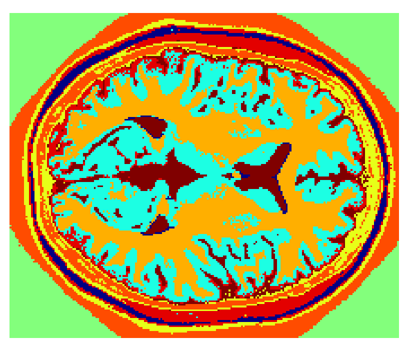
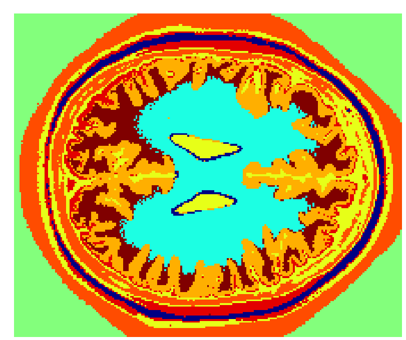
-We compare Fast Global Kernel *k*-Means to Kernel *k*-Means (<u>100 random restarts</u>)

MRI Segmentation - Results

Method/Slice $\sigma = 0.7$ Win=31x31 Bins=70		Slice 60		Slice 80		Slice 100	
		CE	ME	CE	ME	CE	ME
Fast global kernel *k*-means		5208.32	19.89%	5064.99	14.1%	5010.15	15.82%
Kernel *k*-means (100 runs)	**Mean**	5286.95	19.89%	5244.39	14.01%	5094.85	15.97%
	Std	66.29		127.63		141.7	
	Min	5207.65		5064.27		5009.75	
	Max	5364.68		5477.84		5808.77	

- Kernel k-means best: 3, 12, 28 out of 100 runs
- Fast Global Kernel *k*-Means equals the best of Kernel *k*-Means
  - This solution is much better than the average clustering error achieved by Kernel *k*-Means
  - The 100 restarts are 20 times slower than Fast Global Kernel *k*-Means (16 hours vs. 45 minutes)

MRI Segmentation - Examples

	Slice 60	Slice 80	Slice 100
Original MRI			
Ground Truth			
Fast Global kernel *k*-Means			

Conclusions

- We have proposed the Global Kernel k-means:
  - an incremental deterministic approach for clustering in feature space
  - effectively solves the initialization problem of kernel k-means
  - provides near-optimal solutions in terms of the clustering error in feature space
  - Solves all intermediate k-clustering problems for k=1,...,M

- Several techniques can be used to improve computational time
  - fast global kernel k-means
  - Use only a subset with L<<N training data as candidates for the initialization of the new cluster center
  - This subset can be selected through preprocessing using exemplar-based clustering methods (e.g. L-medoids, affinity propagation, convex mixture models).