

Mean-shift Algorithms for Manifold Denoising, Matrix Completion and Clustering



Weiran Wang

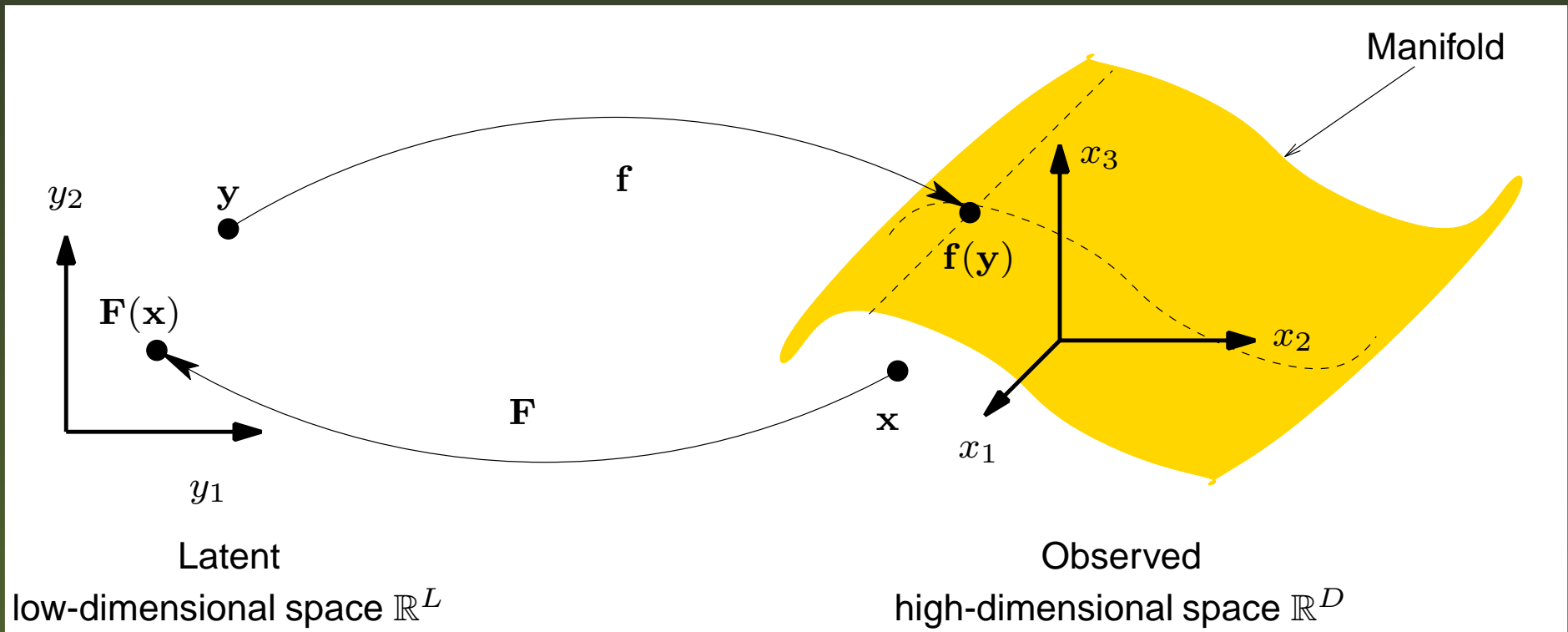
wwang5@ucmerced.edu

EECS Department, UC Merced

Manifold Learning

High dimensional dataset with **manifold structure**.

- ❖ Variations within the dataset can be modeled by a few latent variables.
- ❖ Small variation in latent space leads to small variation in data space.
- ❖ Local neighborhood of each data point can be approximated by a tangent space.



An example: MNIST



Small variations in translation, rotation, scaling and different writing styles change the image appearance slightly, and do not change the identity.

Mean-shift update

Given a set of data points $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N] \subset \mathbb{R}^D$.

- ❖ Maximizes kernel density estimate (mode finding)

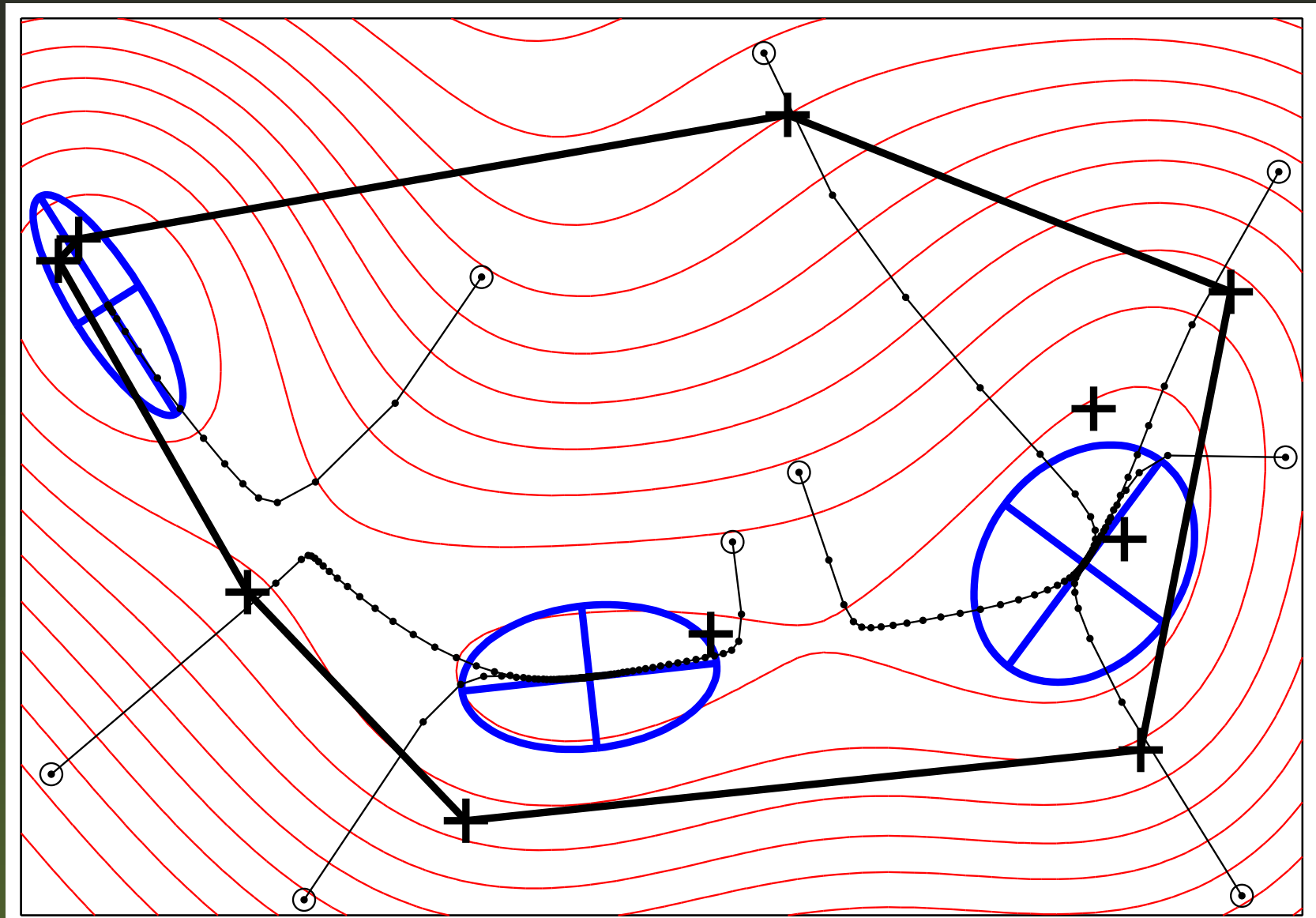
$$p(\mathbf{x}) = \frac{1}{N} \sum_{n=1}^N G\left(\left\|\frac{\mathbf{x} - \mathbf{x}_n}{\sigma}\right\|^2\right), \quad G(t) = e^{-t/2}.$$

- ❖ Applies the mean-shift update (fixed point iteration) iteratively

$$p(n|\mathbf{x}) = \frac{G\left(\left\|\frac{\mathbf{x} - \mathbf{x}_n}{\sigma}\right\|^2\right)}{\sum_{n'=1}^N G\left(\left\|\frac{\mathbf{x} - \mathbf{x}_{n'}}{\sigma}\right\|^2\right)}, \quad \mathbf{x} \leftarrow \mathbf{f}(\mathbf{x}) = \sum_{n=1}^N p(n|\mathbf{x}) \mathbf{x}_n$$

- ❖ Gradient ascent. Linear convergence rate.

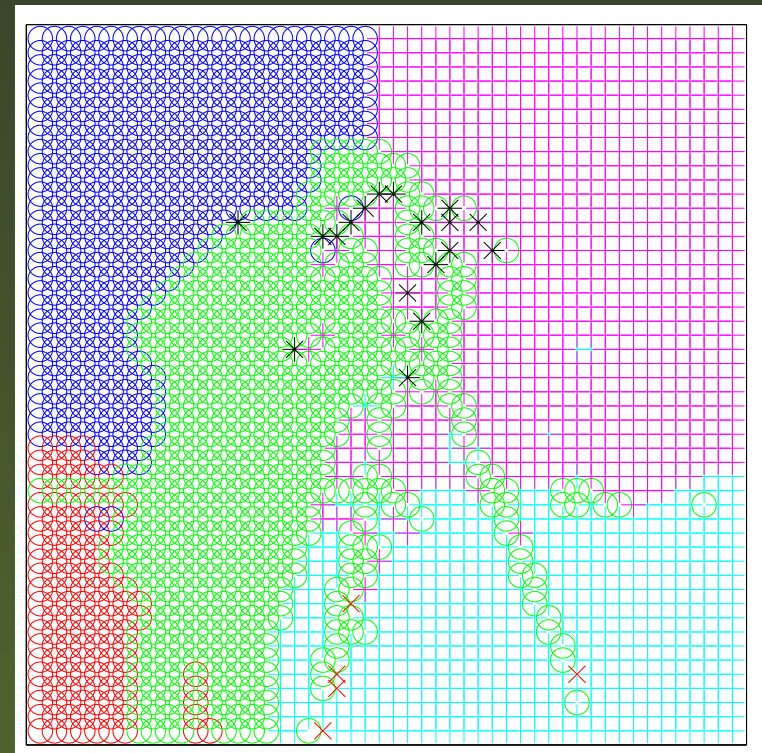
Mean-shift update



Paths followed by GMS for various starting points.

Mean-shift clustering

- ❖ **Gaussian Mean-shift (GMS)**: points that converge to the same mode/centroid define a cluster. Number of clusters depends on σ .
- ❖ **Gaussian Burring Mean-shift (GBMS)**: update dataset after each mean-shift step, has much faster (cubic) convergence rate and strong (isotropic) denoising effect.



Outline

- **Manifold Blurring Mean-shift (MBMS) algorithm for manifold denoising**
- **MBMS for matrix completion**
- **K -modes algorithm for clustering**
- **Laplacian K -modes algorithm for clustering**

Motivation

We develop an algorithm that denoises the dataset, and acts as a **preprocessing** step for unsupervised/supervised learning.

$\tau = 0$

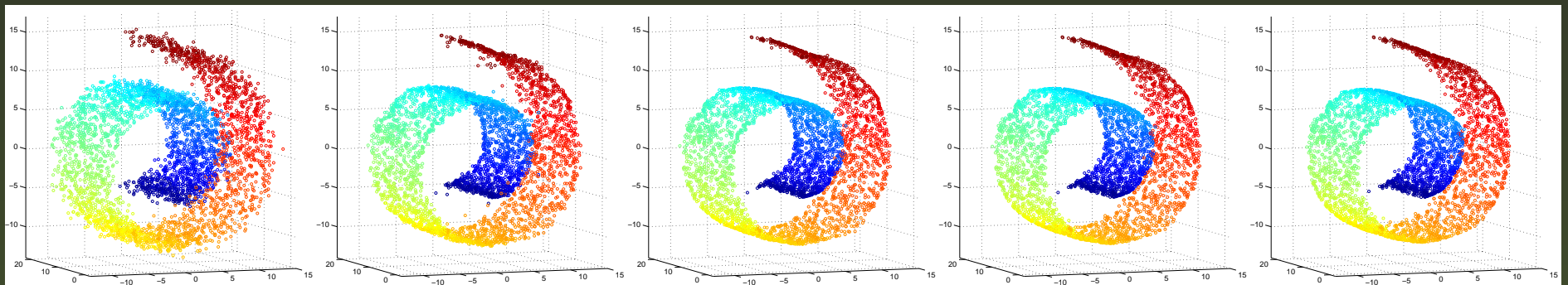
$\tau = 1$

$\tau = 2$

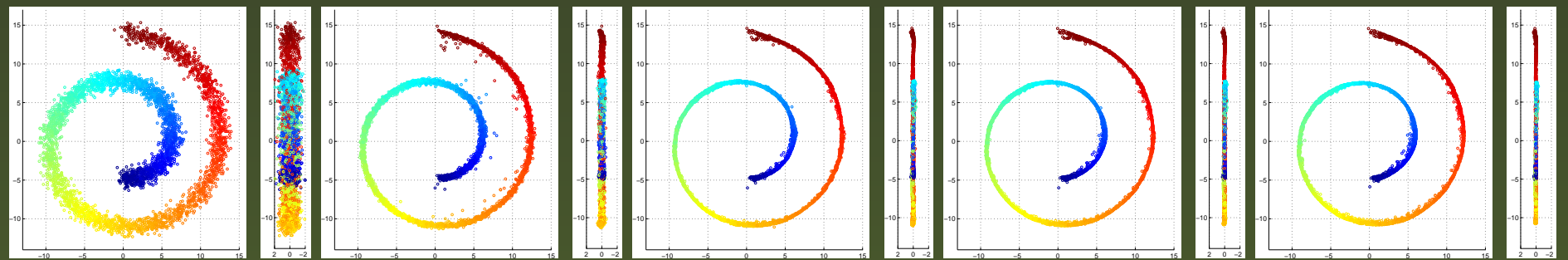
$\tau = 3$

$\tau = 5$

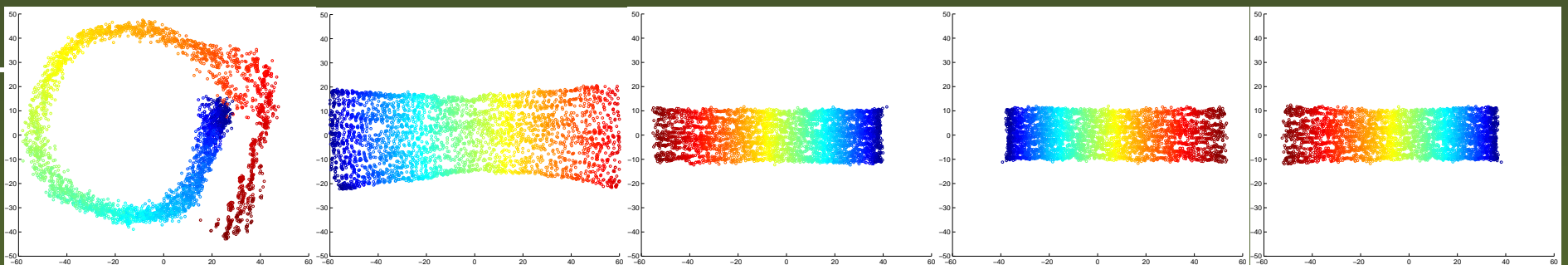
view 0



view 1



Isomap



Manifold Blurring Mean-Shift

- ❖ **Predictor averaging step:** local clustering with GBMS, moves data point to the kernel average of its neighbors

$$\mathbf{x}_n \leftarrow \sum_{m \in \mathcal{N}_n} \frac{G(\|(\mathbf{x}_n - \mathbf{x}_m)/\sigma\|^2)}{\sum_{m' \in \mathcal{N}_n} G(\|(\mathbf{x}_n - \mathbf{x}_{m'})/\sigma\|^2)} \mathbf{x}_m$$

- ❖ **Corrector projective step:** estimate local tangent space with PCA, gives the best linear L -dimensional manifold in terms of reconstruction error (orthogonal projection on the manifold)

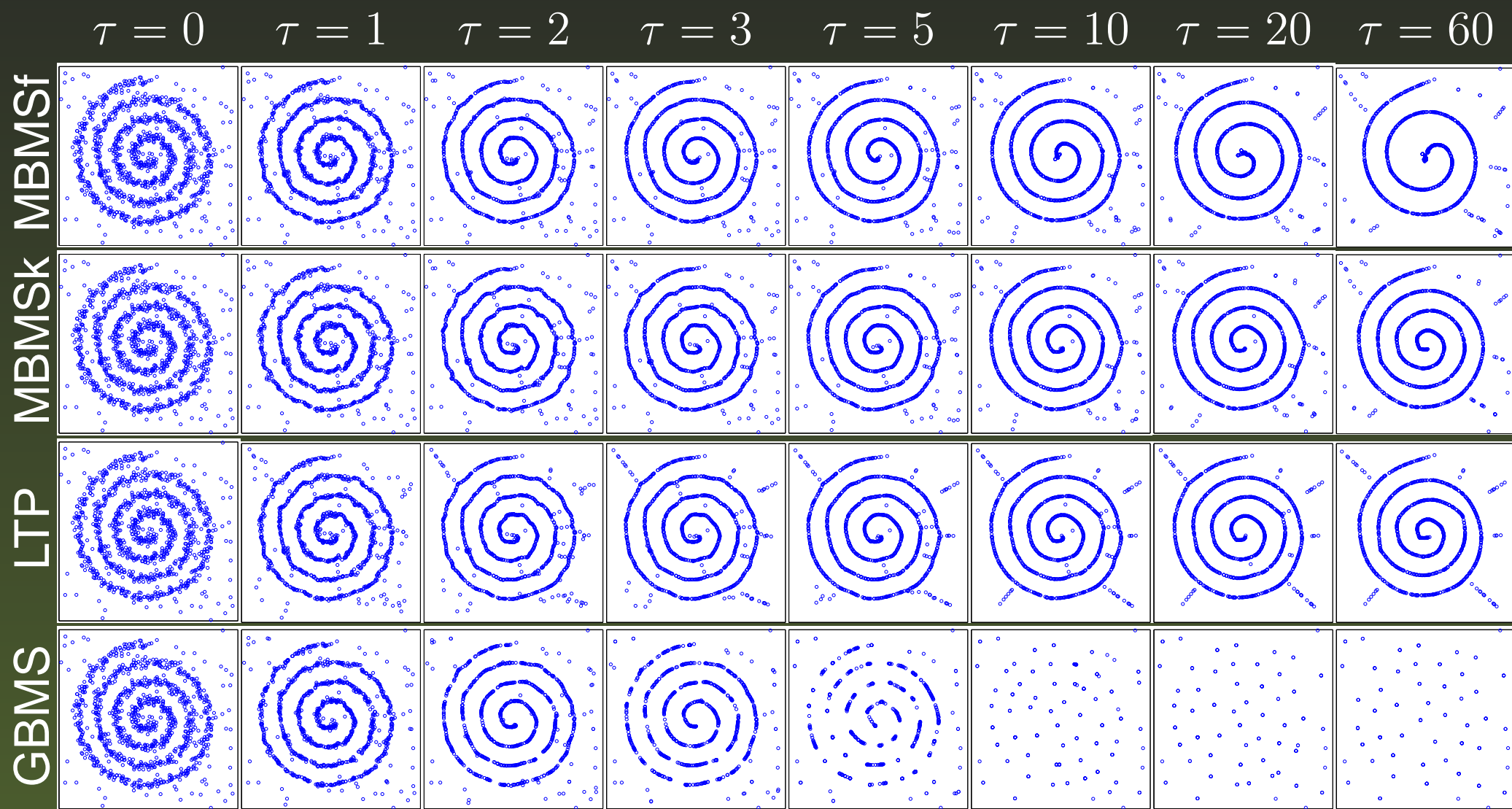
$$\min_{\mu, \mathbf{U}} \sum_{m \in \mathcal{N}'_n} \|\mathbf{x}_m - (\mathbf{U}\mathbf{U}^T(\mathbf{x}_m - \mu) + \mu)\|^2$$

- ❖ User parameters: σ , K , L .

Practicalities

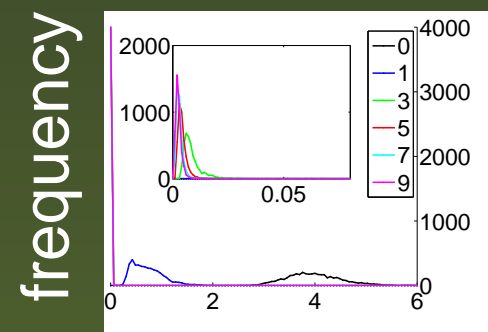
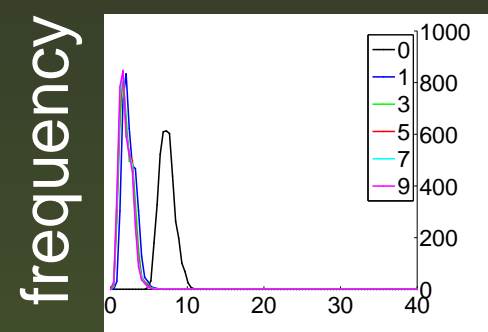
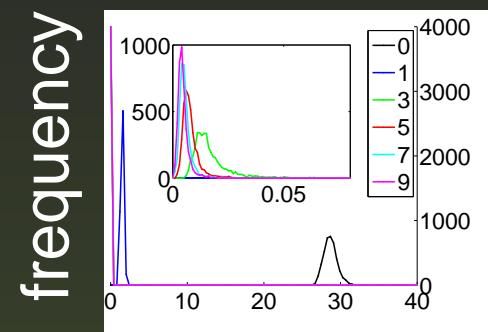
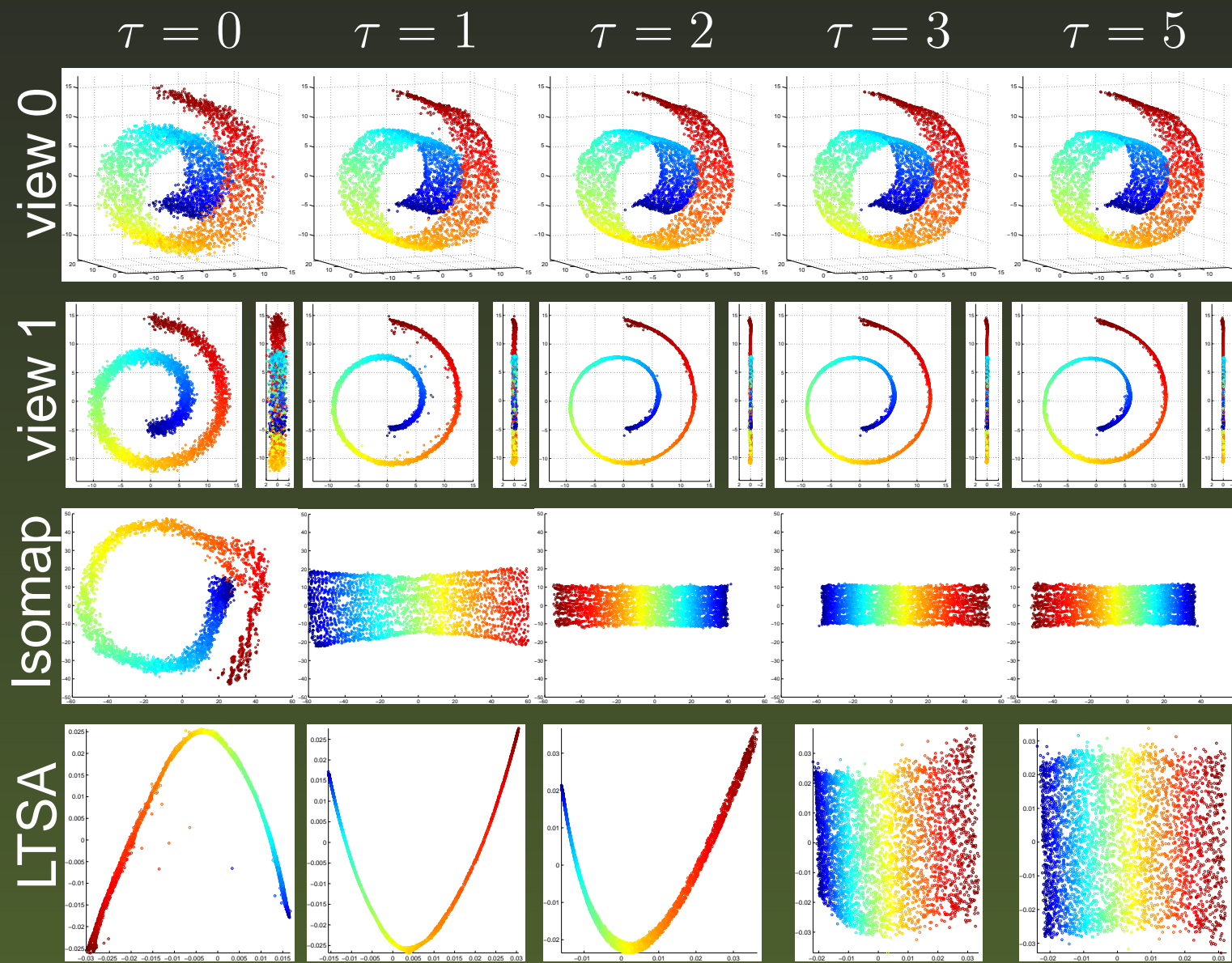
- ❖ Variations of MBMS:
 - ❖ **MBMSf/MBMSk**: use full/knn graph in predictor step.
 - ❖ **Local Tangent Projection (LTP)**: MBMSk with $\sigma = \infty$.
 - ❖ **GBMS**: $L = 0$, no corrector step.
- ❖ User parameters can be determined by cross-validation for supervised problem.
- ❖ Stopping criteria: orthogonal variance λ_{\perp} (sum of the trailing $D - L$ eigenvalues of \mathbf{x}_n 's local covariance) is small.

Experiment: noisy spiral



Denosing a noisy spiral with outliers over iterations. 

Experiment: preprocessing for spectral methods



Dimensionality reduction with Isomap and LTSA for iterations of MBMSk.

Experiment: preprocessing for classifying MNIST

We denoise images of each digit separately using MBMSk.



Sample pairs of (original,denoised) images from the training set.

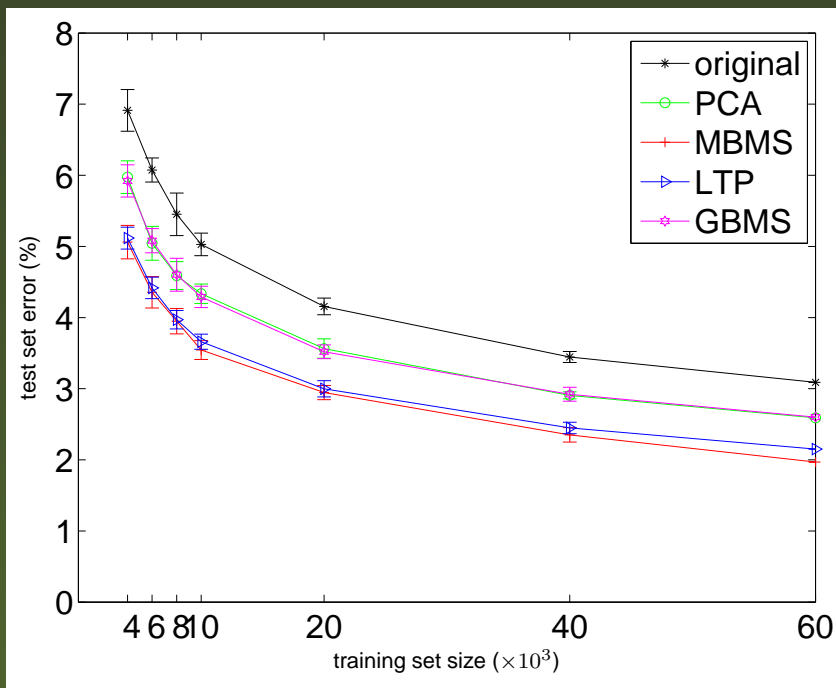
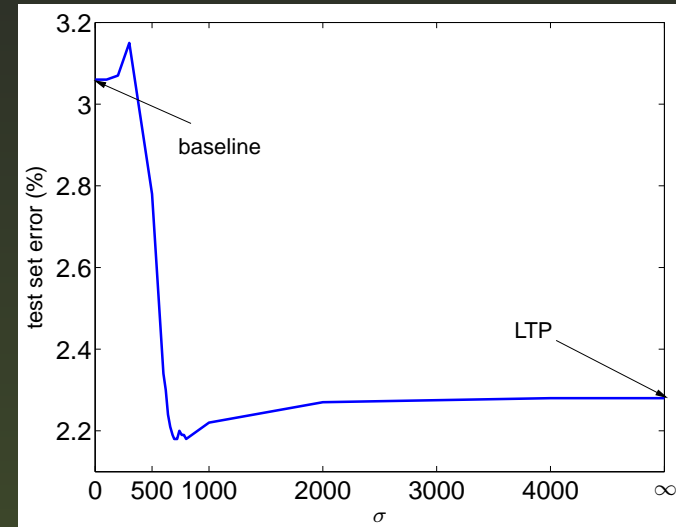
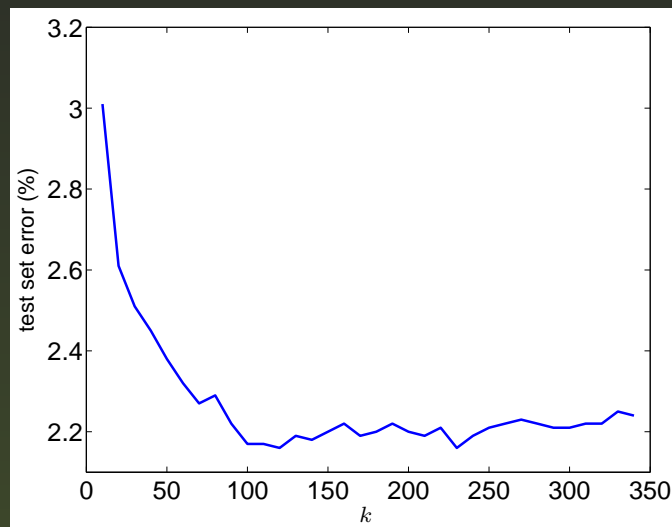
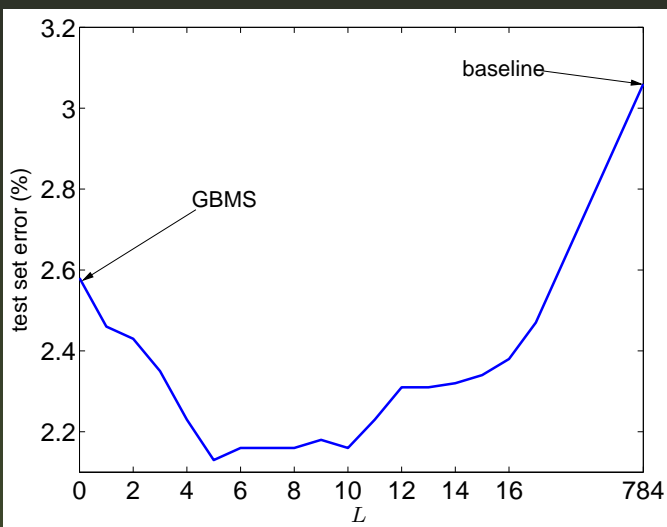
Experiment: preprocessing for classifying MNIST

Classify test set using denoised training set and Nearest Neighbor.



Some misclassified images. Each triplet is (test, original-nearest-neighbor, denoised-nearest-neighbor) and the corresponding label is above each image, with errors highlighted.

Experiment: preprocessing for classifying MNIST



Top 3 plots: 5-fold cross-validation error (%) curves with a nearest-neighbor classifier on training set using MBMSk.

Bottom left plot: denoising and classification of the MNIST test set, by training on the entire training set and smaller subsets.

Conclusion

- ❖ Very effective at denoising in a handful of iterations.
- ❖ Nonparametric and deterministic.
- ❖ Causing very small shrinkage or distortion.
- ❖ Able to handle large noise and extreme outliers.

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- Manifold Blurring Mean-shift (MBMS) algorithm for manifold denoising
- **MBMS for matrix completion**
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Problem Setting

- ❖ Given a set of data points $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_N] \subset \mathbb{R}^D$, where each point may contain missing entries.
 - ❖ $\mathbf{X}^{\mathcal{M}}$ and $\mathbf{X}^{\mathcal{P}}$ indicate the selection of missing or present entries \mathbf{X} , where $\mathcal{P} \subset \mathcal{U}$, $\mathcal{M} = \mathcal{U} - \mathcal{P}$ and $\mathcal{U} = \{(d, n) : d = 1, \dots, D, n = 1, \dots, N\}$.
 - ❖ Indices \mathcal{P} and values $\overline{\mathbf{X}}^{\mathcal{P}}$ of the present entries are the data of the problem.
- ❖ An **ill-posed** problem. Very important in industrial applications.

5	1	?	2	3	?	?
?	2	?	4	1	?	1
?	?	?	5	?	3	2
4	?	?	1	2	?	4
2	3	5	?	?	?	?
?	4	2	?	5	1	3
?	?	3	?	1	2	2

Motivation

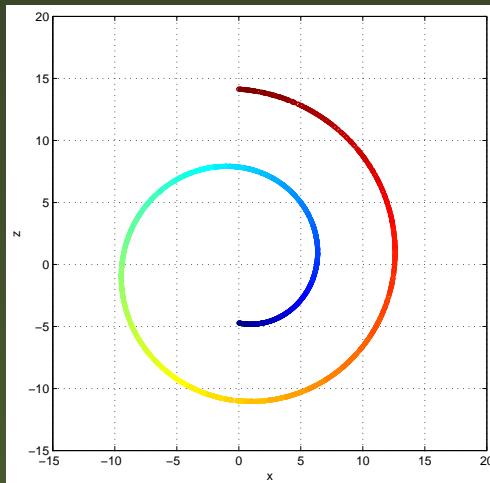
❖ Popular approaches for matrix completion

❖ Low-rank: $\min_{\mathbf{X}} \|\mathbf{X}\|_* \quad \text{s.t.} \quad \mathbf{X}_{\mathcal{P}} = \overline{\mathbf{X}}_{\mathcal{P}}$

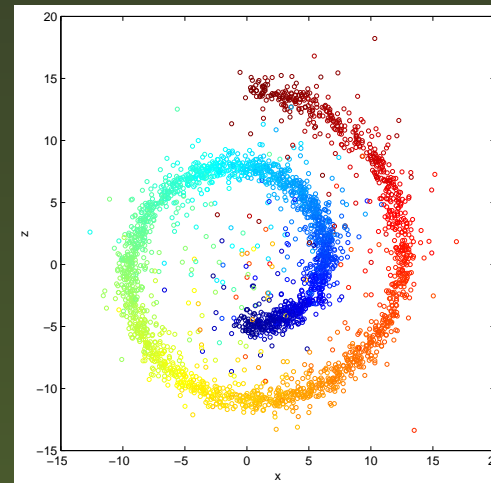
❖ Matrix factorization (probabilistic and nonlinear extensions):

$$\min_{\mathbf{L}, \mathbf{R}} \sum_{(i,j) \in \mathcal{P}} (\mathbf{X}_{ij} - \mathbf{L}_i \mathbf{R}_j^T)^2 + \lambda (\|\mathbf{L}\|_{\text{Fro}}^2 + \|\mathbf{R}\|_{\text{Fro}}^2).$$

❖ Globally low-rank assumption is too restrictive for nonlinear manifold. We use locally low-rank assumption instead.



data



SVP

MBMS for matrix completion

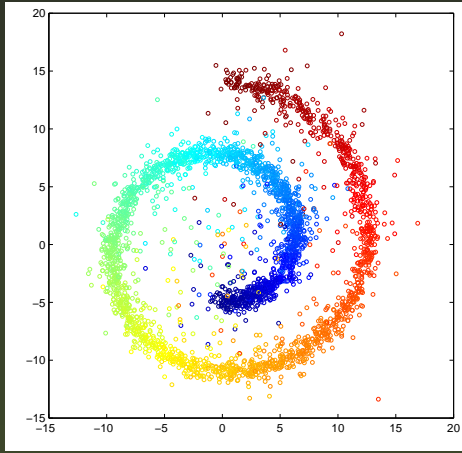
- ❖ GBMS maximizes the following objective function by taking parallel steps of the mean-shift form for each point:

$$E(\mathbf{X}) = \frac{1}{N} \sum_{n,m=1}^N G \left(\left\| \frac{\mathbf{x}_n - \mathbf{x}_m}{\sigma} \right\|^2 \right)$$

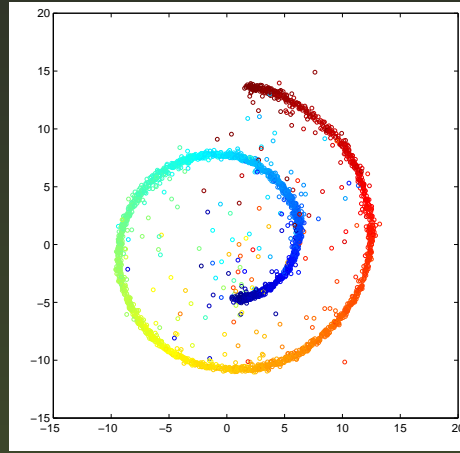
- ❖ Apply GBMS to matrix completion by adding the constraints given by the present values $\mathbf{X}_{\mathcal{P}} = \overline{\mathbf{X}}_{\mathcal{P}}$.
- ❖ We iteratively carry out a GBMS denoising step on \mathbf{X} and refill $\mathbf{X}_{\mathcal{P}}$ to the present values; equivalent to a **gradient projection** algorithm.
- ❖ MBMS can be applied instead to prevent shrinkage.
- ❖ Hyperparameters and number of iterations can be cross-validated on held out present entries.

Synthetic example

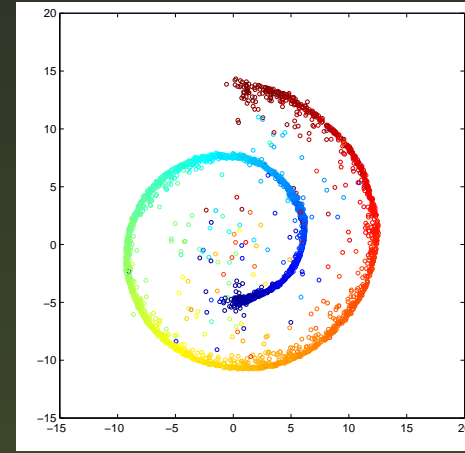
SVP
 $\tau = 0$



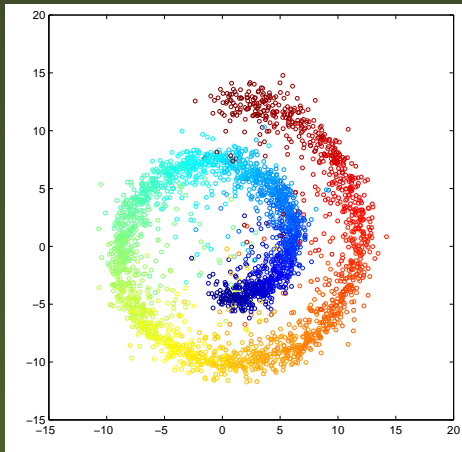
SVP + GBMS
 $\tau = 1$



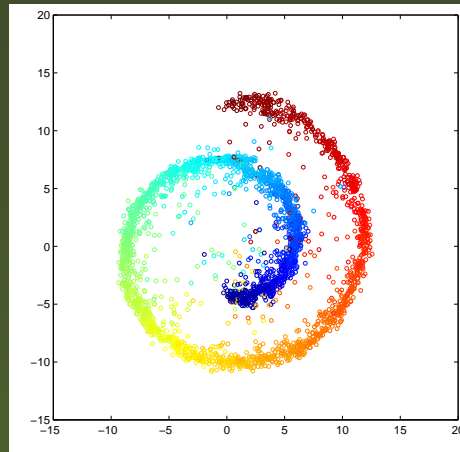
SVP + MBMS
 $\tau = 2$



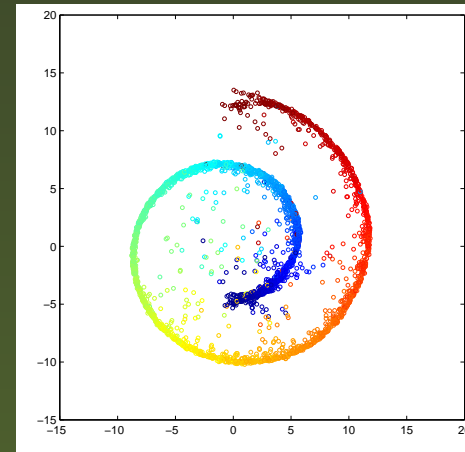
Gaussian
 $\tau = 0$



Gaussian + GBMS
 $\tau = 1$



Gaussian + MBMS
 $\tau = 25$

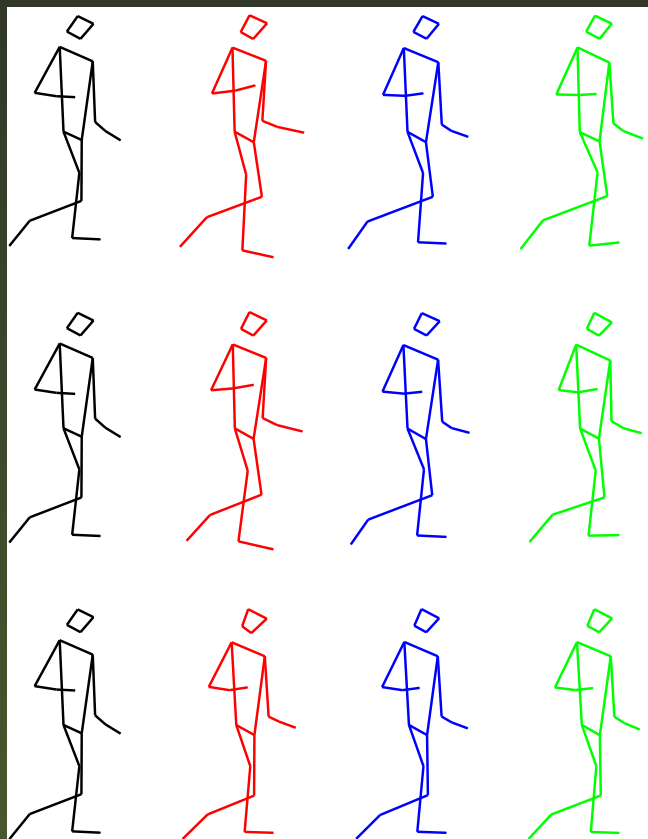


Denosing effect of different algorithms on 100D swissroll.

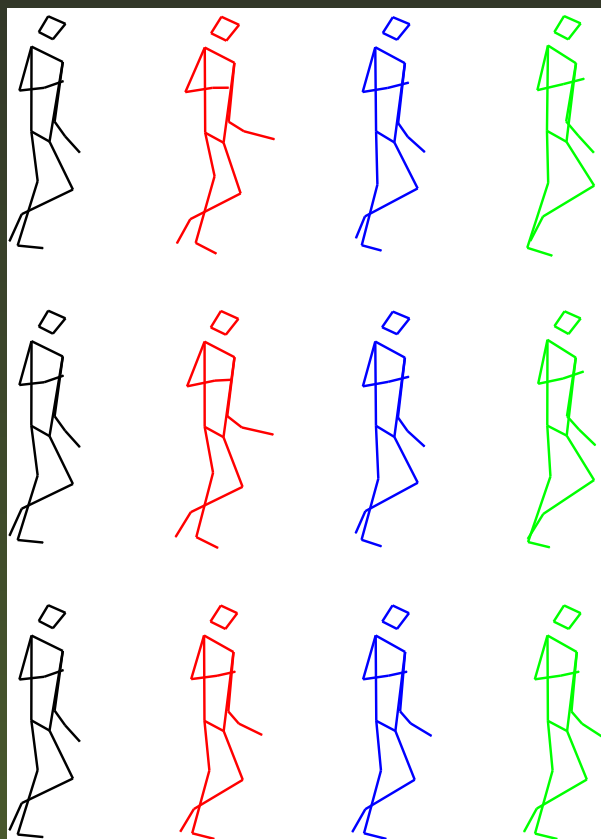
Experiment: Mocap

Running sequence with 148 samples of 150D sensor readings. 

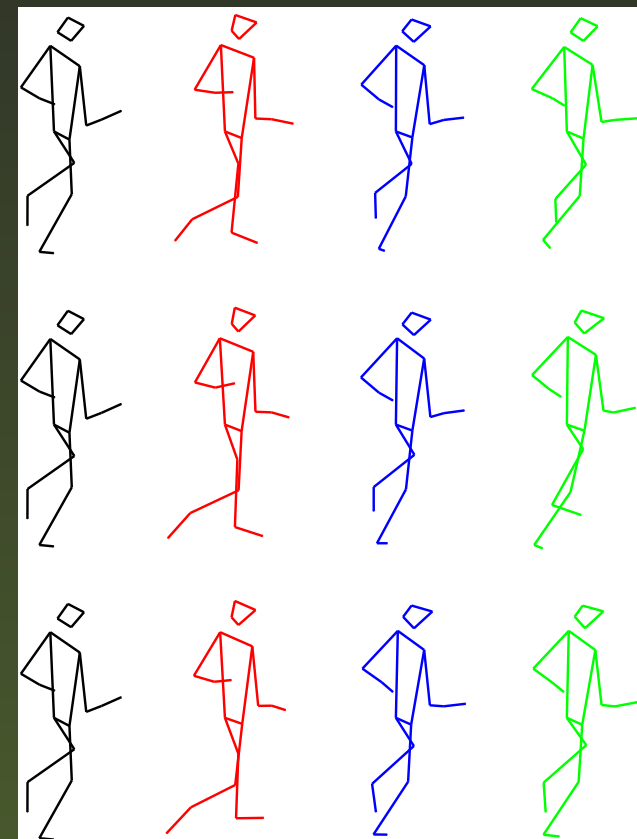
frame 2 (leg distance)



frame 10 (foot pose)

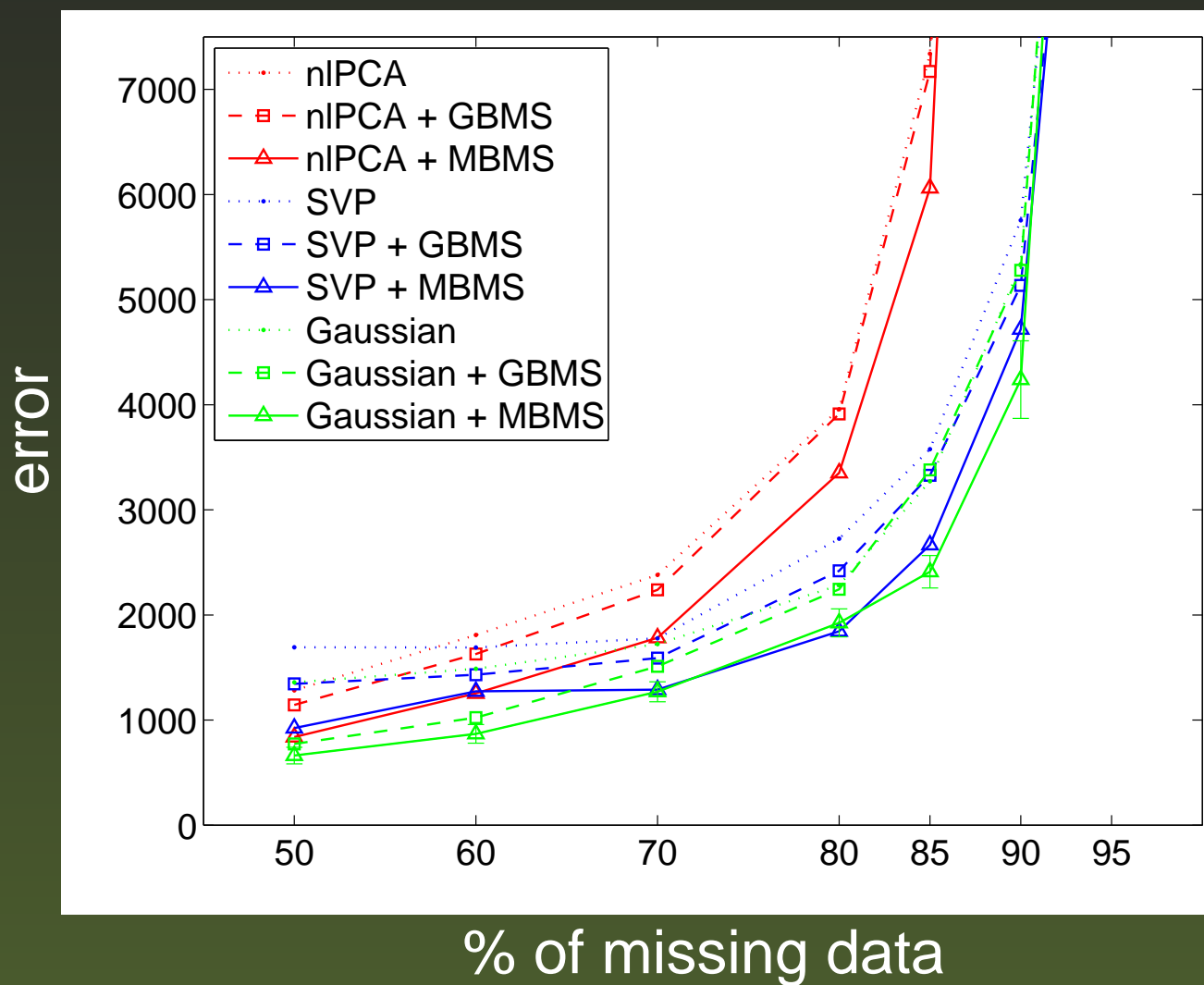


frame 147 (leg pose)



Sample reconstructions when 85% percent data is missing. *Row 1: initialization. Row 2: init+GBMS. Row 3: init+MBMS.* Color indicates different initialization: original data, **n**IPCA, **S**VP, **G**aussian.

Experiment: Mocap



Results on Mocap dataset. Mean of errors (RSSE) of 5 runs obtained by different algorithms for varying percentage of missing values.

Experiment: MNIST digit 7

6 265 greyscale images of size 28×28 , 50% entries missing.

Methods	RSSE	mean	stdev
nIPCA	7.77	26.1	42.6
SVP	6.99	21.8	39.3
+ GBMS (400,140,0,1)	6.54	18.8	37.7
+ MBMS (500,140,9,5)	6.03	17.0	34.9

Reconstruction errors of different algorithms at their optimal parameters.

Experiment: MNIST digit 7

Orig	Missing	nIPCA	SVP	GBMS	MBMS
					
					
					
					
					

Selected reconstructions of MNIST block-occluded digits '7'.

Conclusion

- ❖ We propose new denoising paradigm for matrix completion, which generalizes the commonly used assumption of low rank.
- ❖ MBMS-based algorithm bridges the gap between pure denoising (GBMS) and local low rank.
- ❖ Denoising works due to the fundamental fact that a missing value can be predicted by **averaging nearby present values**, a common approach in recommender systems.

Outline

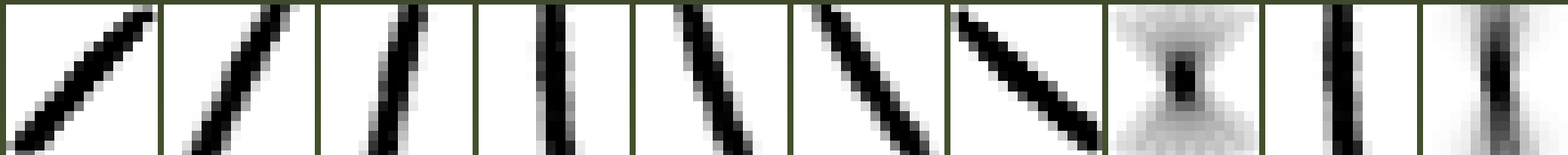
- Manifold Blurring Mean-shift (MBMS) algorithm for manifold denoising
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Motivation

- ❖ Given a dataset $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^D$, centroids-based clustering
 - ❖ partition data points into groups,
 - ❖ estimate a representative $\mathbf{c}_k \in \mathbb{R}^D$ of each cluster k .
- ❖ Popular algorithms of this type: K -means, mean-shift, K -medoids.
- ❖ **No K -modes algorithm exists.** Mode \Rightarrow high density \Rightarrow representativeness.

data

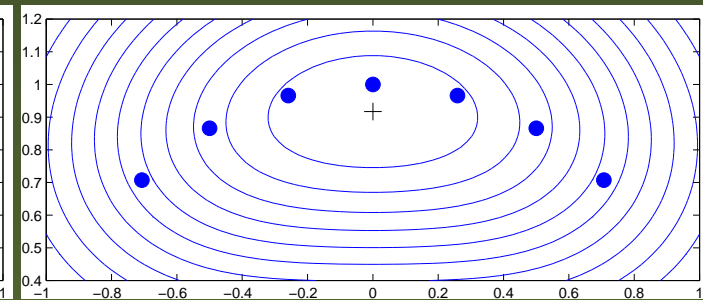
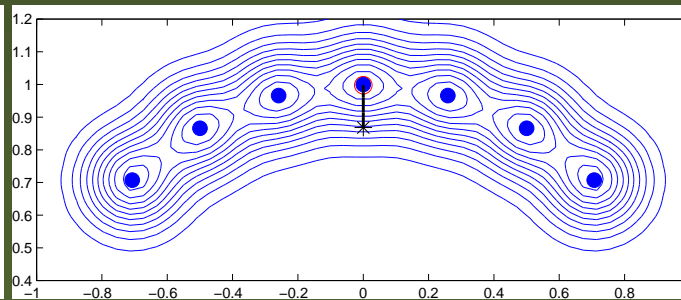
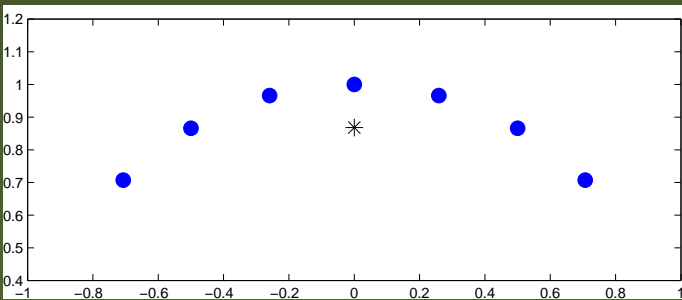
K -means K -modes GMS



K -means

K -modes ($\sigma = 0.1$)

GMS ($\sigma = 0.45$)



K-means algorithm

Optimizes over assignment Z and centroids C

$$\min_{Z, C} \sum_{k=1}^K \sum_{n=1}^N z_{nk} \|\mathbf{x}_n - \mathbf{c}_k\|^2$$

$$\text{s.t. } z_{nk} \in \{0, 1\}, \sum_{k=1}^K z_{nk} = 1, \text{ for } n = 1, \dots, N.$$

- ❖ Efficient algorithm alternates Z -step (computes assignment) and C -step (computes mean).
- ❖ Can only produce convex clusters (Voronoi tessellation).
- ❖ Cluster mean may not be valid pattern.
- ❖ Sensitive to noise and outliers.

K -modes: objective function

$$\max_{\mathbf{Z}, \mathbf{C}} \sum_{n=1}^N \sum_{k=1}^K z_{nk} G \left(\left\| \frac{\mathbf{x}_n - \mathbf{c}_k}{\sigma} \right\|^2 \right)$$

$$\text{s.t. } z_{nk} \in \{0, 1\}, \quad \sum_{k=1}^K z_{nk} = 1, \quad \text{for } n = 1, \dots, N,$$

- ❖ Sum of KDE but separately for each cluster.
- ❖ Combines the notions of assignment and density estimation.
- ❖ Two limit cases: “ K -medoids” when $\sigma \rightarrow 0$, K -means when $\sigma \rightarrow \infty$.
- ❖ Alternating optimization with guaranteed convergence
 - ❖ Z-step: decouples over points, [same assignment rule as \$K\$ -means](#).
 - ❖ C-step: decouples over clusters, [mode-finding within each cluster](#).

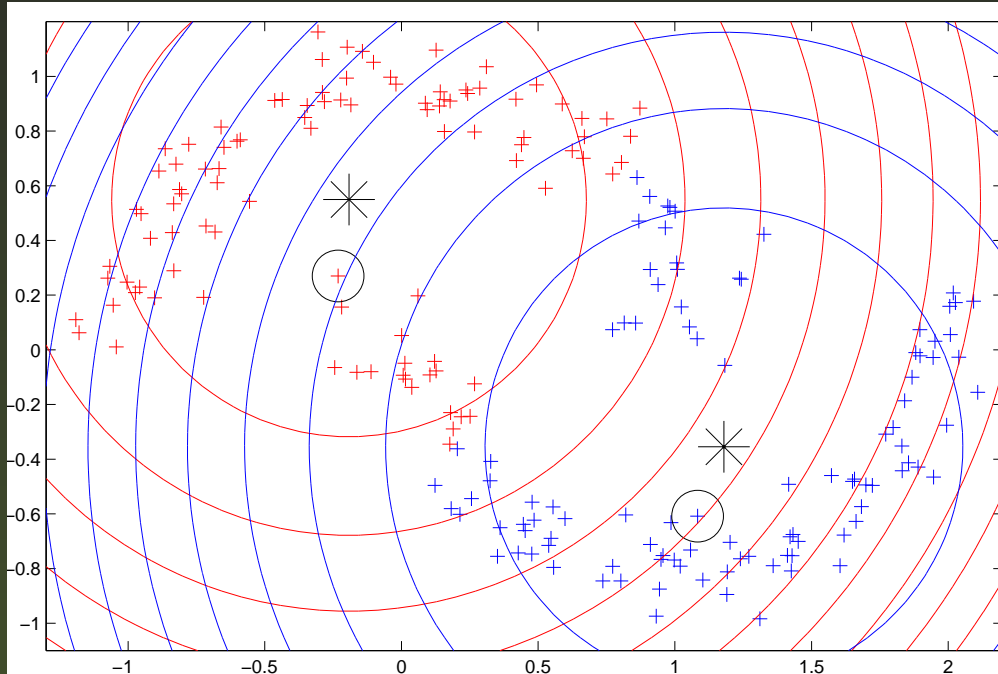
K-modes: homotopy algorithm

Start with $\sigma = \infty$ (*K*-means), gradually decrease σ while running J iterations of the fixed- σ *K*-modes algorithm for each value of σ , until reach a target value σ^* .

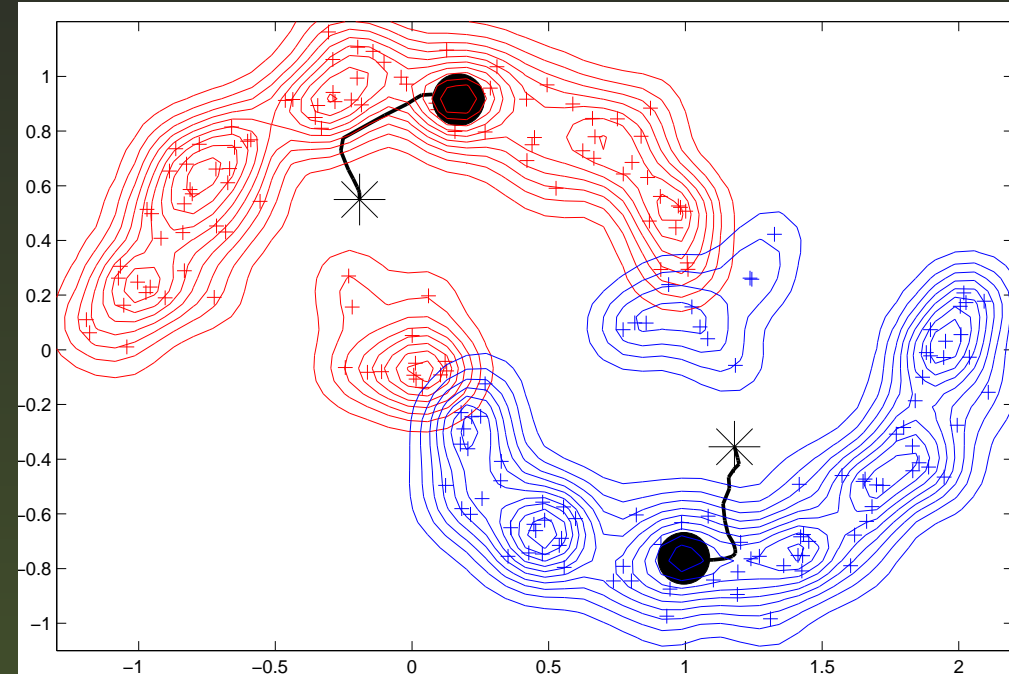
- ❖ A deterministic algorithm given local optimum found by *K*-means.
- ❖ Follows an optimum path $(\mathbf{Z}(\sigma), \mathbf{C}(\sigma))$ for $\sigma \in [\sigma^*, \infty)$.
- ❖ Homotopy techniques tends to find better optima than starting directly at the target value σ^* .
- ❖ Representative, valid centroids are obtained for a wide range of intermediate σ values.

K -modes: homotopy algorithm

$\sigma = \infty$



$\sigma = 0.1$

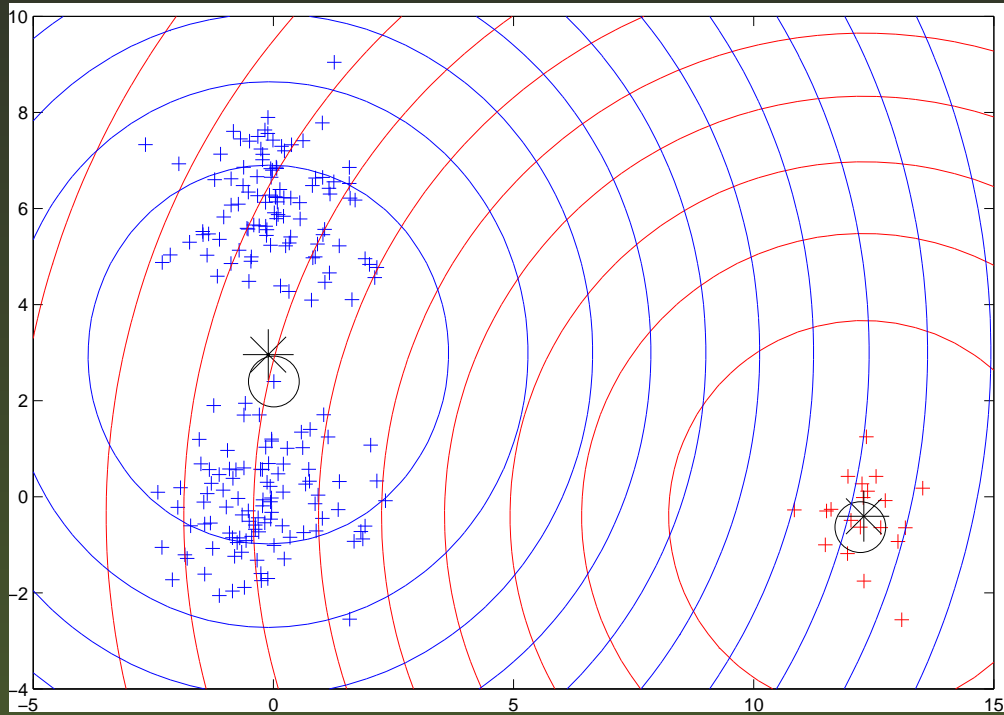


👉 $K = 2$. No value of σ results in two modes that separate the (nonconvex) moons.

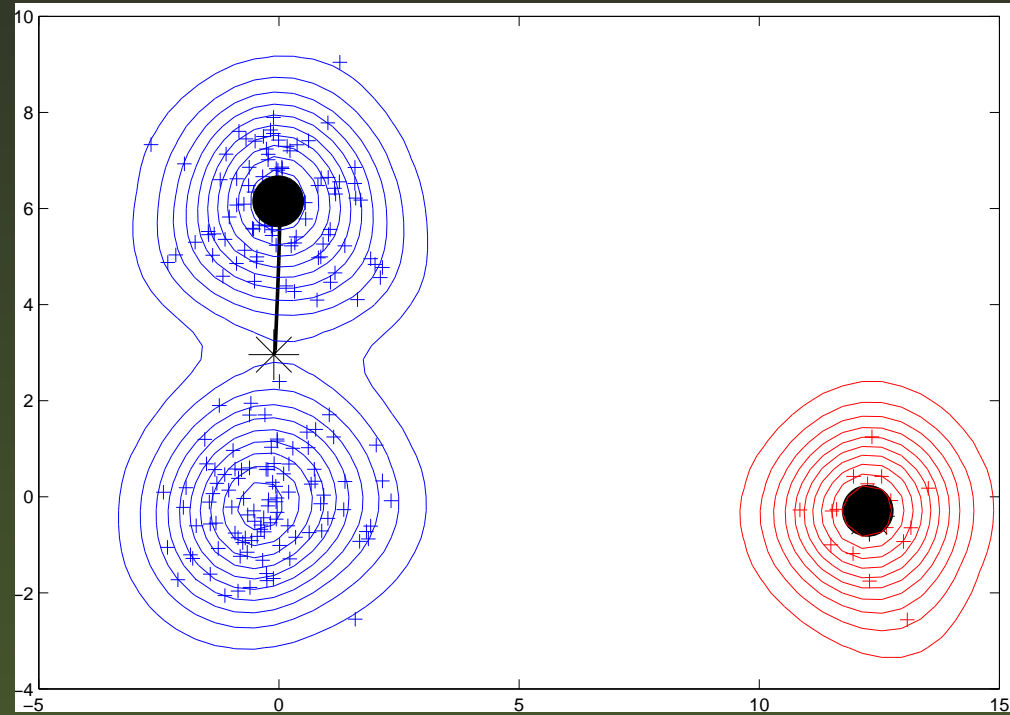
Experiment: misspecification of K

3 natural clusters, but use $K = 2$. 

$\sigma = \infty$

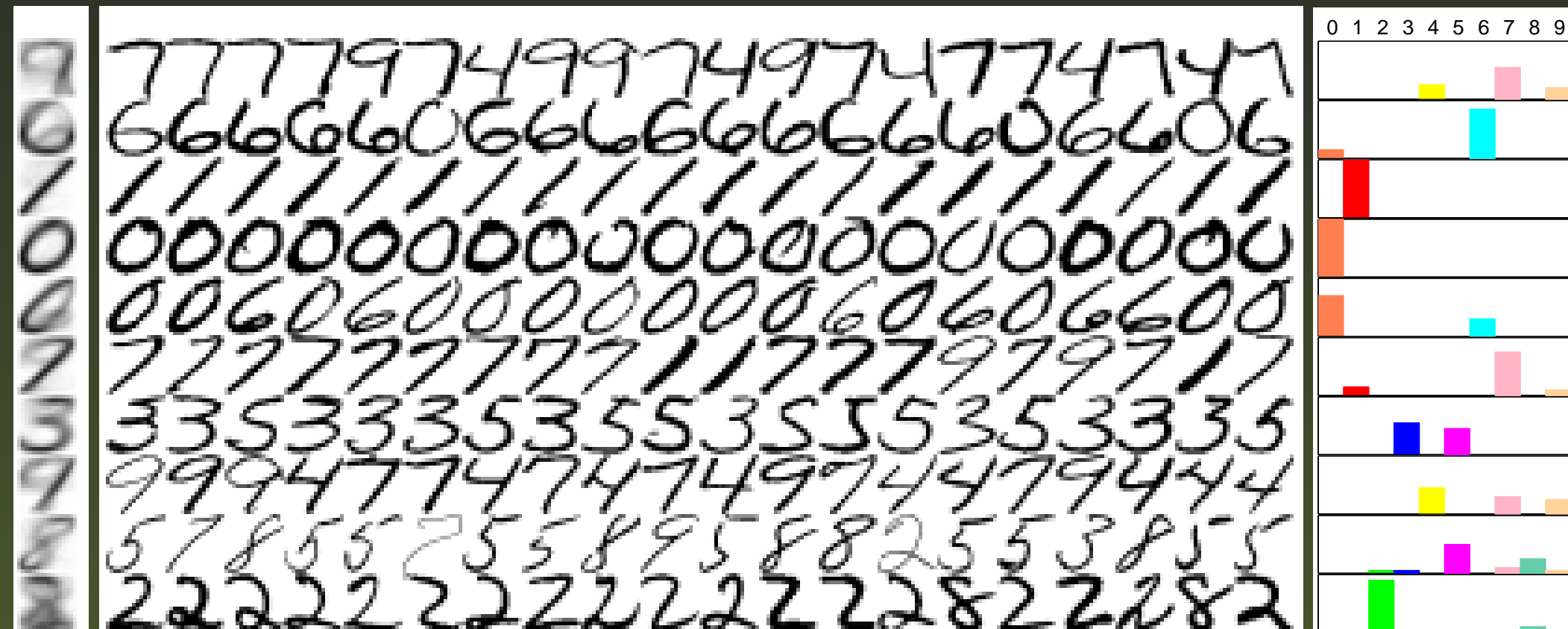


$\sigma = 1$



Experiment: handwritten digit images

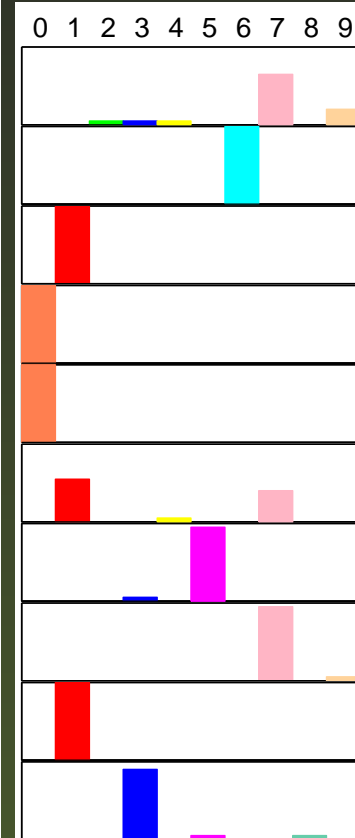
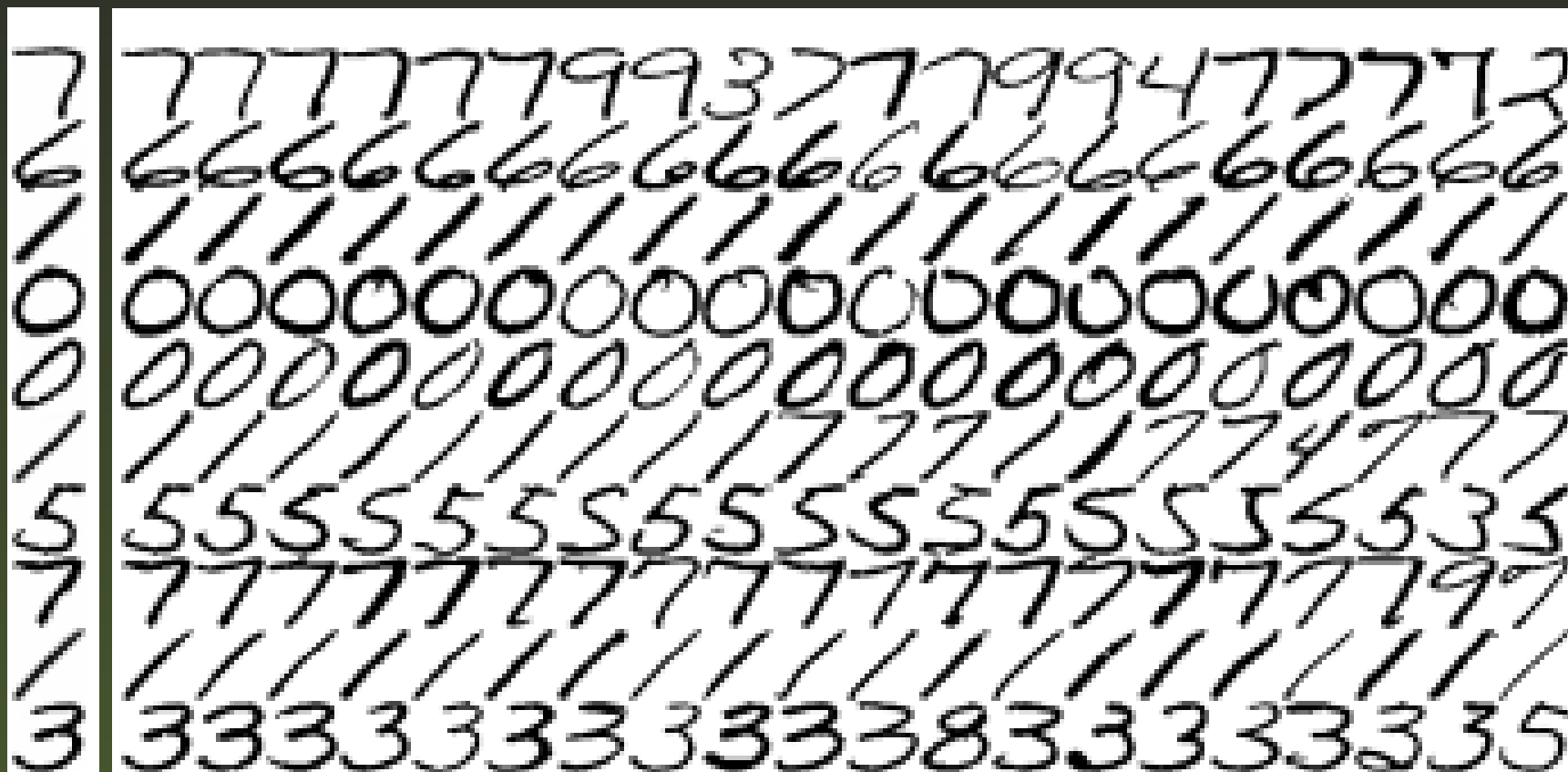
K -means result ($K = 10, \sigma = \infty$)



- ❖ Centroids are average of different classes.
- ❖ Neighborhoods are not homogeneous/pure.

Experiment: handwritten digit images

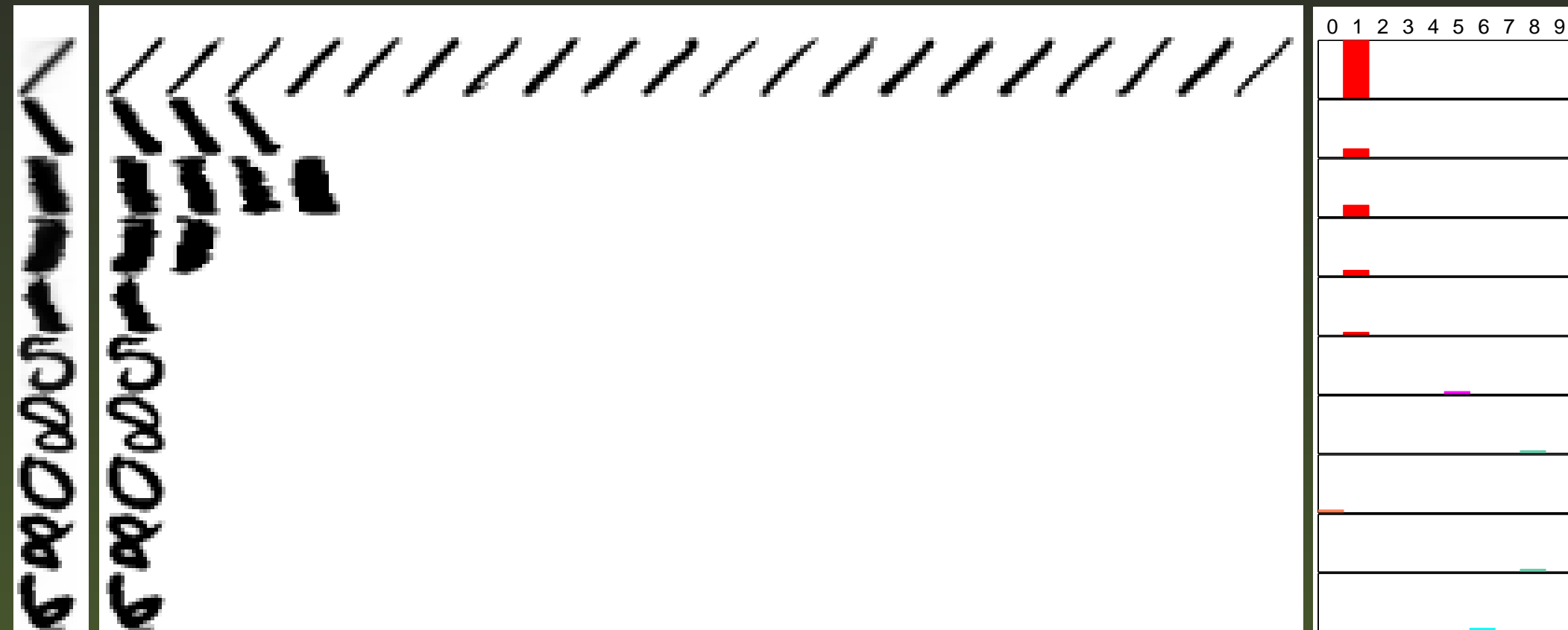
K -modes result ($K = 10, \sigma = 1$)



- ❖ Centroids are very representative.
- ❖ Neighborhoods are homogeneous/pure.

Experiment: handwritten digit images

Mean-shift result ($\sigma = 1.8369$)



- ❖ In high dimensions, many modes have very few associated points.

Summary

- ❖ K -modes is more robust than K -means and GMS to outliers and parameter misspecification.
- ❖ K -modes will return exactly K modes (one per cluster) no matter the value of σ , and whether the dataset KDE has more or fewer than K modes.
- ❖ Centroids are representative, valid patterns.

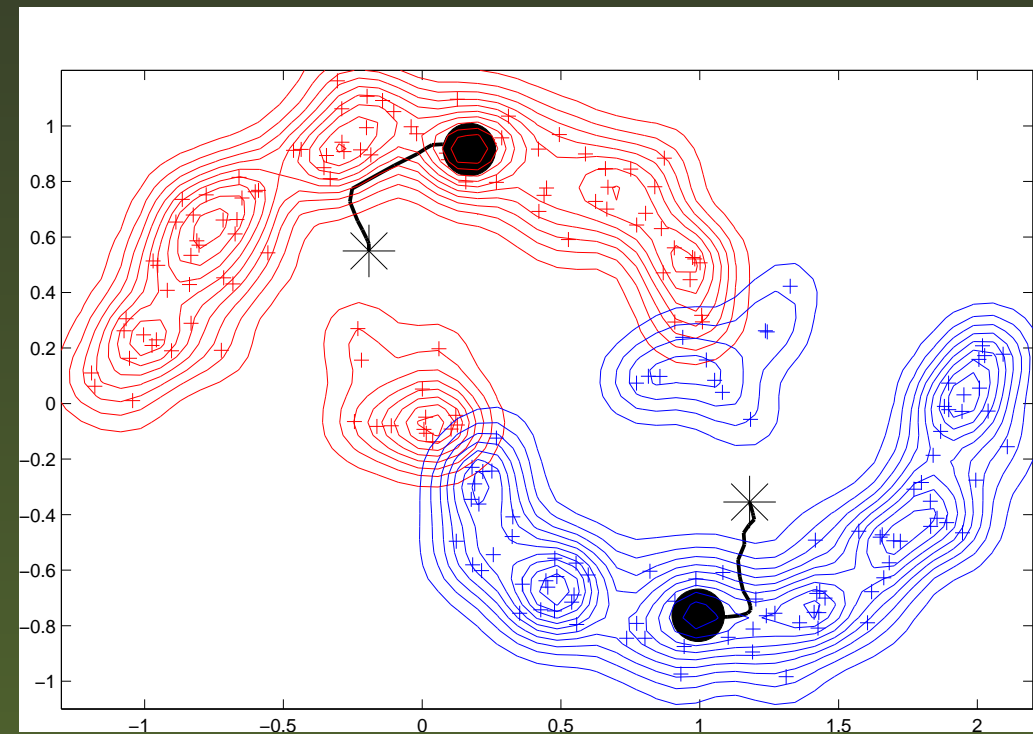
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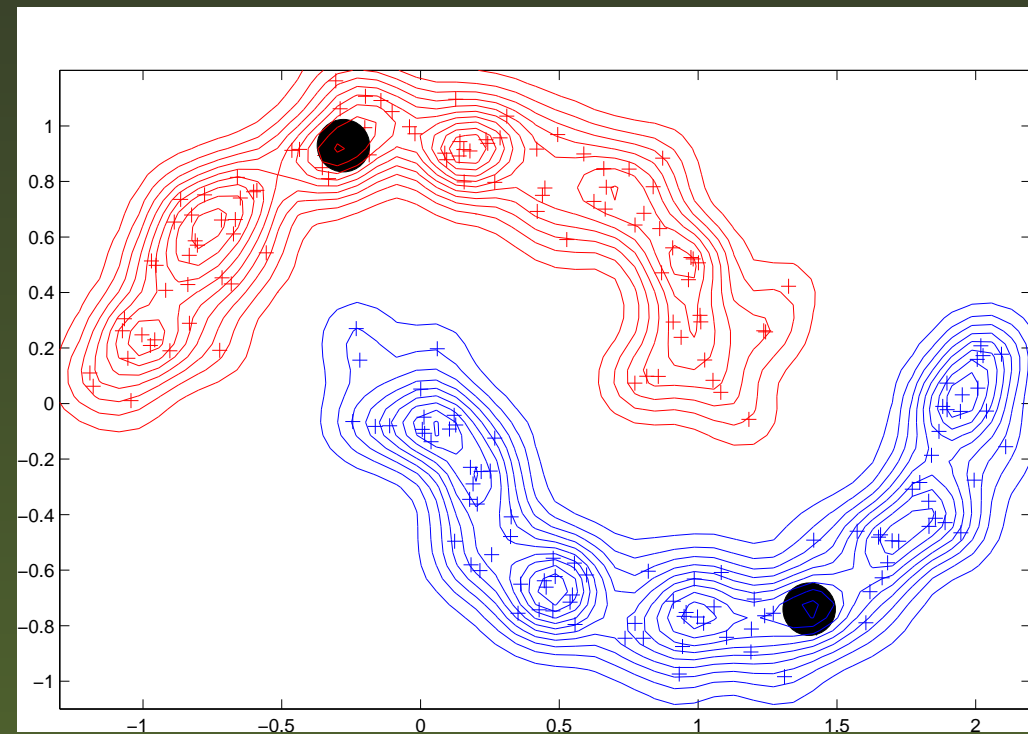
Motivation

- ❖ Limitation of K -modes assignment: can only find convex clusters.
- ❖ In addition to representative centroids and density estimate, we want more **flexible assignment**.

K -modes ($\sigma = 0.1$)



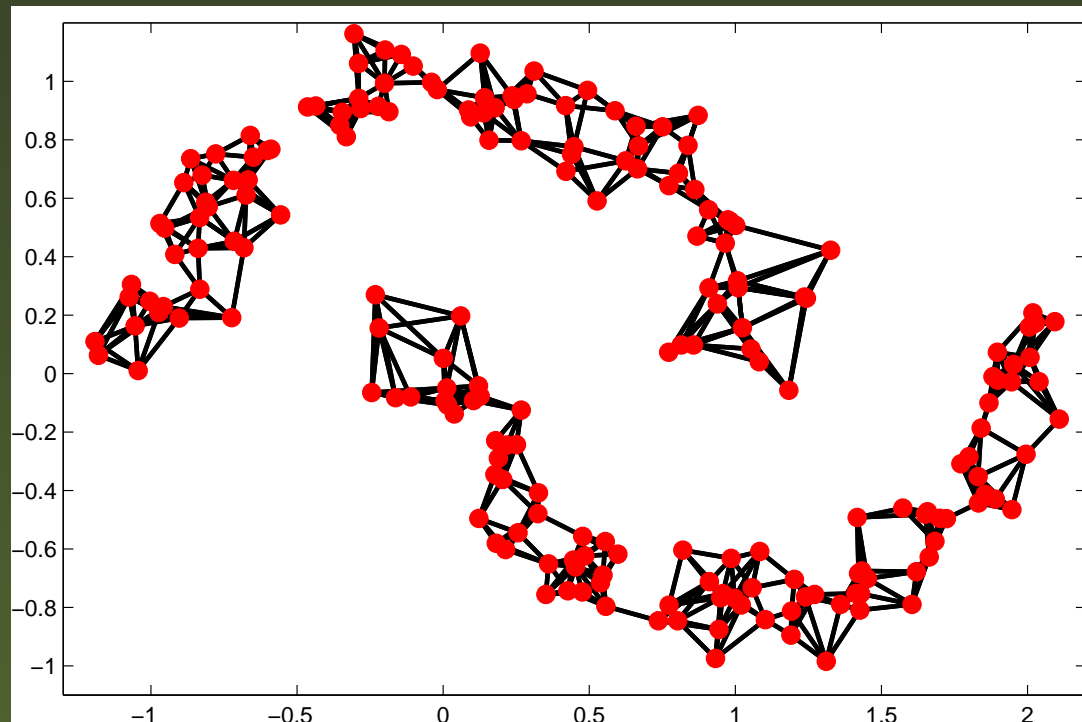
Laplacian K -modes ($\sigma = 0.1$)



Laplacian smoothing

Key to separate clusters with manifold structure: **nearby data points should have similar assignment.**

1. Relax the assignment to be continuous, but constrain them to probabilities.
2. Build a graph on the dataset, let w_{mn} be the weight between \mathbf{x}_m and \mathbf{x}_n .
3. Add Laplacian smoothing term $\frac{\lambda}{2} \sum_{m=1}^N \sum_{n=1}^N w_{mn} \|\mathbf{z}_m - \mathbf{z}_n\|^2$.



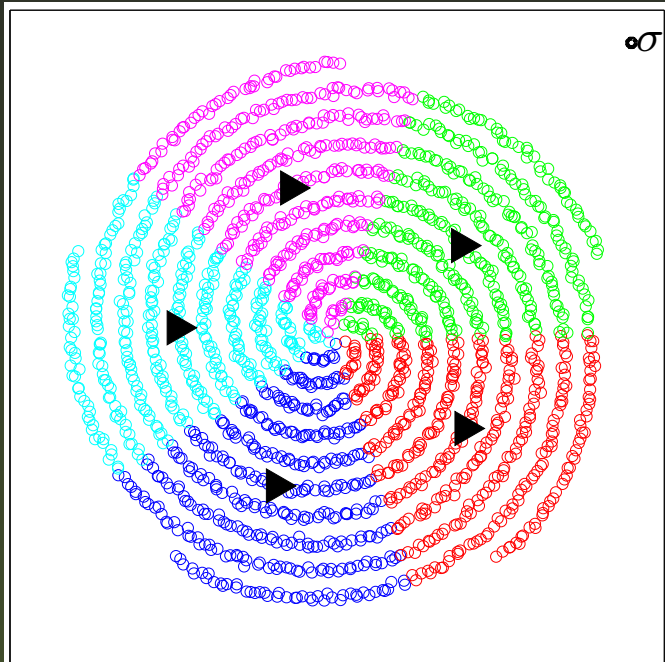
Laplacian K -modes: objective function

$$\begin{aligned} \min_{\mathbf{Z}, \mathbf{C}} \quad & \frac{\lambda}{2} \sum_{m=1}^N \sum_{n=1}^N w_{mn} \|\mathbf{z}_m - \mathbf{z}_n\|^2 - \sum_{n=1}^N \sum_{k=1}^K z_{nk} G \left(\left\| \frac{\mathbf{x}_n - \mathbf{c}_k}{\sigma} \right\|^2 \right) \\ \text{s.t.} \quad & \sum_k z_{nk} = 1, \text{ for } n = 1, \dots, N, \\ & z_{nk} \geq 0, \text{ for } n = 1, \dots, N, k = 1, \dots, K. \end{aligned}$$

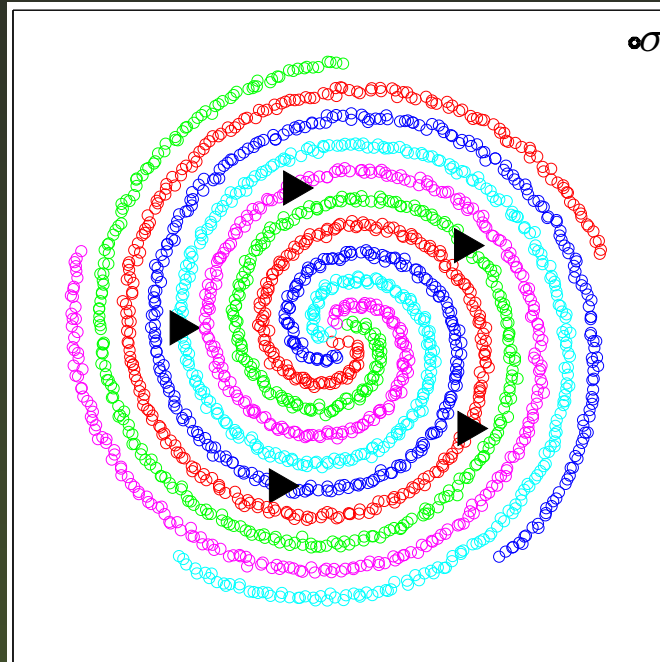
- ❖ Obtain hard assignment by choosing largest assignment probability.
- ❖ Alternating optimization
 - ❖ C-step: decouples over clusters, **mode-finding within each cluster**.
 - ❖ Z-step: **convex quadratic program**, solved with gradient projection.
- ❖ Homotopy in (σ, λ) can be done similarly as in K -modes.

Effect of Laplacian smoothing

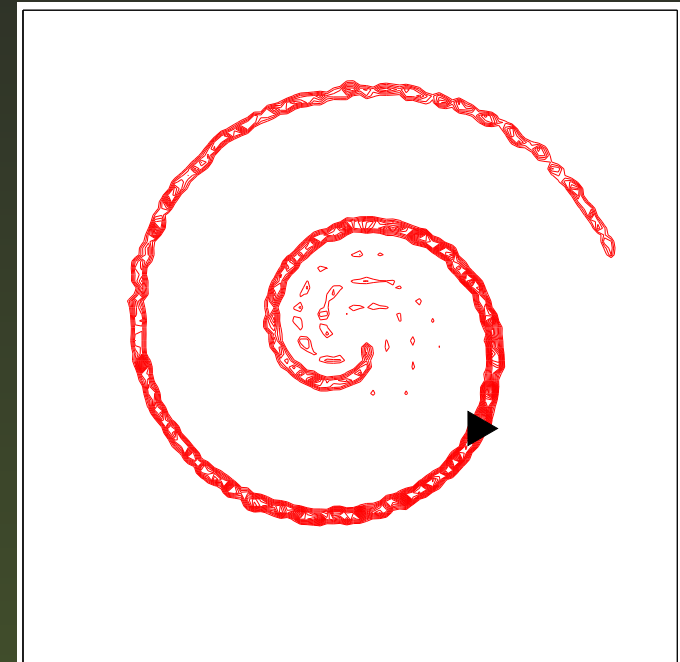
K -modes



Laplacian K -modes



KDE



❖ $K=5$. K -modes assignment rule can never separate the spirals.

Out-of-sample problem

- ❖ Optimize assignment \mathbf{z} of new point \mathbf{x} given \mathbf{Z} and \mathbf{C} from training.
- ❖ The out-of-sample problem is equivalently

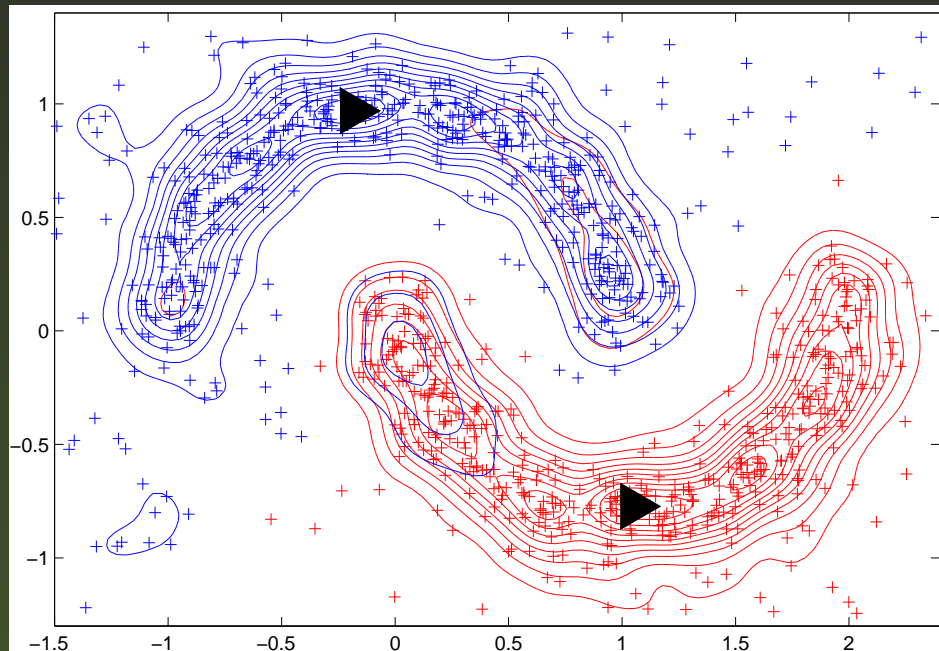
$$\begin{aligned} \min_{\mathbf{z}} \quad & \frac{1}{2} \|\mathbf{z} - \bar{\mathbf{z}} - \gamma \mathbf{q}\|^2, \\ \text{s.t.} \quad & \mathbf{z}^\top \mathbf{1}_K = 1, \quad \mathbf{z} \geq 0, \end{aligned}$$

where $\bar{\mathbf{z}}$ is the weighted mean of training assignments, \mathbf{q} is soft distance to centroids.

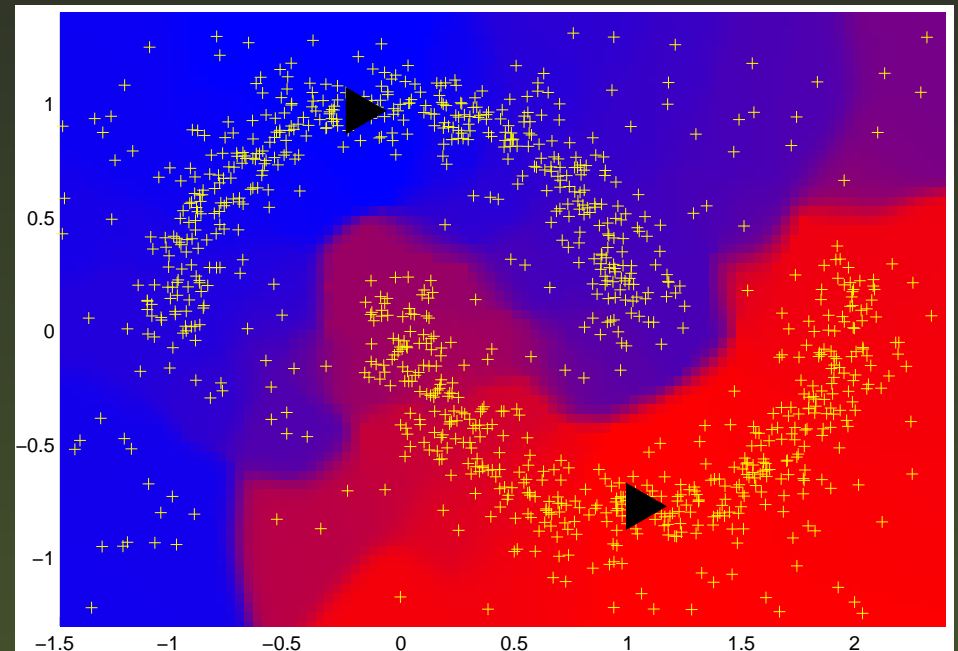
- ❖ **Projection of $\bar{\mathbf{z}} + \gamma \mathbf{q}$ onto the probability simplex.**
- ❖ It is a mixture of two assignment rules and a nonlinear mapping.

Out-of-sample problem

Laplacian K -modes



Out-of-sample



☞ $K = 2$. Homotopy in σ for Laplacian K -modes.

Clustering analysis

Statistics of datasets.

dataset	size (N)	dimensionality (D)	# of classes (K)
MNIST (digit image)	2000	768	10
COIL20 (object image)	1440	1024	20
TDT2 (document)	9394	36771	30

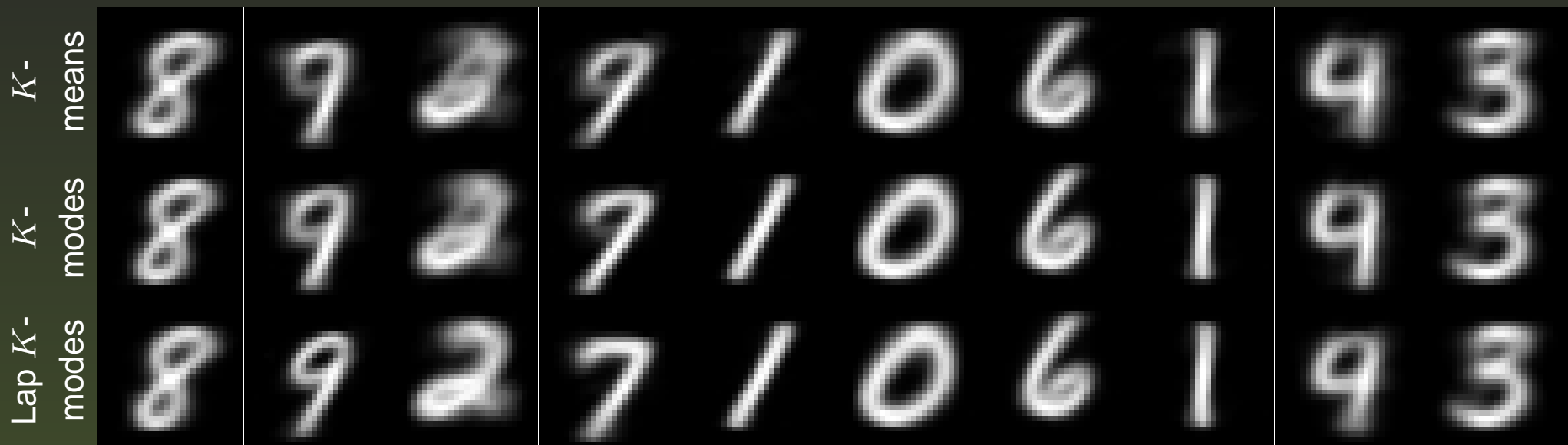
Clustering accuracy (%).

dataset	K -means	K -modes	GMS	NCut	GNMF	DCD	Lap. K -modes
MNIST	58.2	59.2	15.9	65.5	66.2	69.4	70.5
COIL-20	66.5	67.2	27.2	79.0	75.3	71.5	81.0 (81.5)
TDT2	68.9	70.0	N/A	88.4	88.6	55.1	91.4

Normalized Mutual Information (%).

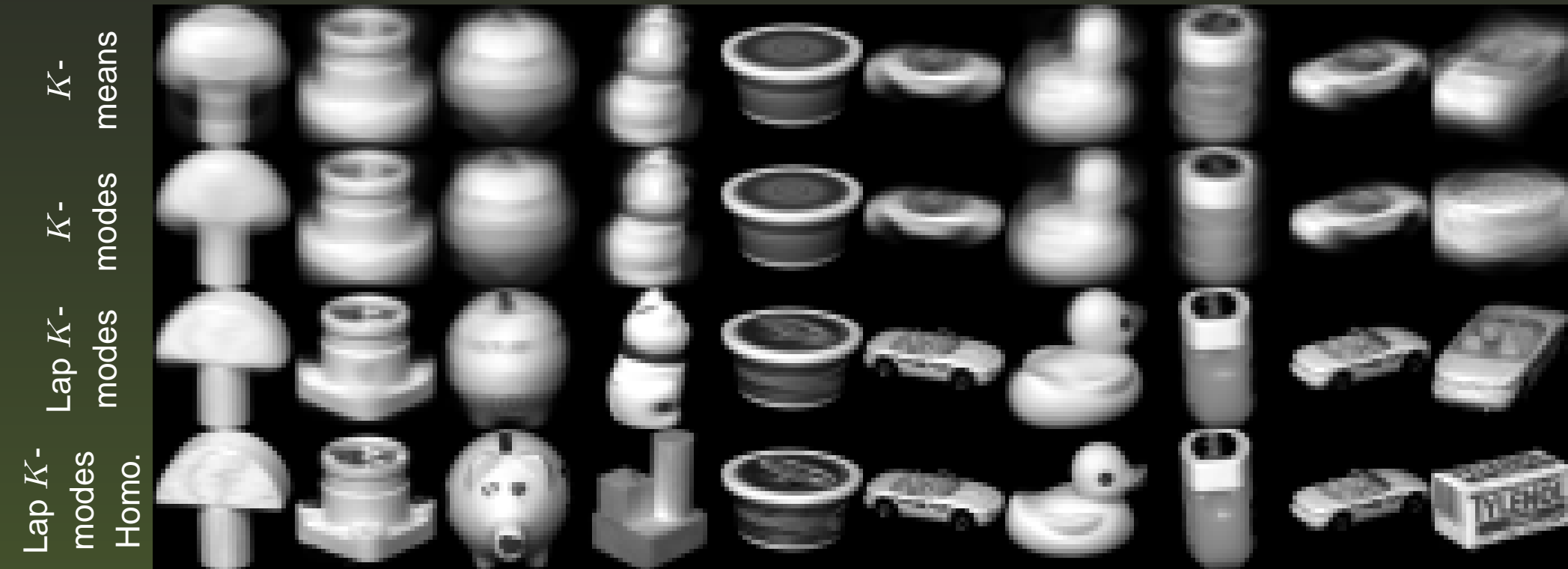
dataset	K -means	K -modes	GMS	NCut	GNMF	DCD	Lap. K -modes
MNIST	53.3	53.6	6.51	66.9	64.9	65.6	68.8
COIL-20	75.3	75.9	38.9	88.0	87.5	77.6	87.3 (88.0)
TDT2	75.3	75.8	N/A	83.7	83.7	68.6	88.8

Clustering analysis



Centroids found by different algorithms on MNIST.

Clustering analysis



Centroids found by different algorithms on COIL-20.

Summary

Comparison of different clustering algorithms.

	<i>K</i> -means	<i>K</i> -medoids	Mean-shift	Spectral clustering	<i>K</i> -modes	Laplacian <i>K</i> -modes
Centroids	likely invalid	“valid”	“valid”	N/A	valid	valid
Nonconvex clusters	no	depends	yes	yes	no	yes
Density	no	no	yes	no	yes	yes
Assignment	hard	hard	hard	hard	hard	soft
Cost/iteration	KND	KN^2D	N^2D	$N^2 \sim N^3$	KND	KND

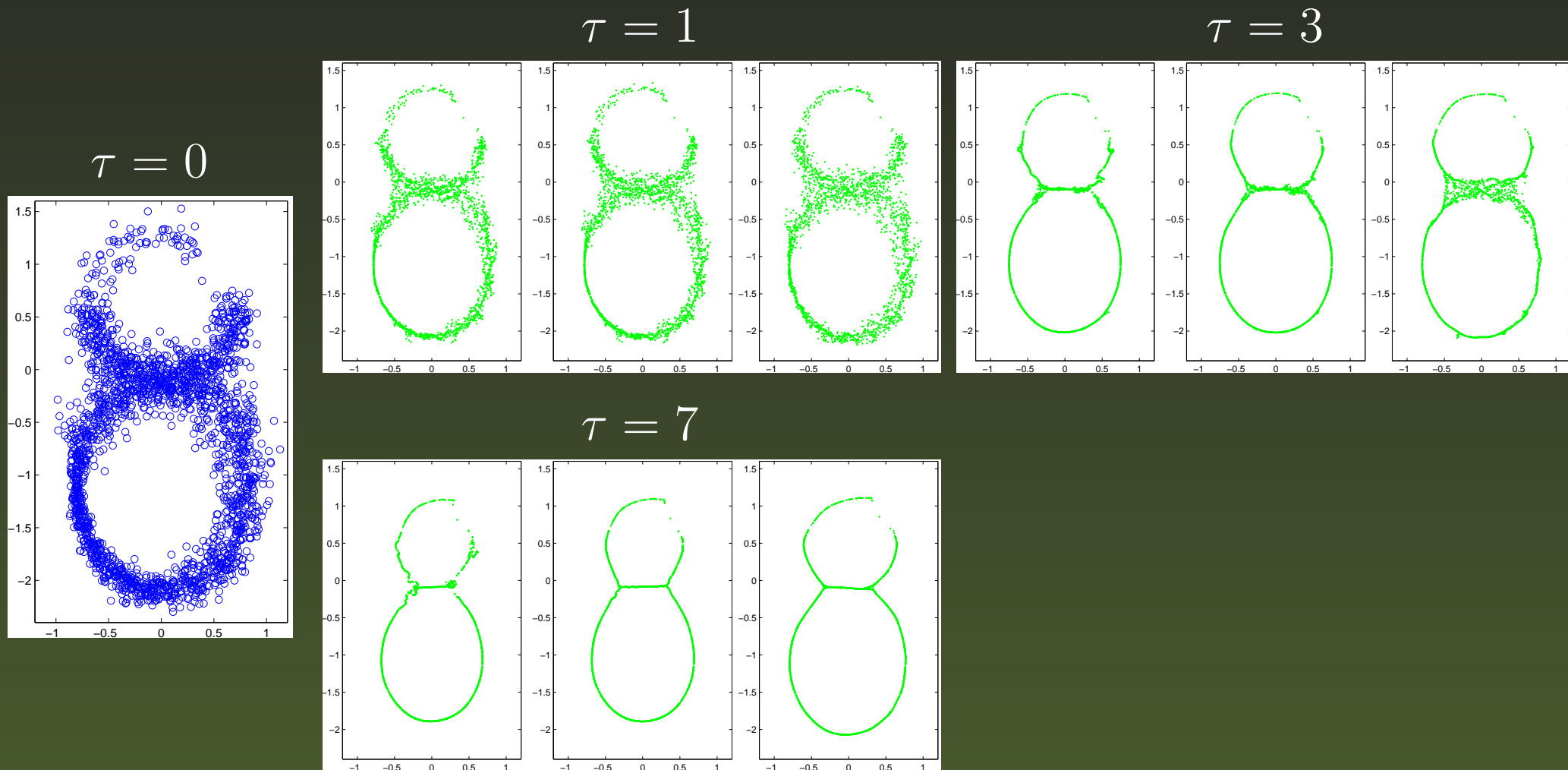
Conclusion

- ❖ We develop mean-shift algorithms to analyze dataset with low degrees of freedom.
- ❖ Future directions:
 - ❖ Theoretical analysis
 - ❖ Speedup training and testing
 - ❖ Incorporating more domain knowledge

Papers

- ❖ Miguel A. Carreira-Perpinan and Weiran Wang. *A simple assignment model with Laplacian smoothing*. Unpublished manuscript.
- ❖ Weiran Wang and Miguel A. Carreira-Perpinan. *The role of dimensionality reduction in classification*. Unpublished manuscript.
- ❖ Weiran Wang and Miguel A. Carreira-Perpinan. *The Laplacian K-modes algorithm for clustering*. Unpublished manuscript.
- ❖ Miguel A. Carreira-Perpinan and Weiran Wang. *The K-modes algorithm for clustering*. Unpublished manuscript, Apr. 23, 2013, arXiv:1304.6478 [cs.LG].
- ❖ Miguel A. Carreira-Perpinan and Weiran Wang. *Distributed optimization of deeply nested systems*. Unpublished manuscript, Dec. 24, 2012, arXiv:1212.5921 [cs.LG].
- ❖ Weiran Wang and Miguel A. Carreira-Perpinan. *Nonlinear low-dimensional regression using auxiliary coordinates*. AISTATS 2012.
- ❖ Weiran Wang, Miguel A. Carreira-Perpinan and Zhengdong Lu. *A denoising view of matrix completion*. NIPS 2011.
- ❖ Weiran Wang and Miguel A. Carreira-Perpinan. *Manifold blurring mean shift algorithms for manifold denoising*. CVPR 2010.

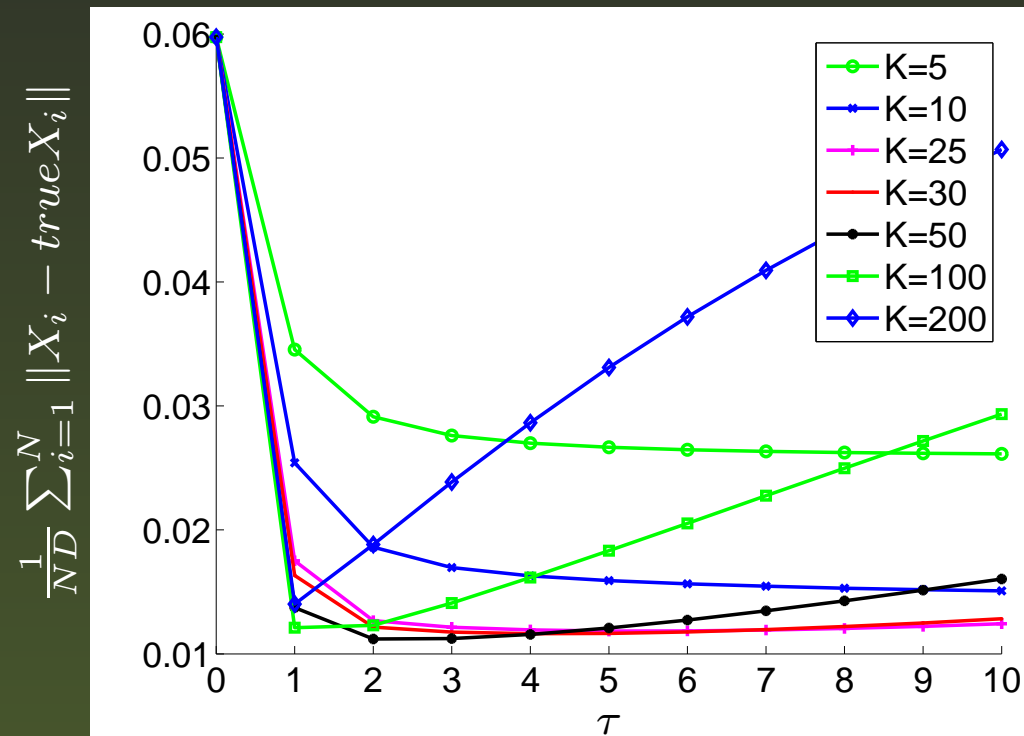
MBMS Experiment: complex shape



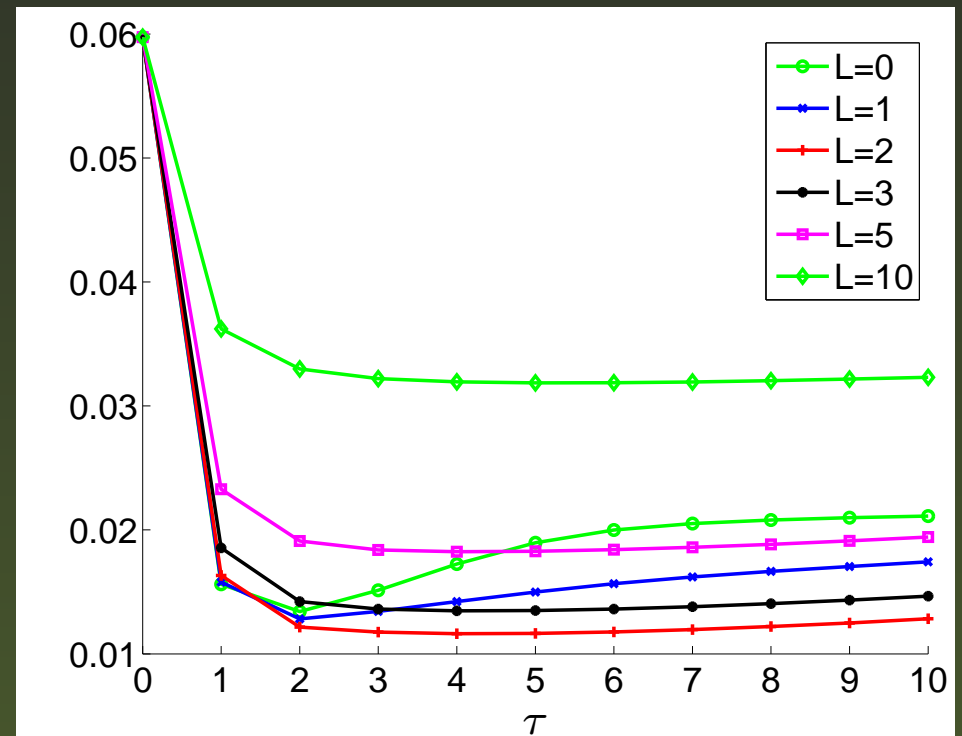
Denosing a complex shape with nonuniform density and noise with MBMSf using different affinity (left: normal, middle: diffusion maps, right: entropic affinity).

MBMS Experiment: Robustness to parameters choice

For swissroll dataset, there is a wide range for each parameter in which MBMS works well.



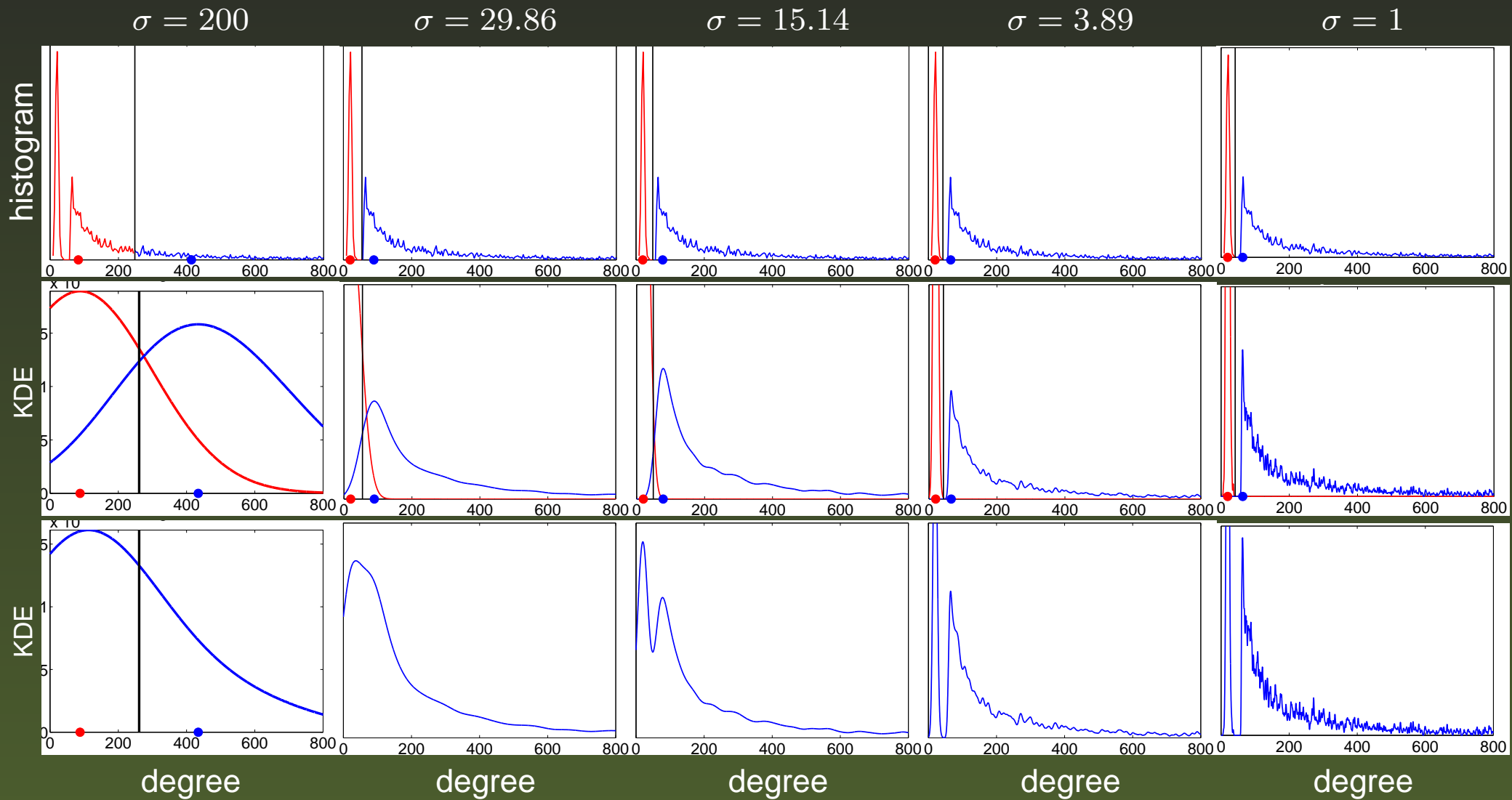
$$\sigma = \infty, L = 2$$



$$\sigma = \infty, K = 30$$

Behavior of LTP for different parameters K and L . Error decreases for all parameter choices.

K-modes Experiment: heavy tailed distribution



👉 $K = 2$. Separating mixture of a Gaussian component and a power-law component.

Laplacian K -modes: alternating optimization

- ❖ C-step: decouples over different cluster. For cluster k , solve $\max_{c_k} \sum_{\{n: z_{nk} > 0\}} z_{nk} G\left(\left\|\frac{\mathbf{x}_n - \mathbf{c}_k}{\sigma}\right\|^2\right)$ with mean-shift updates.
- ❖ Z-step: **nolonger decouples** over different points.

$$\begin{aligned} \min_{\mathbf{Z}} \quad & \lambda \operatorname{tr}(\mathbf{Z}^\top \mathbf{L} \mathbf{Z}) - \operatorname{tr}(\mathbf{B}^\top \mathbf{Z}) \\ \text{s.t.} \quad & \mathbf{Z} \mathbf{1}_K = \mathbf{1}_N, \\ & \mathbf{Z} \geq 0, \end{aligned}$$

where $\mathbf{B}_{nk} = G\left(\left\|\frac{\mathbf{x}_n - \mathbf{c}_k}{\sigma}\right\|^2\right)$, \mathbf{L} is the **graph Laplacian**.

- ❖ Quadratic program of NK variables.
- ❖ Interior point method is too slow for large dataset.
- ❖ We use first order method instead.

Laplacian K -modes: Z-step

- ❖ The ISTA/FISTA framework (gradient proximal method):
 - ❖ Solves $\min_{\mathbf{x}} f(\mathbf{x}) = g(\mathbf{x}) + h(\mathbf{x})$. g is convex and has Lipschitz continuous gradient (with constant L). h is convex and not necessarily differentiable.
 - ❖ $\mathbf{x}_{n+1} = \arg \min_{\mathbf{y}} \frac{L}{2} \|\mathbf{y} - (\mathbf{x}_n - \frac{1}{L} \nabla g(\mathbf{x}_n))\|^2 + h(\mathbf{y})$.
 - ❖ Convergence: $f(\mathbf{x}_T) - f(\mathbf{x}^*) \approx \mathcal{O}(\frac{1}{T})$ for **constant stepsize** $\frac{1}{L}$.
 - ❖ Nesterov's acceleration scheme improves the rate to $\mathcal{O}(\frac{1}{T^2})$.
- ❖ Apply to our Z-step:
 - ❖ g is the quadratic objective function, with $L = 2\lambda\sigma_1(\mathbf{L})$.
 - ❖ h is the indicator function of probability simplex, therefore the proximal step is computing Euclidean projection.

Accelerated gradient projection for Z-step

Input: Initial $\mathbf{Z}_0 \in \mathbf{R}^{N \times K}$, $s = \frac{1}{2\lambda\sigma_1(\mathbf{L})}$.

1: Set $\mathbf{Y}_1 = \mathbf{Z}_0$, $t_1 = 1$, $k = 1$.

2: **repeat**

3: Compute gradient at \mathbf{Y}_k : $\mathbf{G}_k = 2\lambda\mathbf{L}\mathbf{Y}_k - \mathbf{B}$,

4: $\mathbf{Z}_k = \text{SimplexProj}(\mathbf{Y}_k - s\mathbf{G}_k)$ where $\text{SimplexProj}()$ projects each row of the argument onto the probability simplex,

5: $t_{k+1} = \frac{1 + \sqrt{1 + 4t_k^2}}{2}$,

6: $\mathbf{Y}_{k+1} = \mathbf{Z}_k + \left(\frac{t_k - 1}{t_{k+1}}\right)(\mathbf{Z}_k - \mathbf{Z}_{k-1})$,

7: $k = k + 1$,

8: **until** convergence.

Output: \mathbf{Z}_k is the solution of \mathbf{Z} given \mathbf{C} .

Projection onto the probability simplex

Input: A vector $\mathbf{v} \in \mathbb{R}^K$

1: Sort \mathbf{v} into $\mathbf{u} : u_1 \geq u_2 \geq \dots \geq u_K$

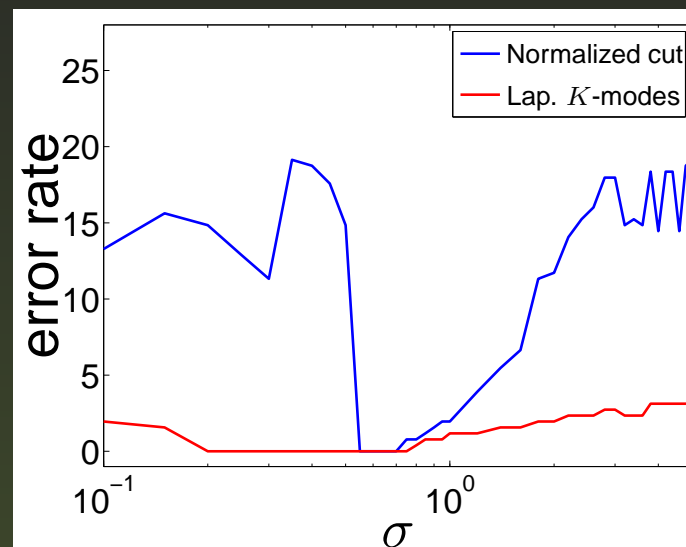
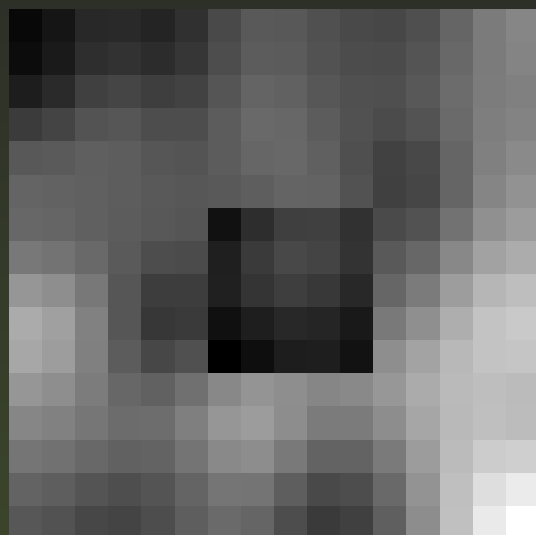
2: Find $\rho = \max\{1 \leq j \leq K : u_j - \frac{1}{j}(\sum_{r=1}^j u_r - 1) > 0\}$

3: Define $\theta = \frac{1}{\rho}(\sum_{r=1}^{\rho} u_r - 1)$

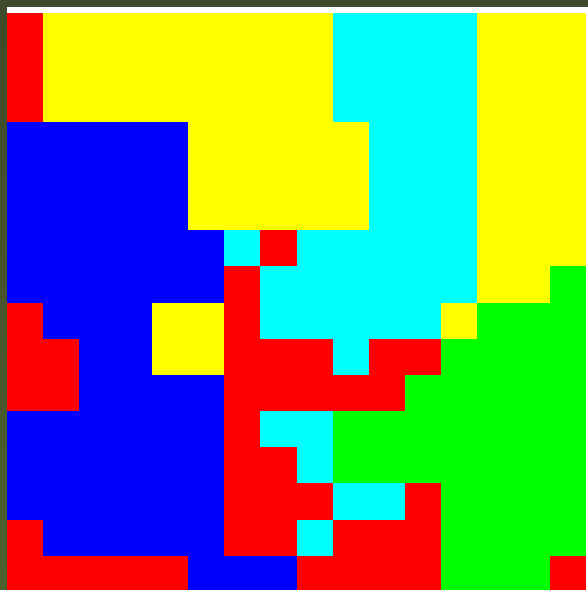
Output: \mathbf{w} s.t. $w_i = \max\{v_i - \theta, 0\}$

Computational complexity: $\mathcal{O}(K \log K)$.

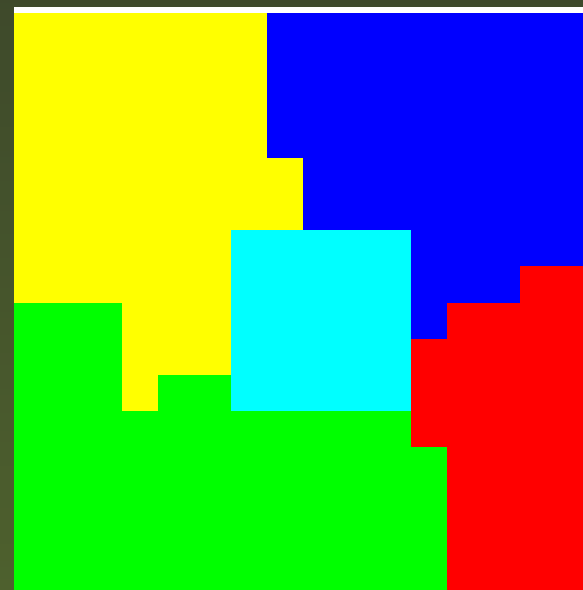
Laplacian K -modes: occluder segmentation



Normalized cut ($\sigma = 0.2$)



Laplacian K -modes ($\sigma = 0.2$)



 $K = 5$. Each pixel is connected with nearby eight pixels with edge weighted using heat kernel.