Learning & Exploiting Low-Dimensional Structure in High-Dimensional Data

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with Didong Li & Minerva Mukhopadhyay

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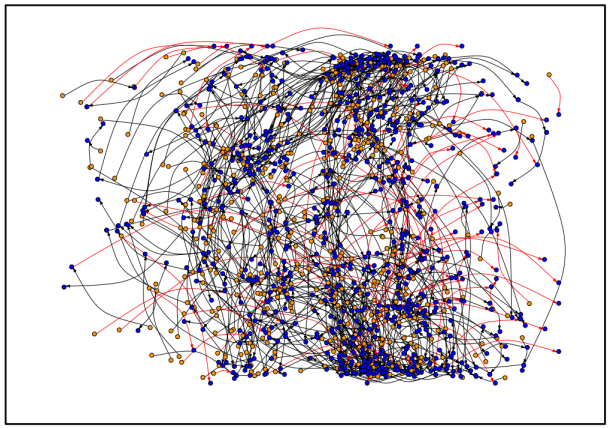
Overview

1. Background and Motivation
2. Manifold learning
   - New Dictionary: Spherelets
   - Spherical Principal Component Analysis (SPCA)
   - Algorithm & Examples
3. Density estimation
   - Fisher-Gaussian Kernel
   - Examples
4. Classification
5. Geodesic distance estimation

Motivation



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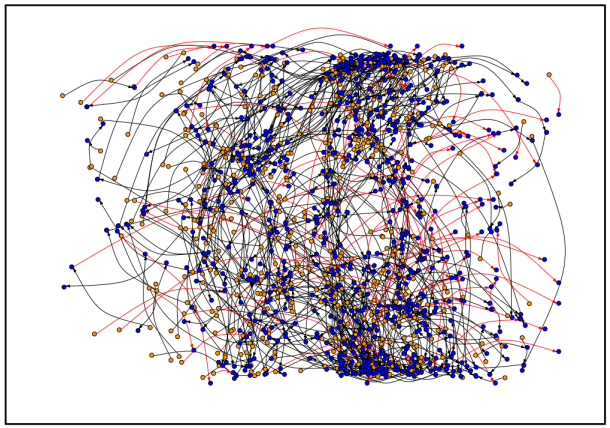

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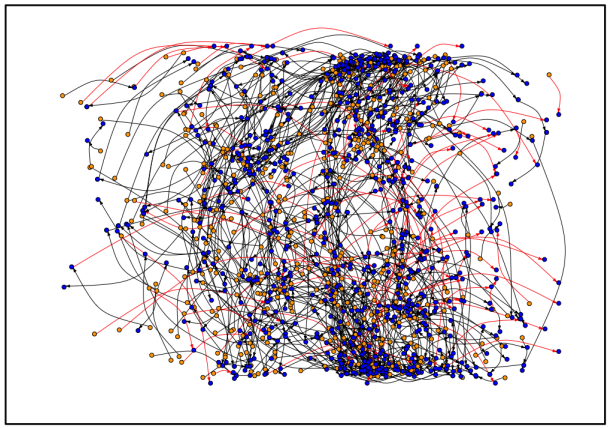

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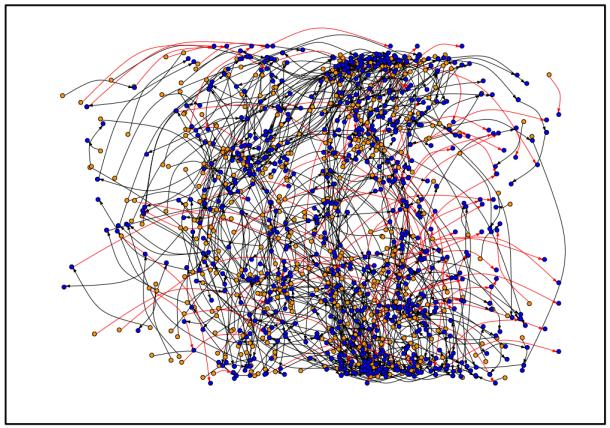

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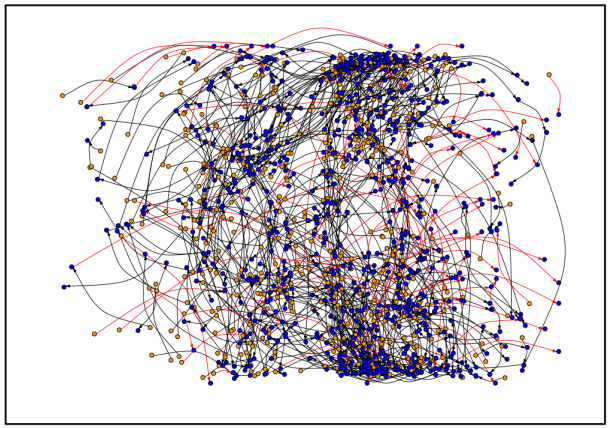

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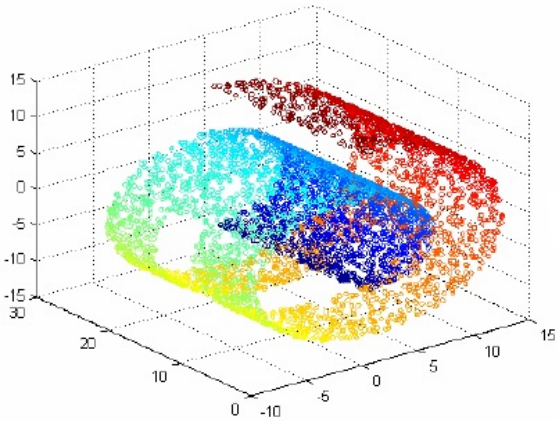
- Uncertainty quantification is of paramount importance

Dimensionality Reduction



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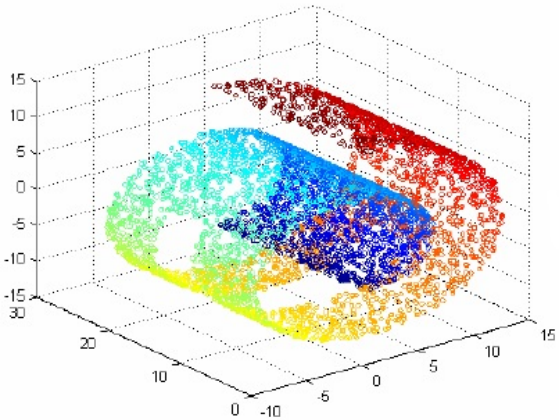

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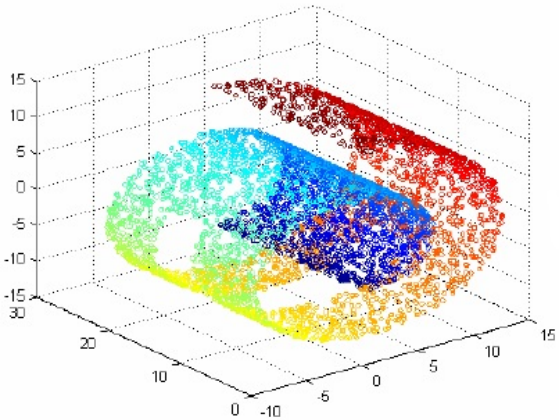

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- Then, dimension reduction can be based on the model:

$$X_i = f(\eta_i) + \epsilon_i,$$

where $\eta_i = (\eta_{i1}, \ldots, \eta_{id})'$ are latent factors, $f(.)$ is an unknown function, and ϵ_i is a zero-mean measurement error

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- Our goal: develop simpler approaches including non-linear alternatives to PCA & model-based methods

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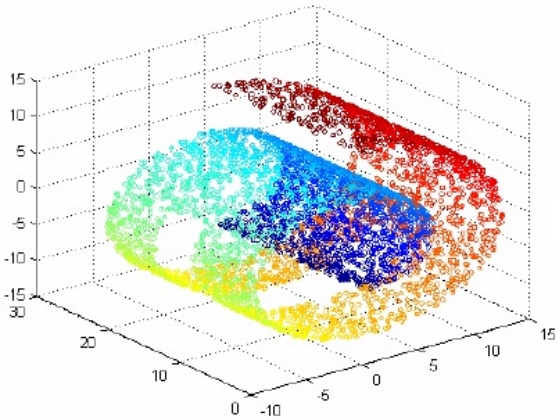

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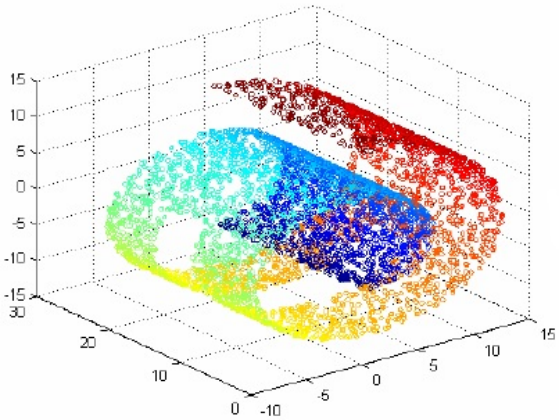

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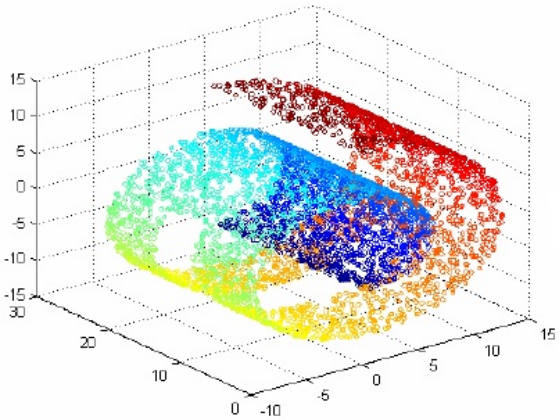

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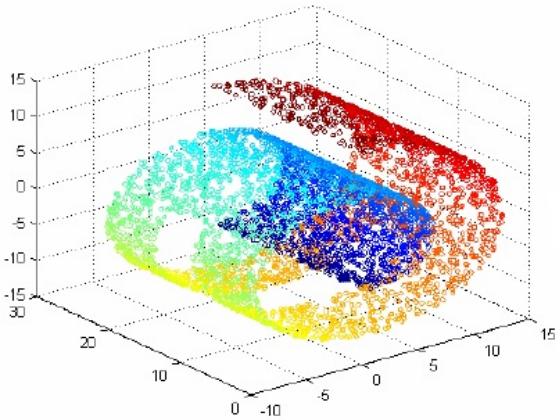

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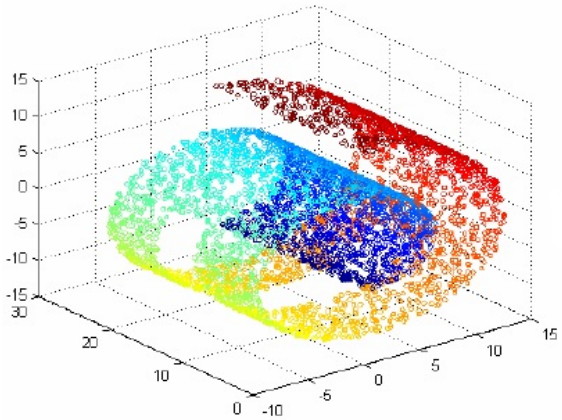

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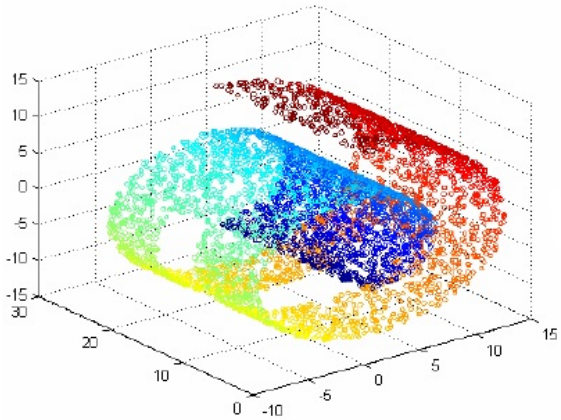

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- Misnomer in that manifold estimates are typically not produced - black box for dimensionality reduction

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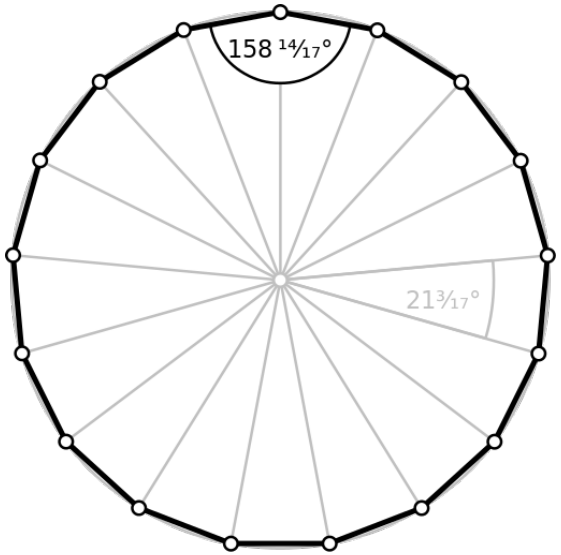
- BUT too many pieces are needed when $\mathcal{M}$ has large curvature



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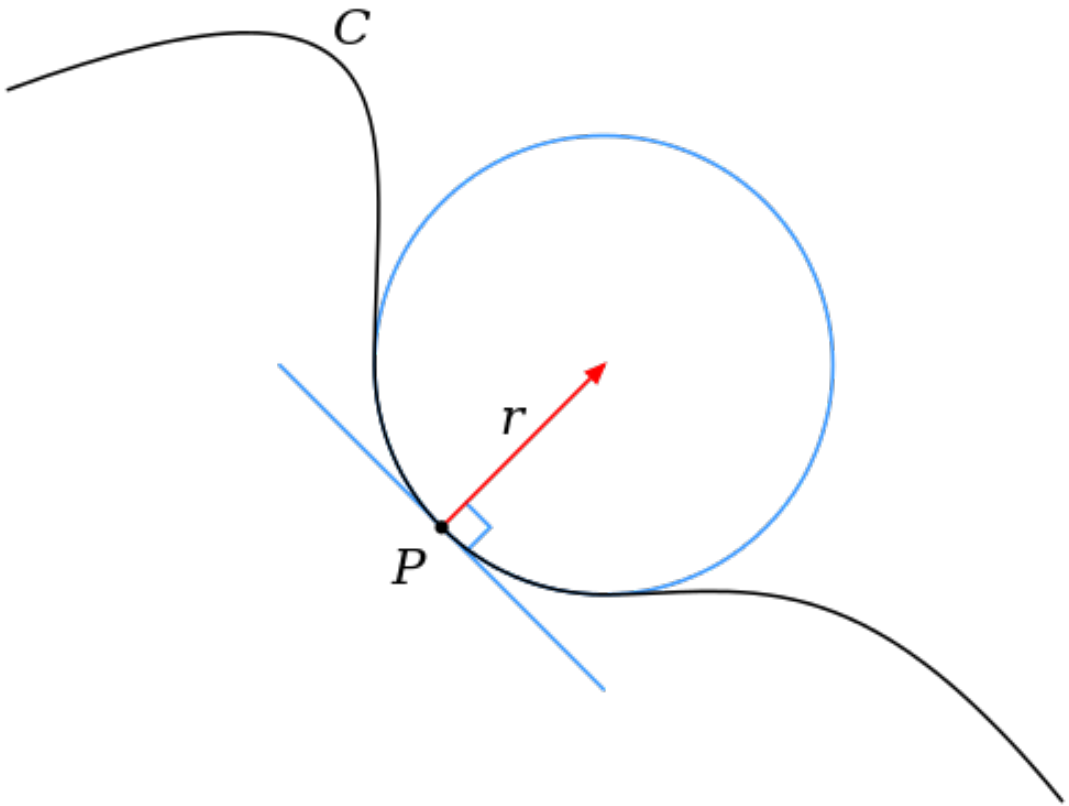
- An alternative is “osculating” circles/spheres



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- Before considering algorithms for fitting spherelets, we (briefly) consider their approximation properties

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- K=max curvature, T=maximum rate of change in curvature, V = Vol($\mathcal{M}$).

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Theorem (Li, Mukhopadhyay, D., 18')

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$$N_S(\epsilon, \mathcal{M}) \leq V_\epsilon\left(\frac{6\epsilon}{3+T}\right)^{-\frac{d}{3}} + (V - V_\epsilon)\left(\frac{2\epsilon}{K}\right)^{-\frac{d}{2}}$$

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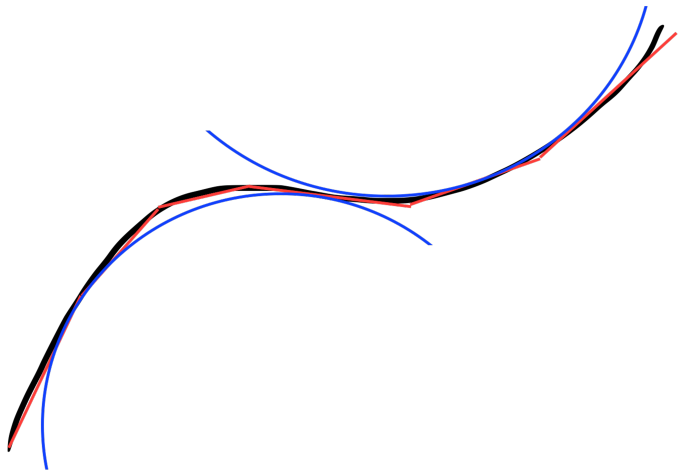

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$$\widehat{c} = -\frac{1}{2}\left(\sum_{i=1}^n (\bar{Y} - Y_i)(\bar{Y} - Y_i)^\top\right)^{-1} \sum_{i=1}^n \left(\|Y_i^\top Y_i\| - \frac{1}{n}\sum_{j=1}^n \|Y_j^\top Y_j\|\right)(\bar{Y} - Y_i).$$

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Spherical principal component analysis (SPCA)

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- SPCA minimizes the loss function

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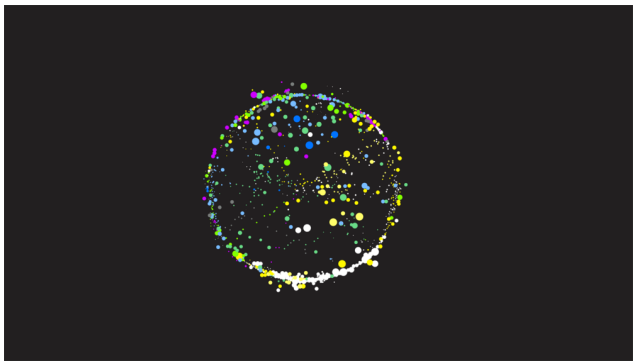

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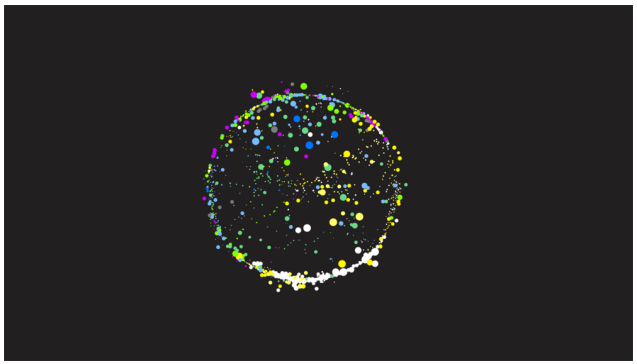

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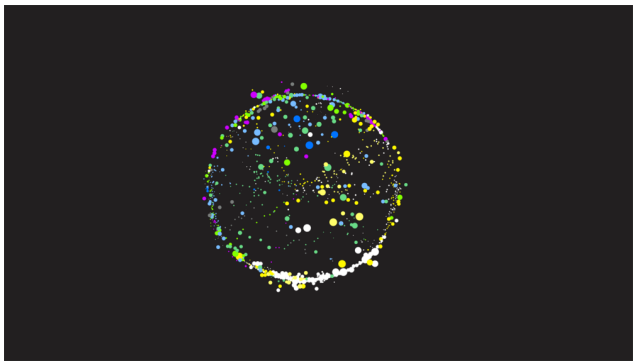

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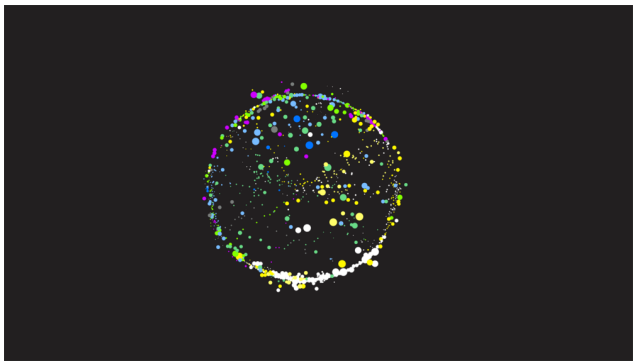

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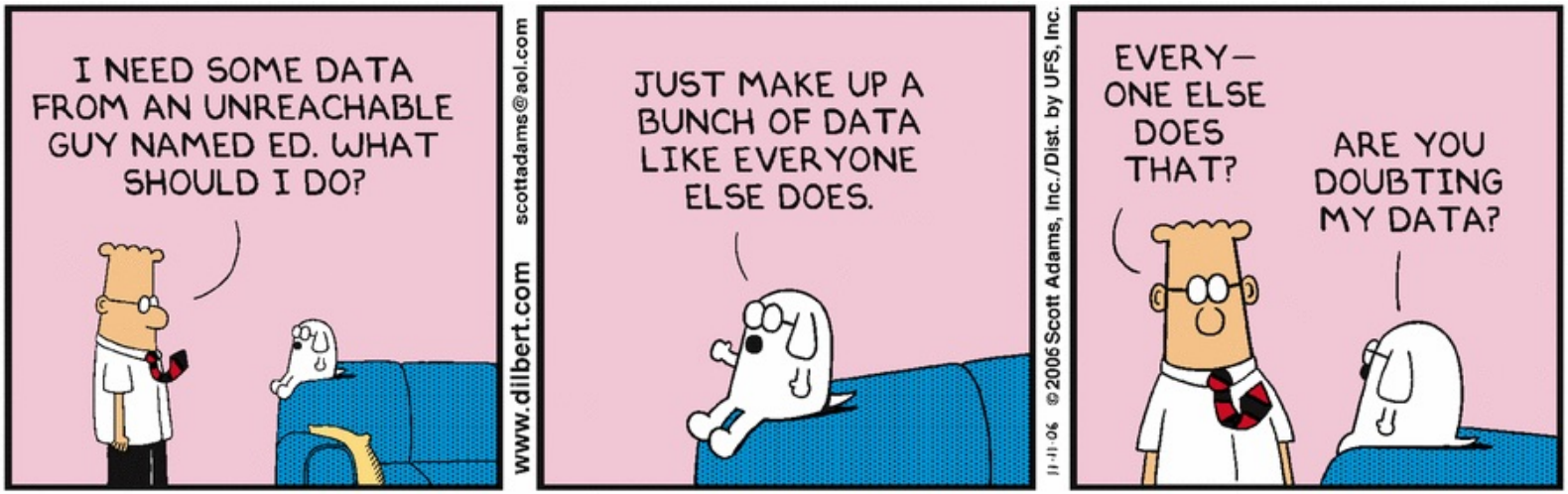
Analyzing data using spherelets



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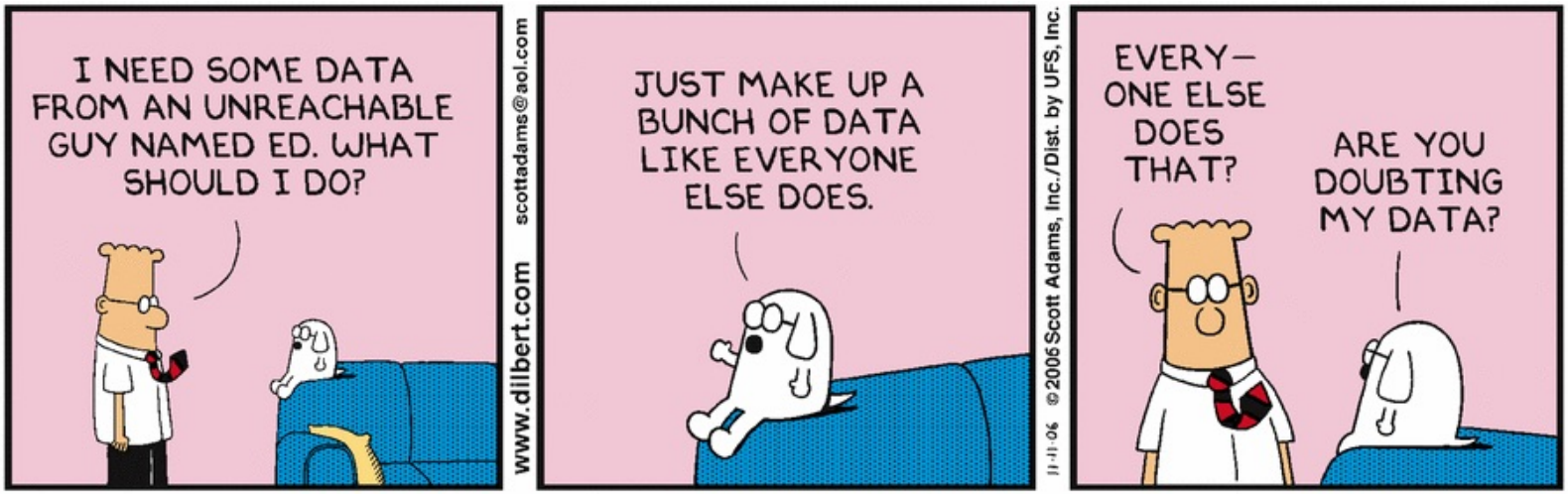

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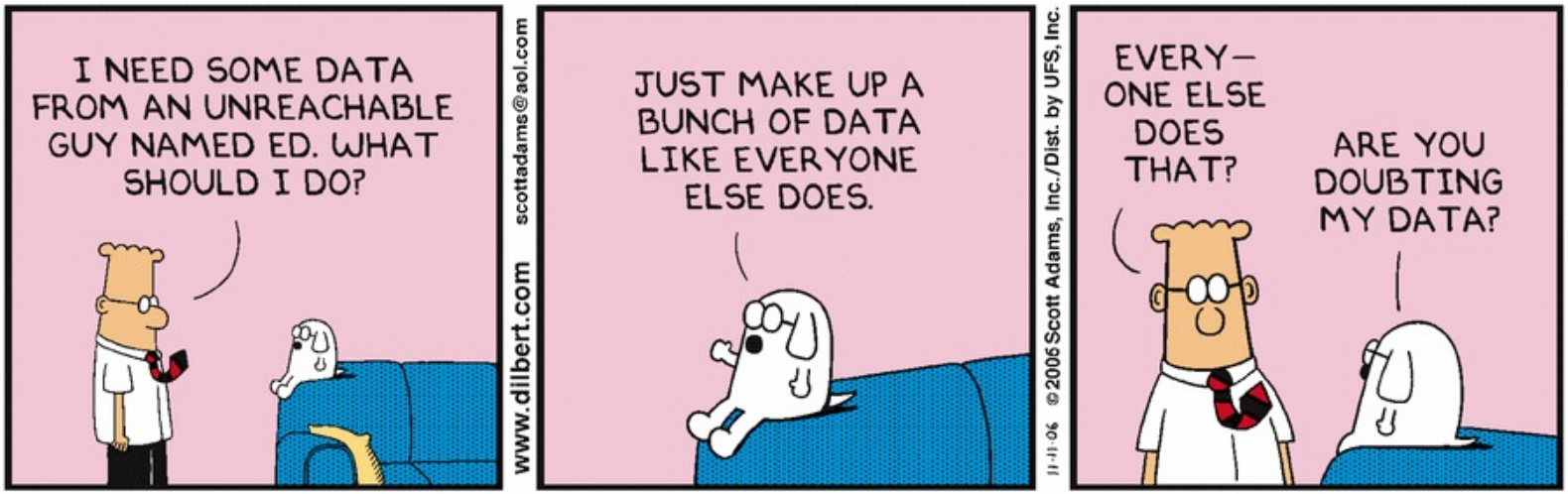

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- Initially develop simple local SPCA algorithm & compared to local PCA

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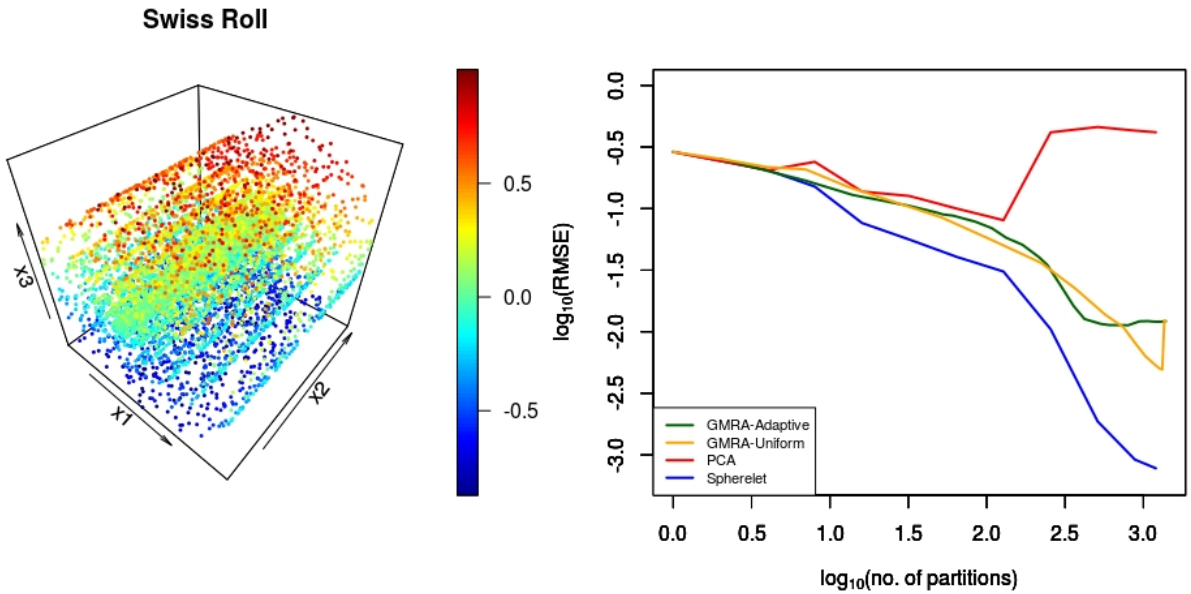

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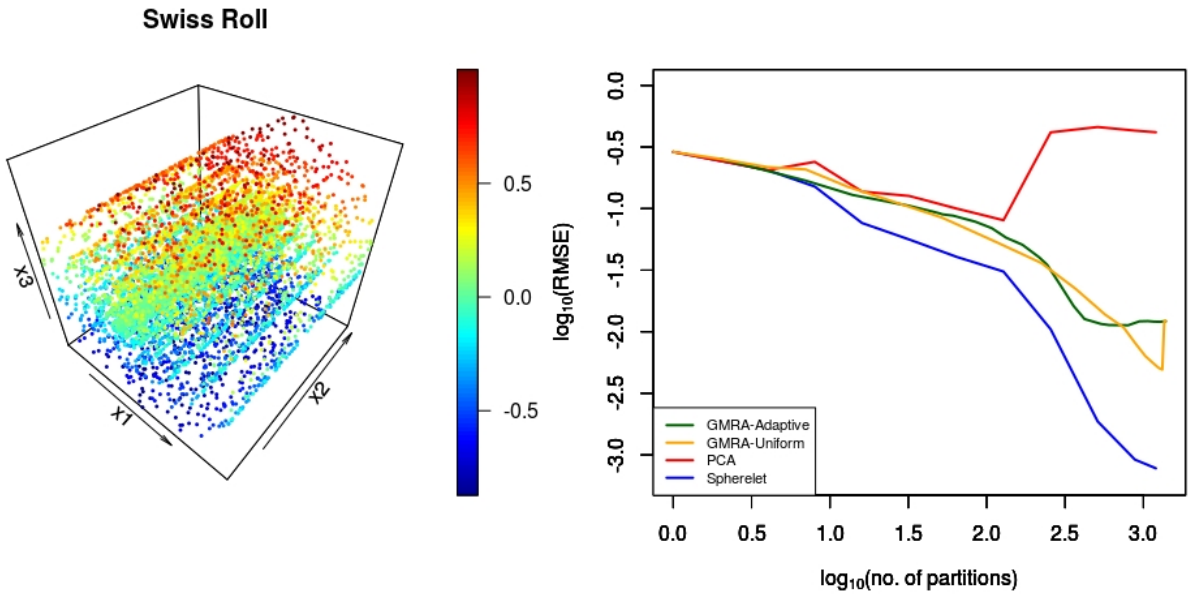

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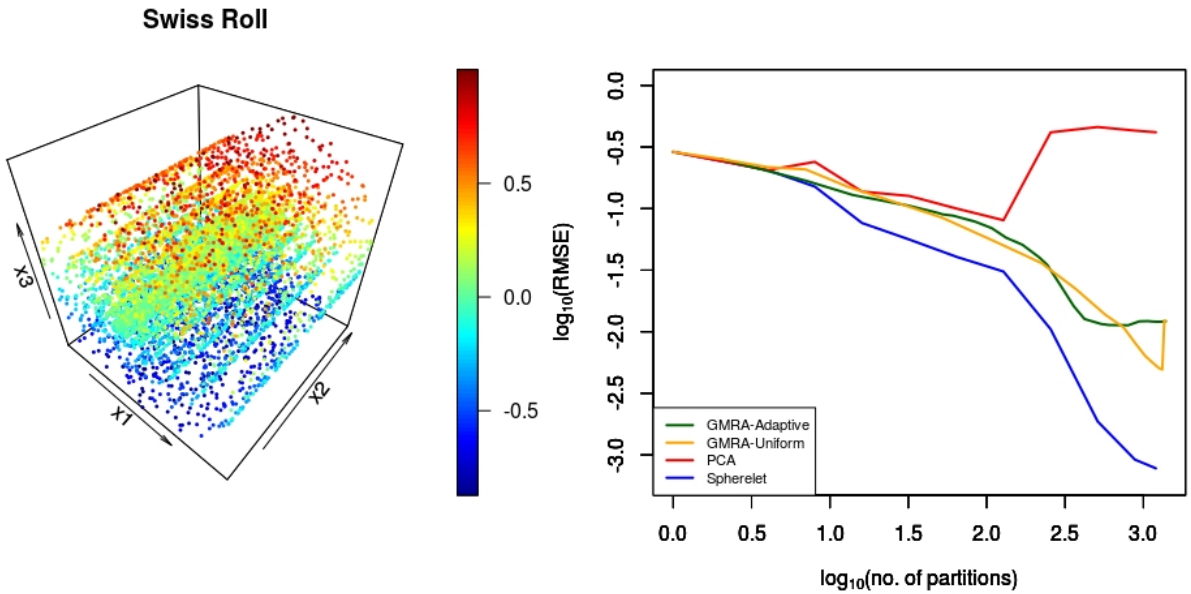

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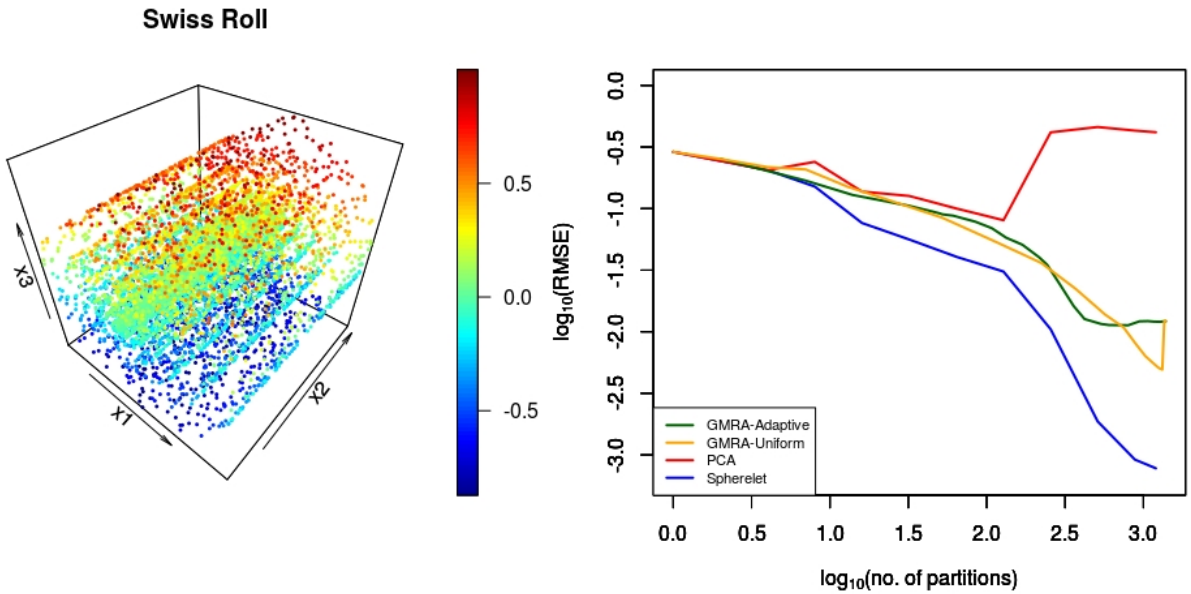

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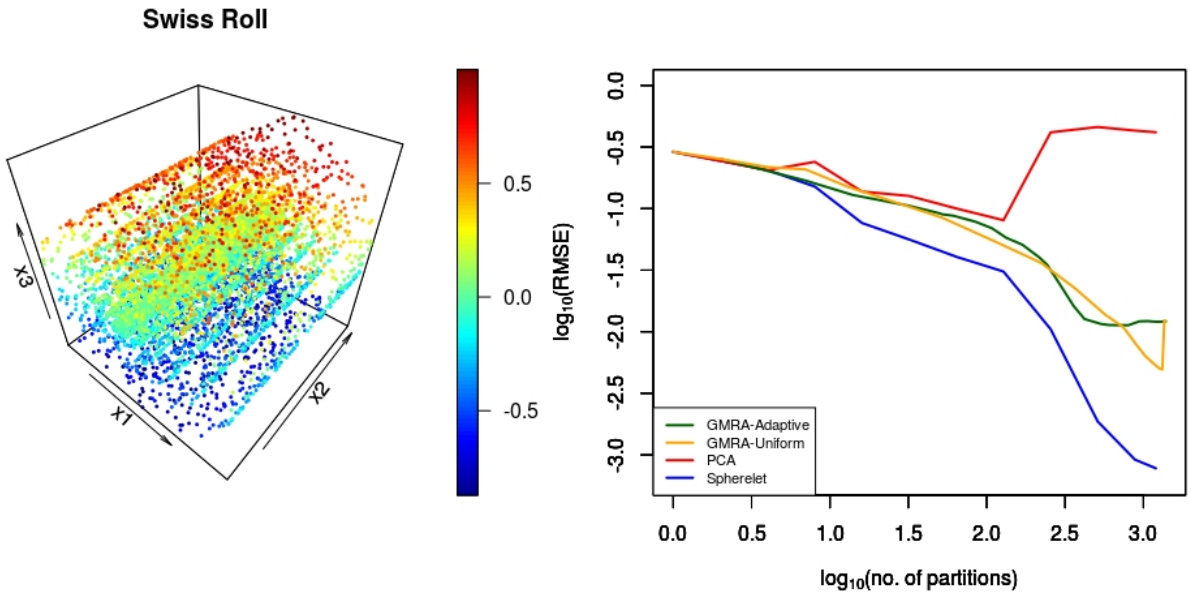

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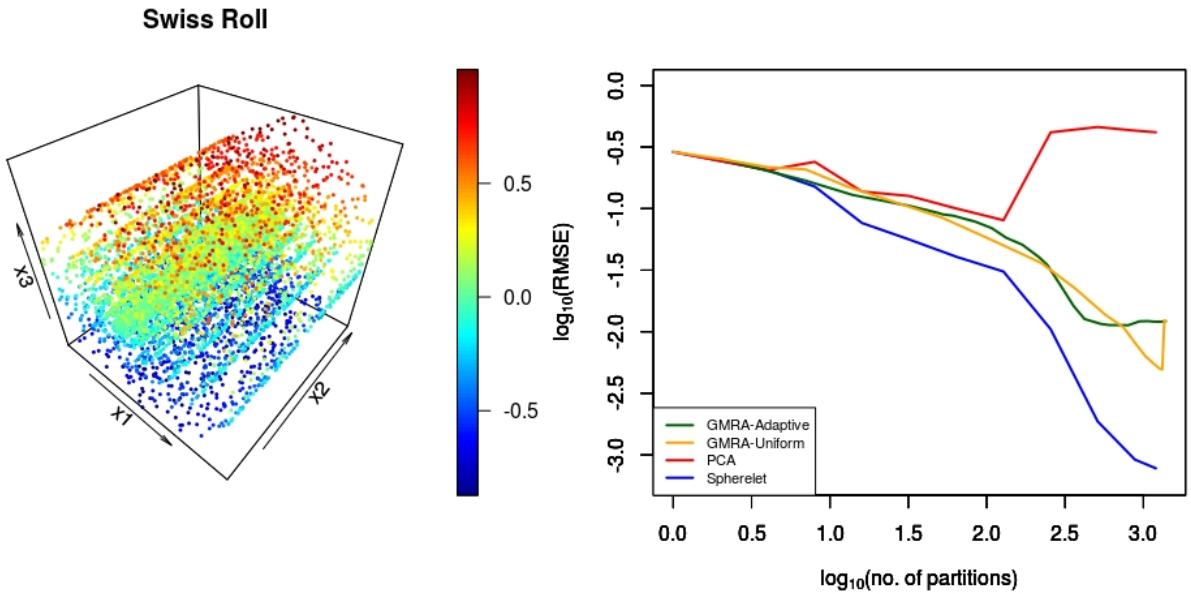

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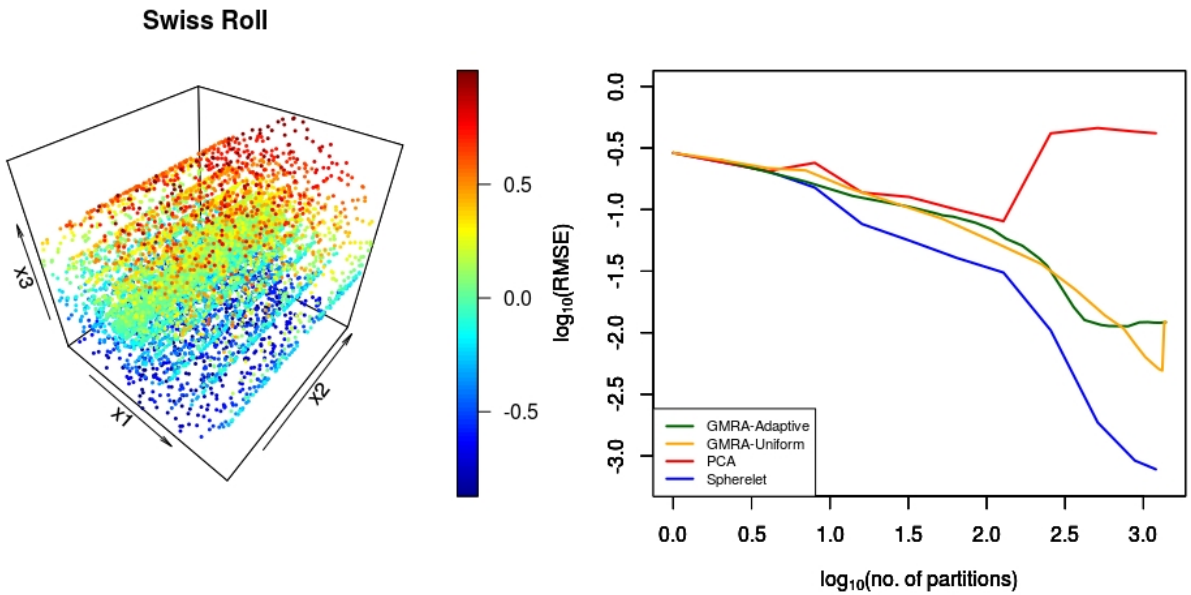

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- Spirals, olympic rings, swiss roll, armadillo, dragon & real datasets (Iris, EUStockMarkets, Seals, banknotes, quakes)

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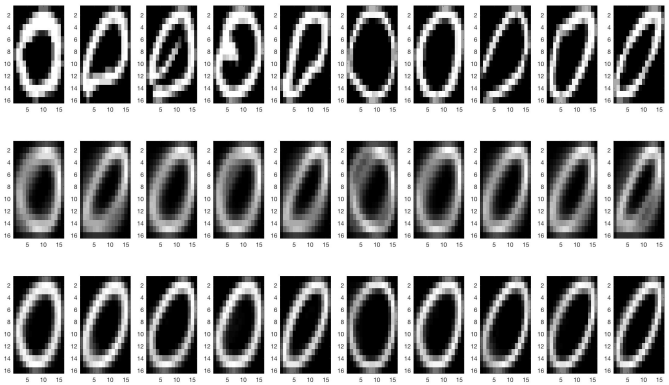
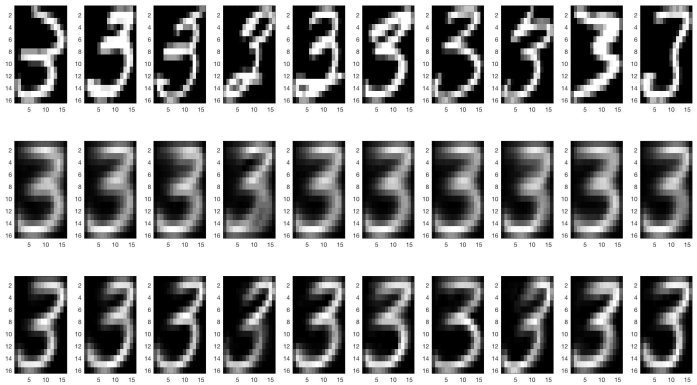
- We modify MBMS by applying spherelets to provide a locally spherical projection instead of linear by replacing local PCA by local SPCA.

Denoising

Application on USPS Hand written digits images ($D = 256$).





The first row: original data;
The second row: denoised data by MBMS;
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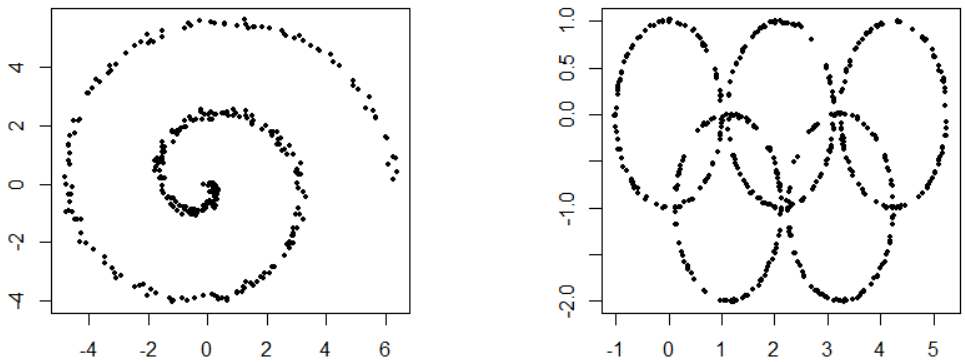
- Also, we want to incorporate uncertainty quantification & allow easy extensions to more complex settings

Density estimation with non-linear support



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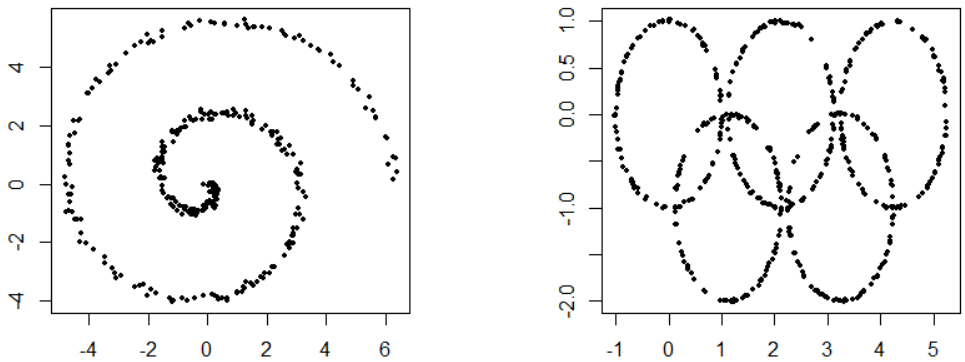

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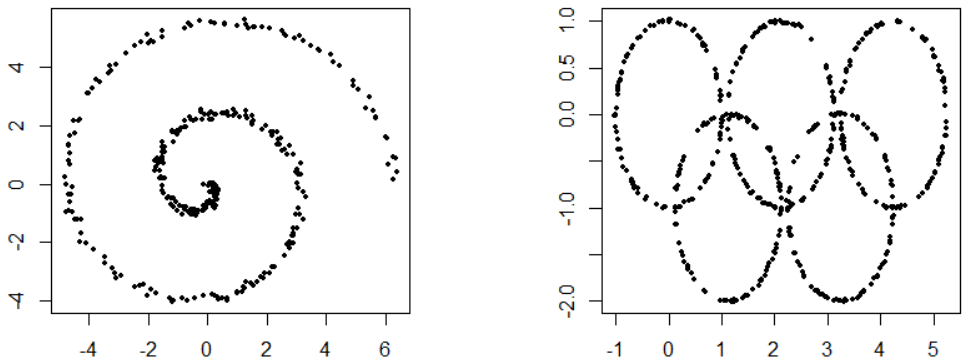

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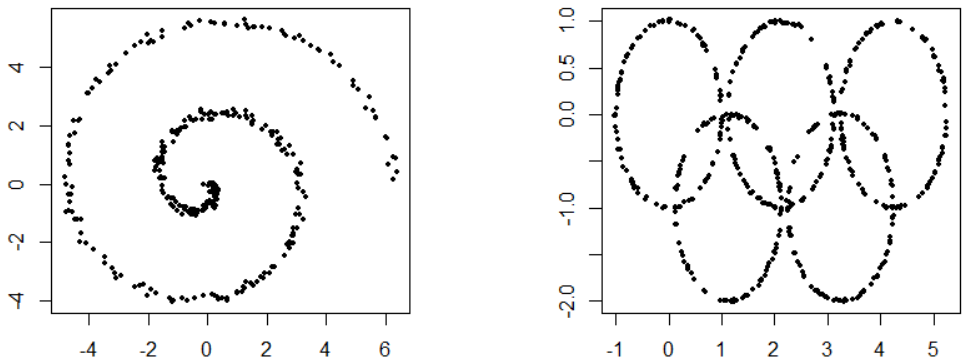

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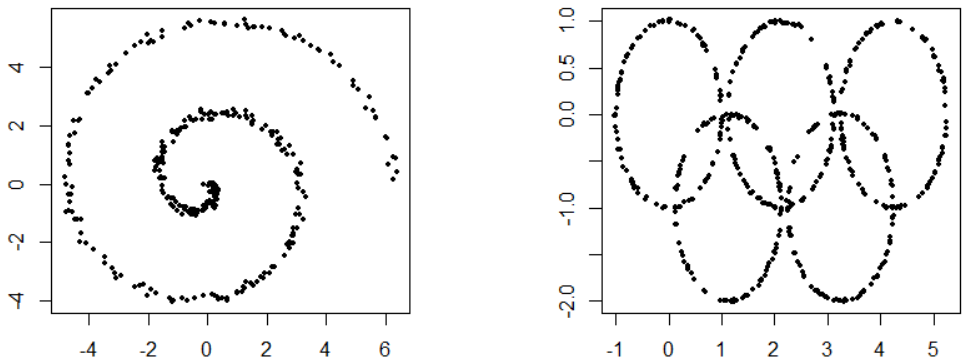

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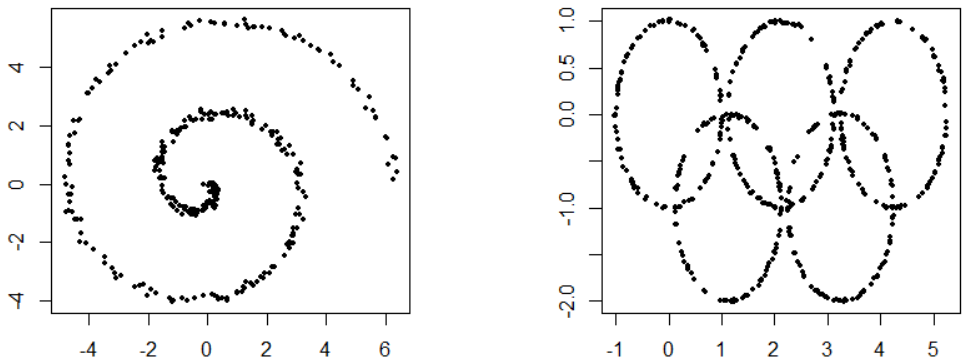

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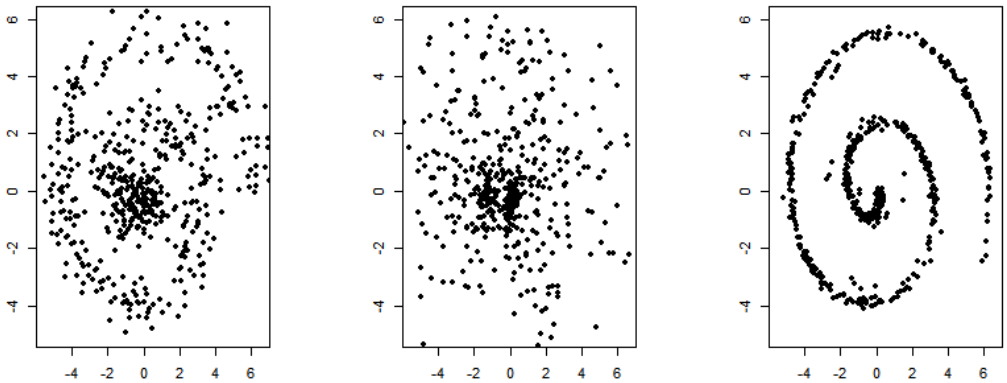
- Are current density estimation methods adequate in the presence of such relationships?

Current density estimation methods



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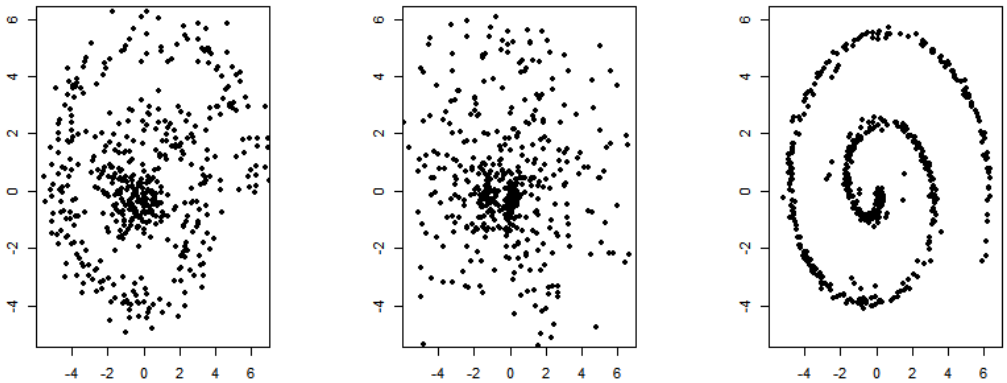

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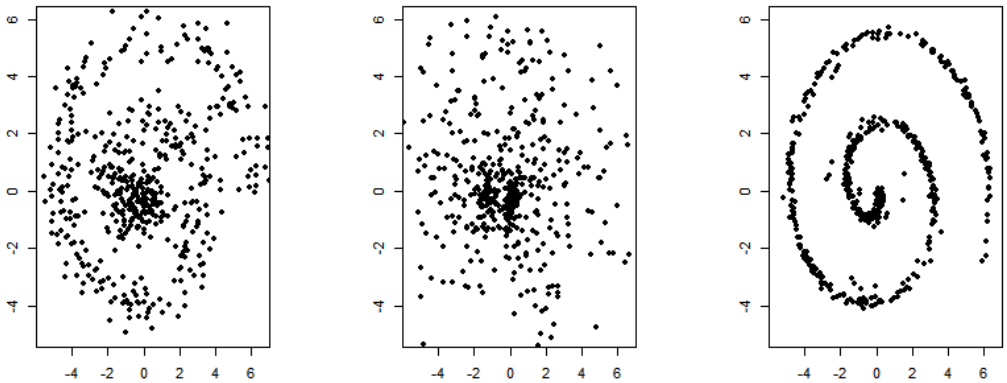

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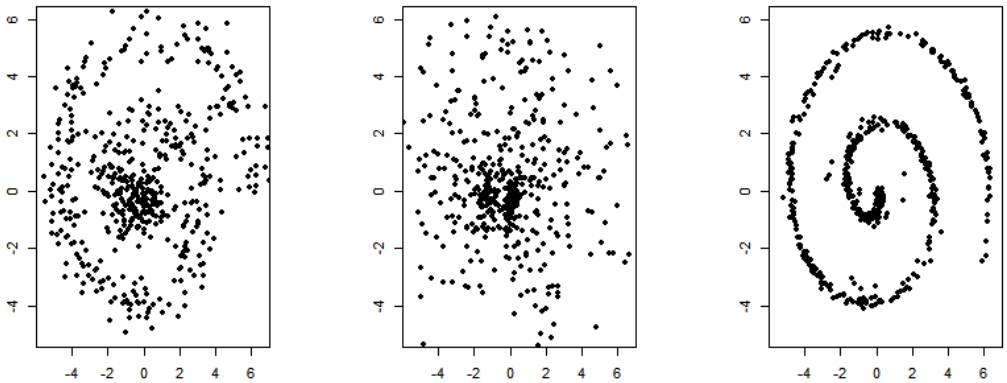

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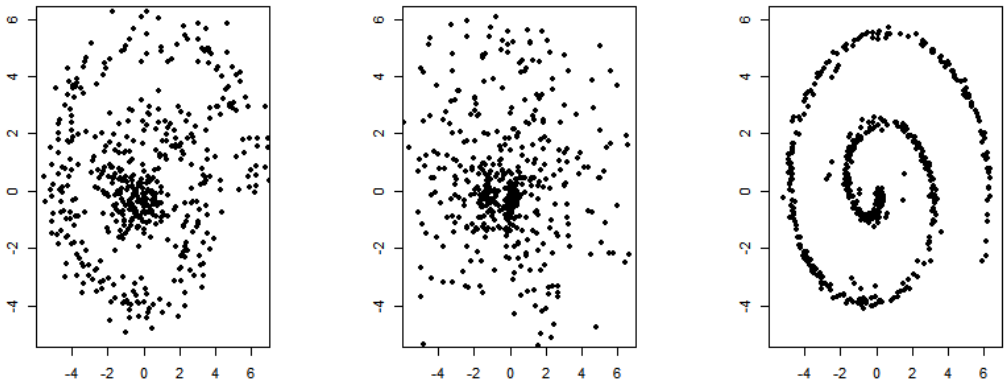

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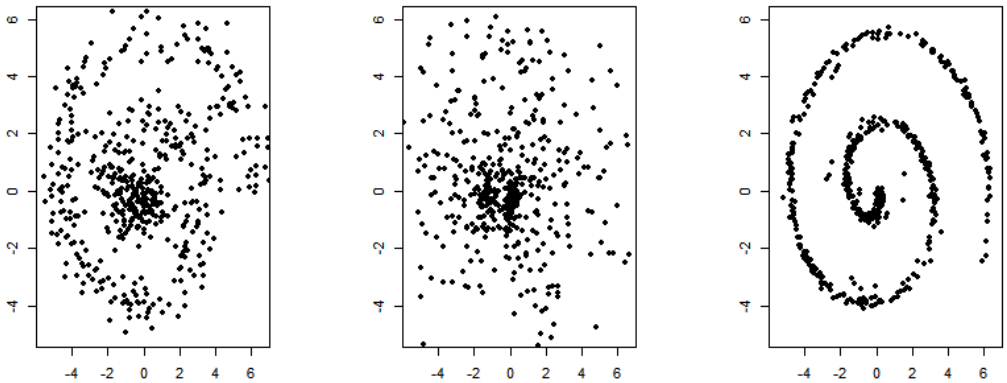

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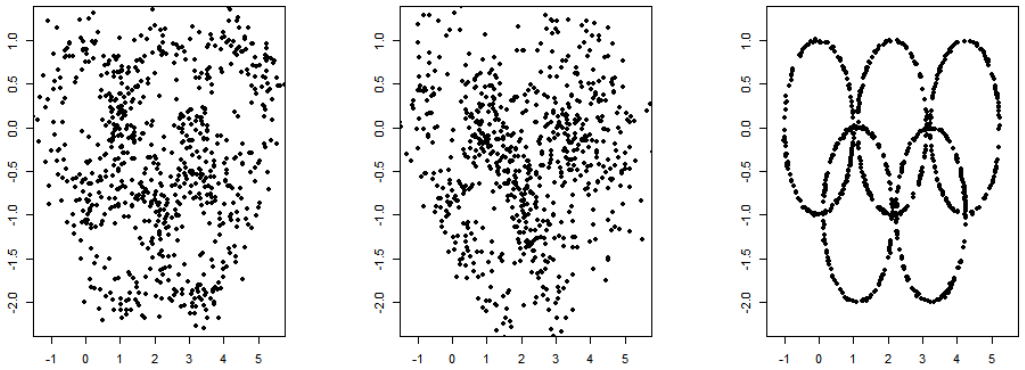
- MIDDLE = samples from density estimated with KMM; using Dirichlet process (DP) mixture of multivariate Gaussians

Current density estimation methods



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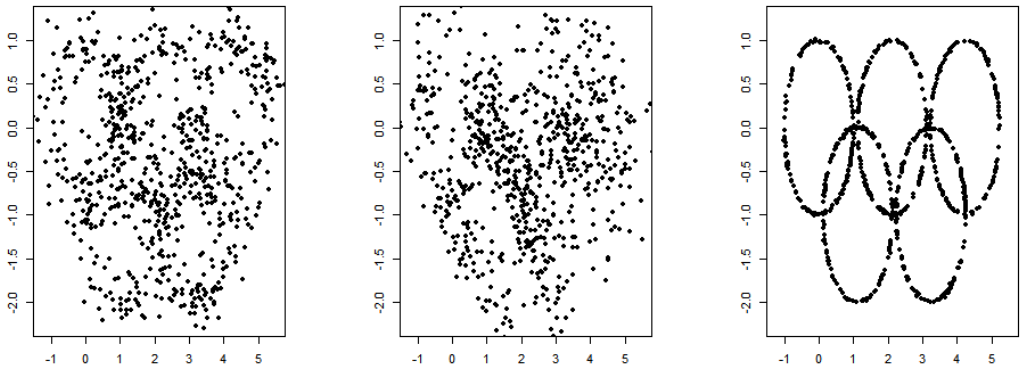

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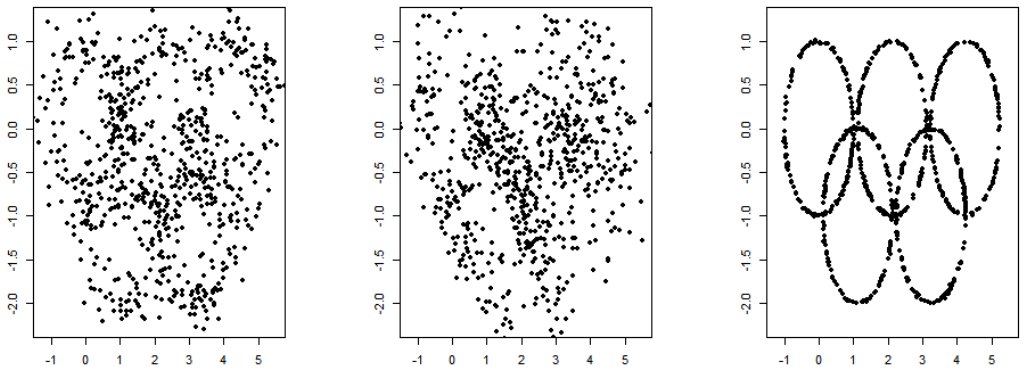

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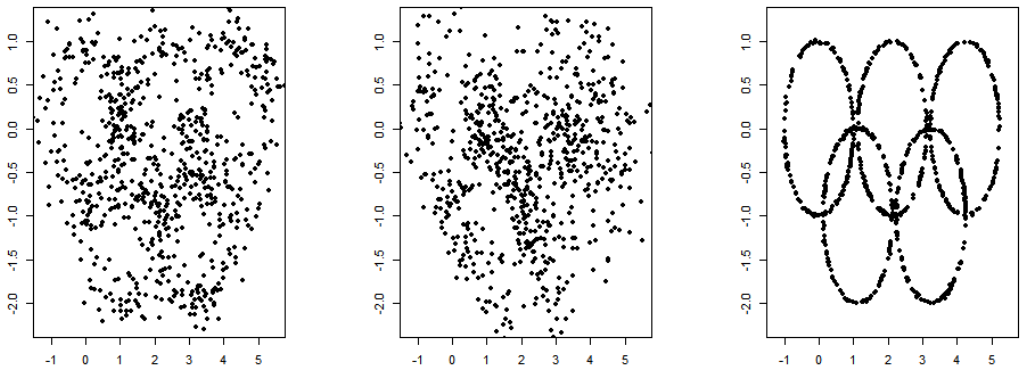

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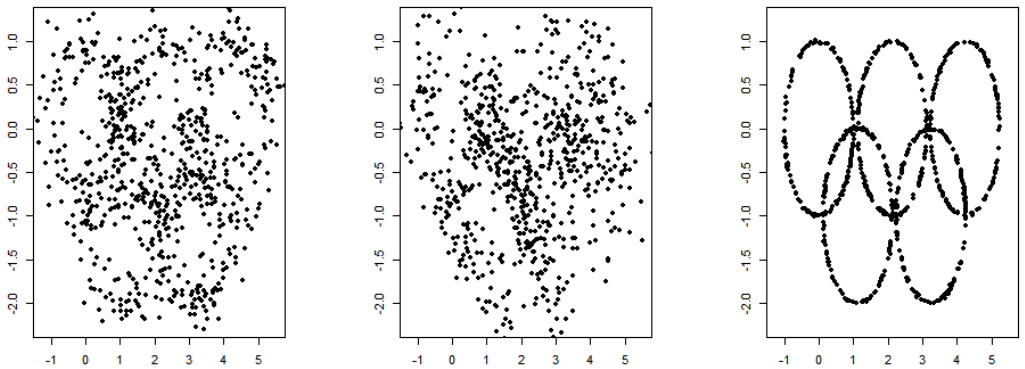

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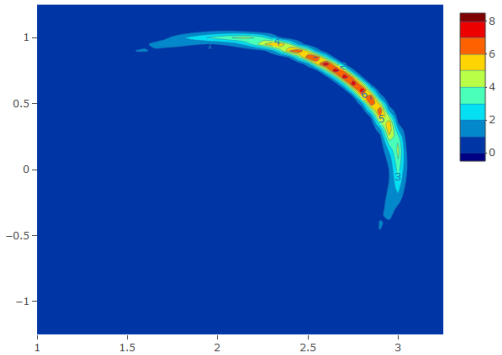
- MCMC mixing becomes a significant issue, as posterior sampling algorithms struggle here

Choosing a better kernel



- Why does the Gaussian kernel suck so bad?

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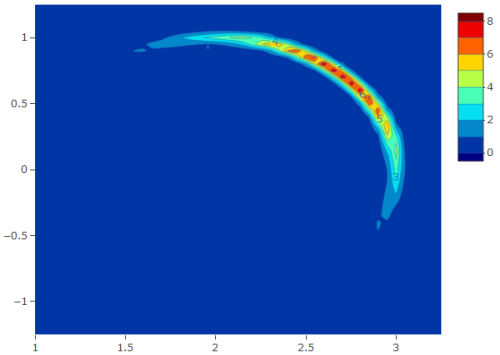

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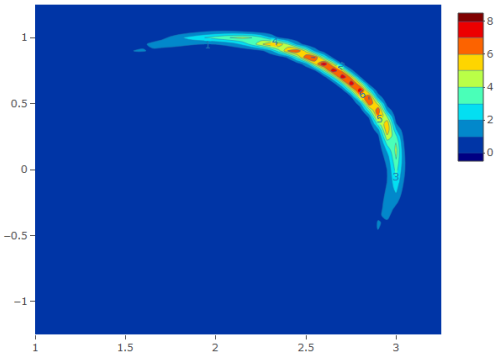

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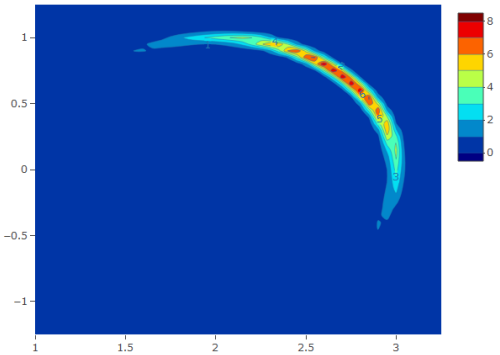

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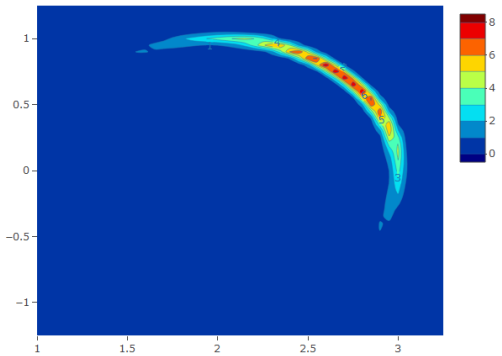

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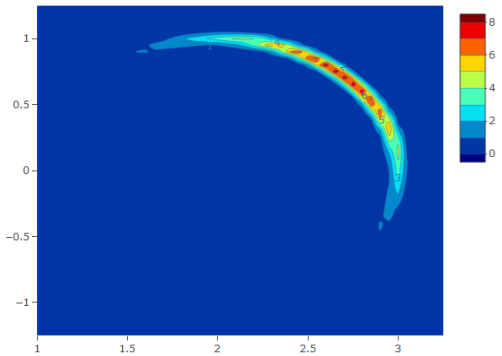

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- There is a huge literature on kernels/multivariate pdfs but mostly on skewed, heavy tails etc

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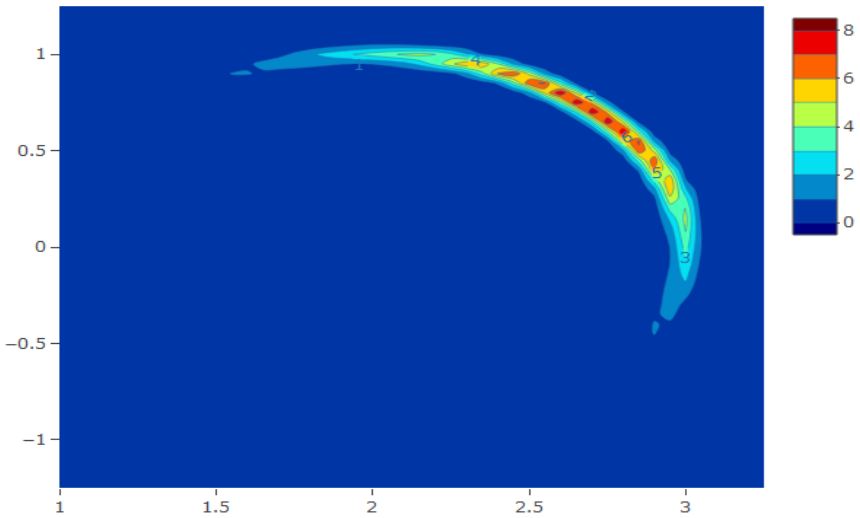
- The resulting FG density has parameters $\rho = (c, r, \mu, \tau)$:

$$FG_\sigma(x \mid \rho) = \frac{c(\tau)(2\pi\sigma^2)^{-d/2}}{c\left(\|\tau\mu + r(x-c)x/\sigma^2\|\right)} \exp\left\{-\frac{1}{2\sigma^2}\left(\|x-c\|^2 + r^2\right)\right\},$$

with $c(\tau) = \frac{\tau^{d/2-1}}{(2\pi)^{d/2} I_{d/2-1}(\tau)}$ & I_ν the modified Bessel function of the first kind of order ν

Examples of FG kernels



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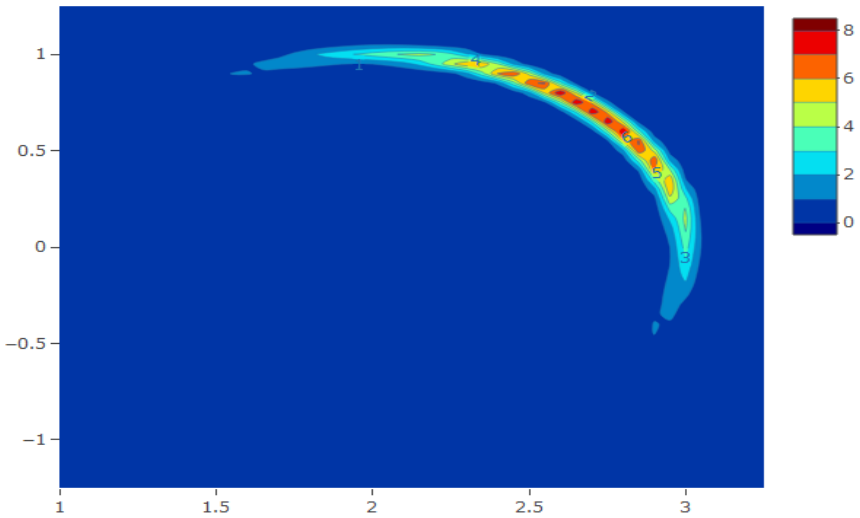

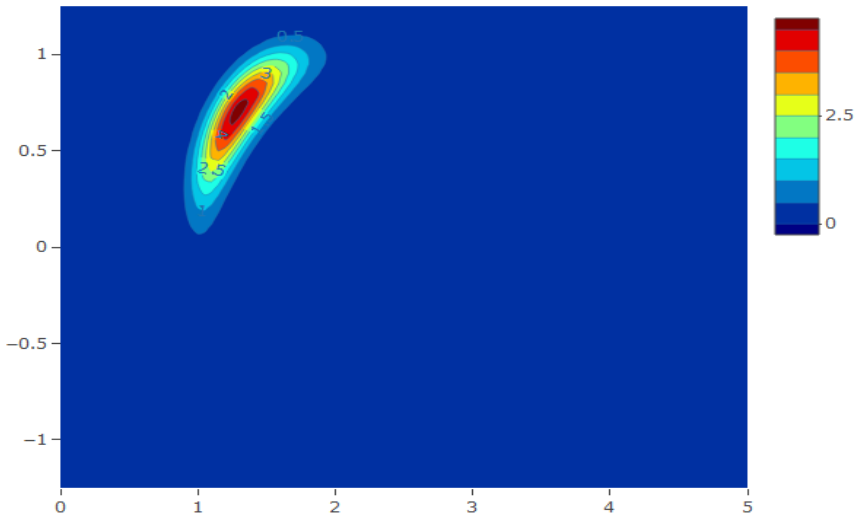

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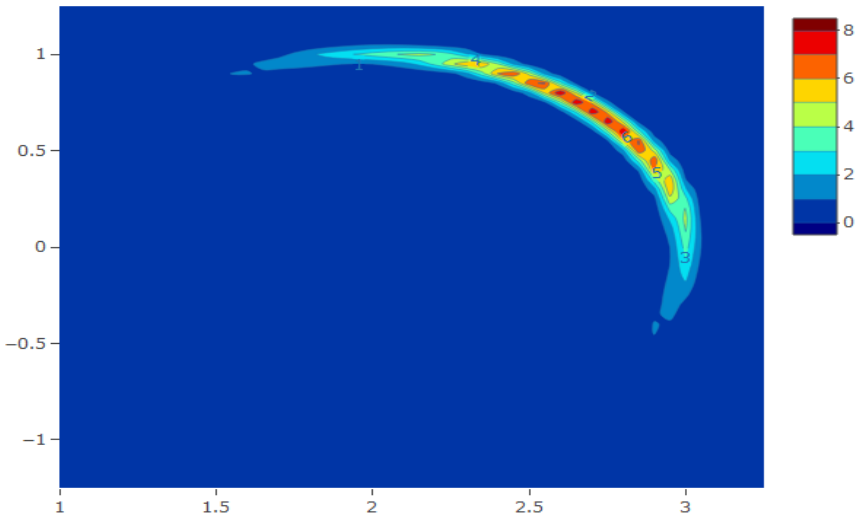

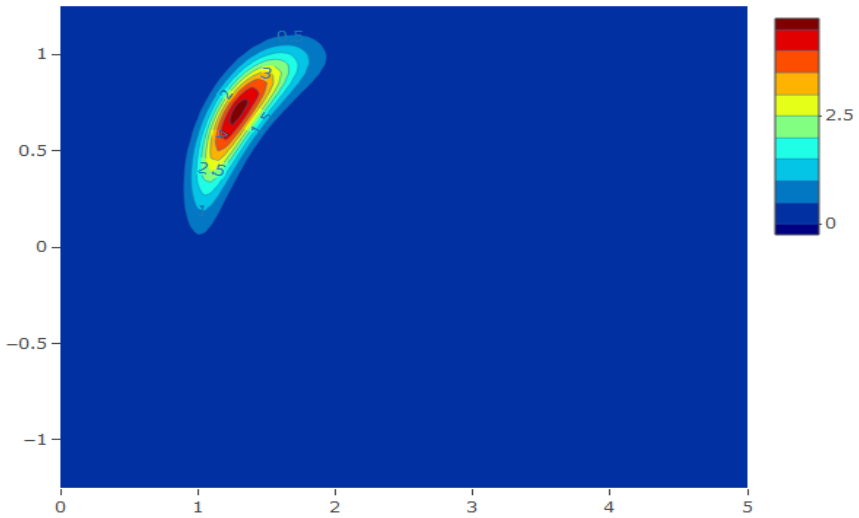

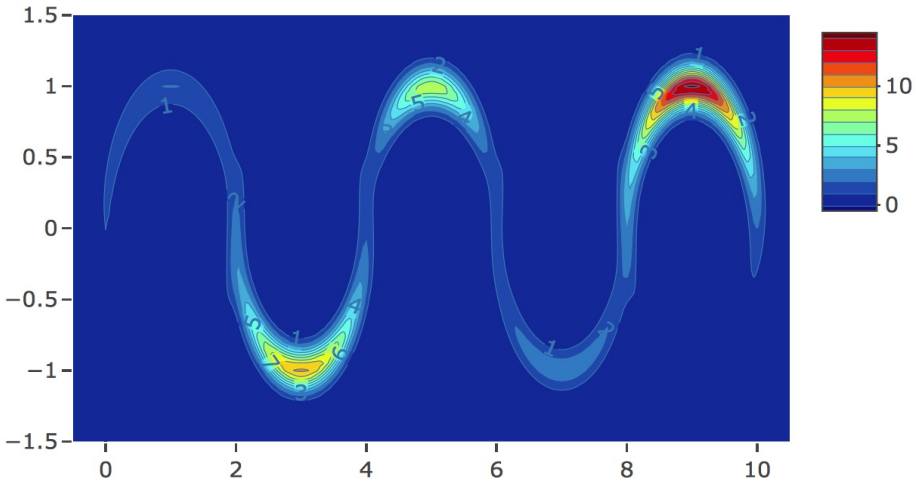

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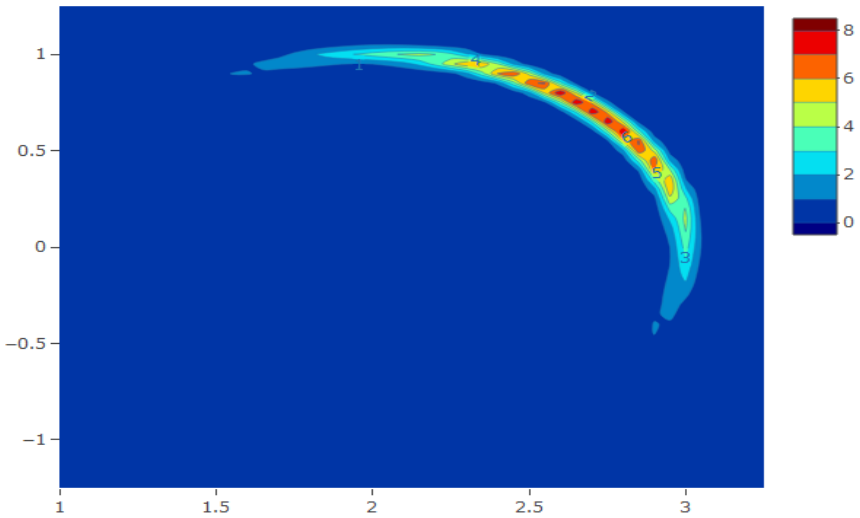

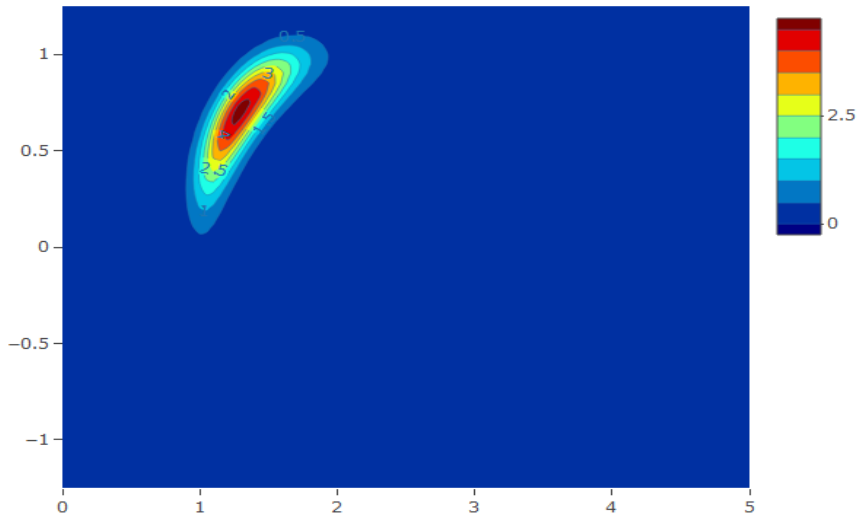

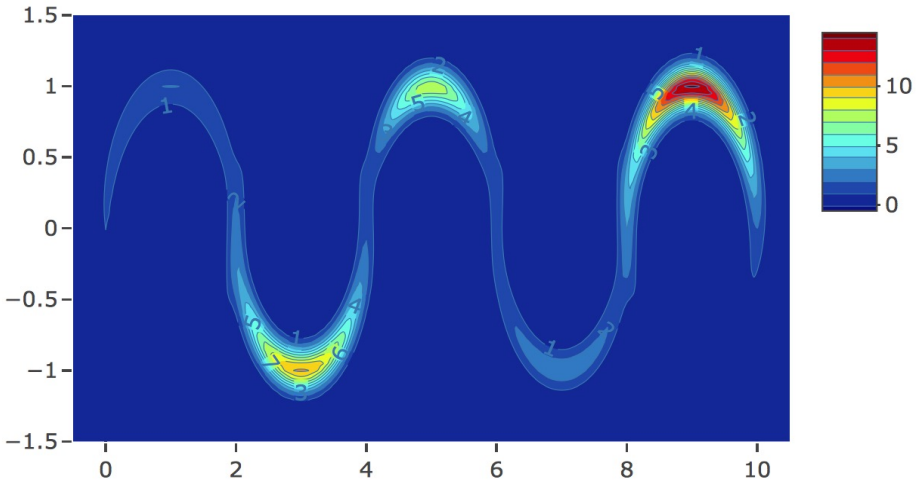

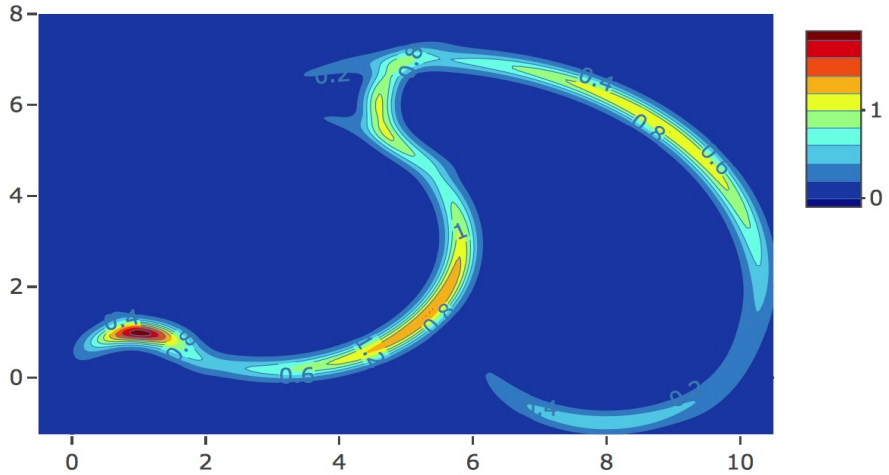

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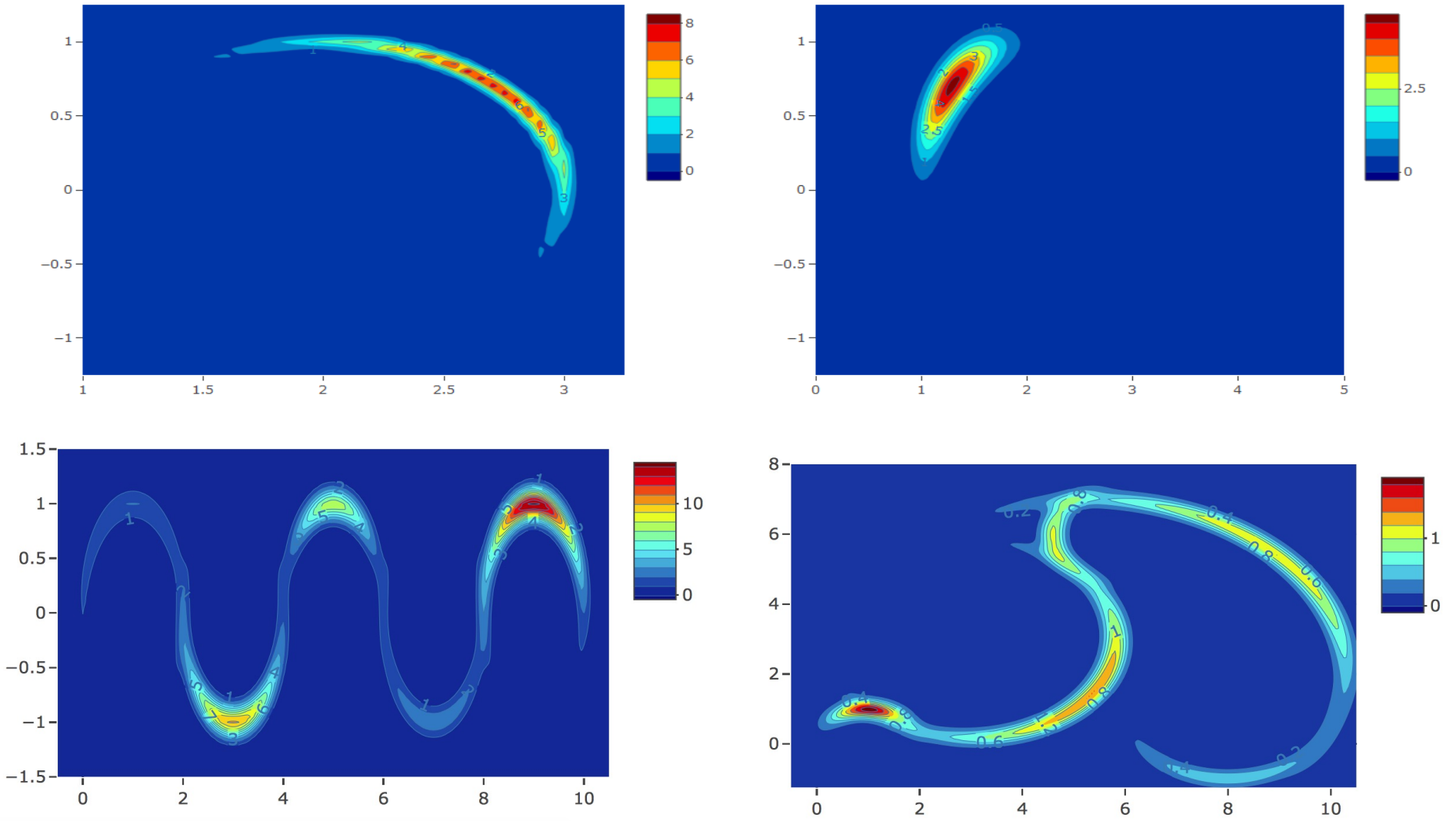
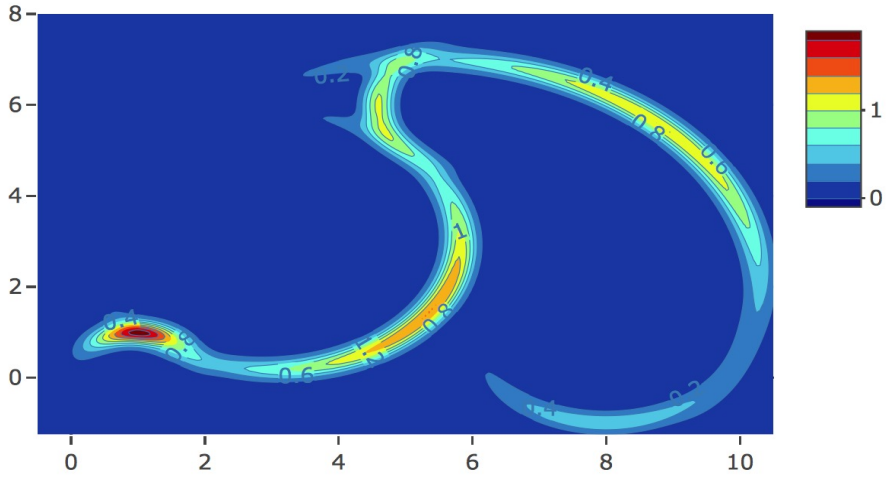


Two single FG kernels and two mixtures of five FG kernels.

FG Mixtures & Implementation



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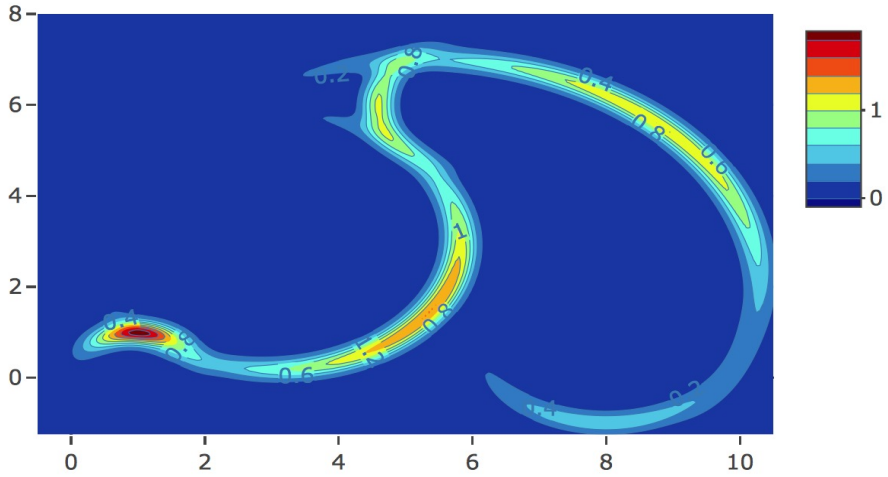

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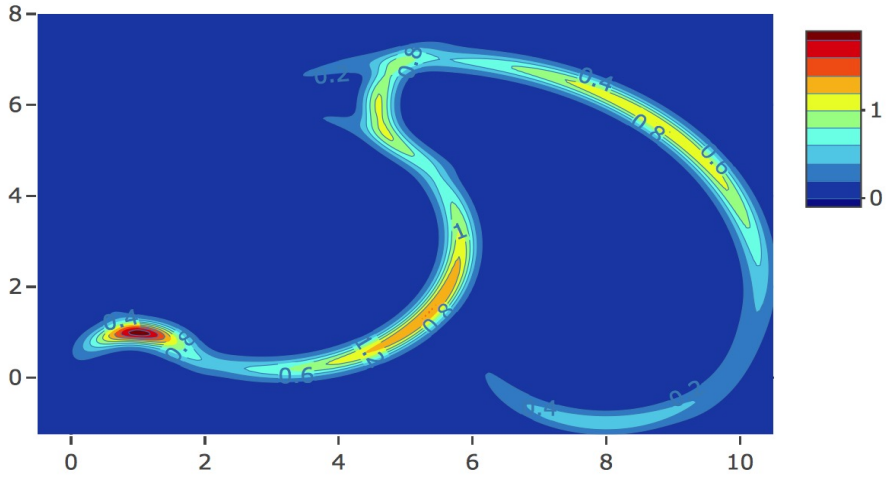

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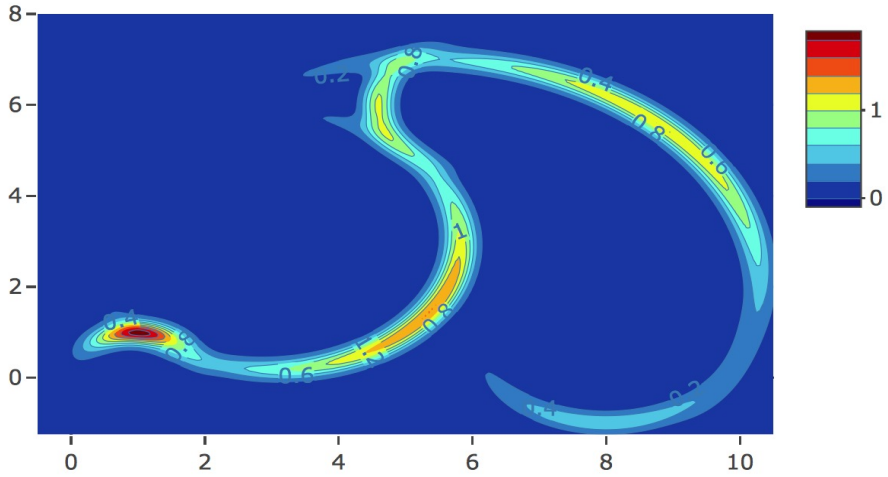

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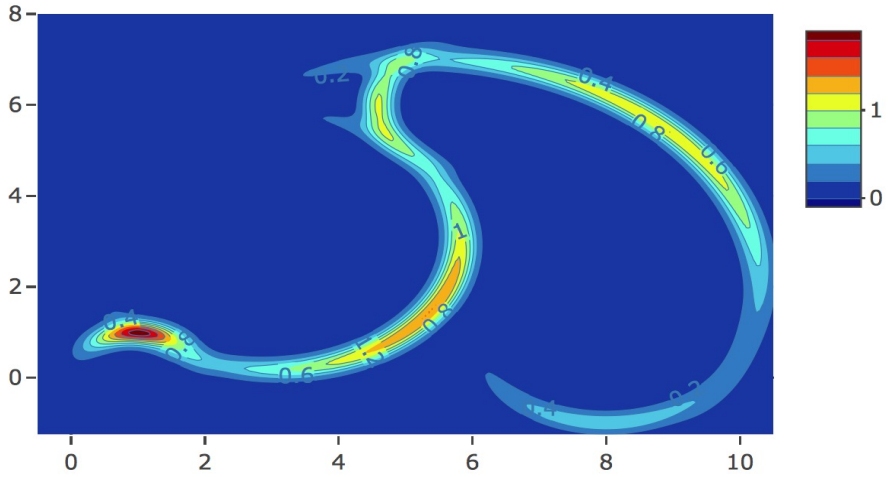

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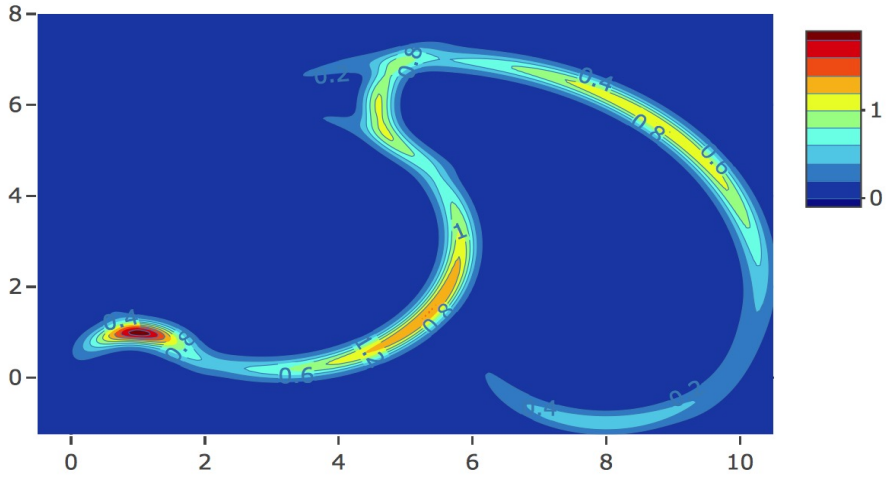

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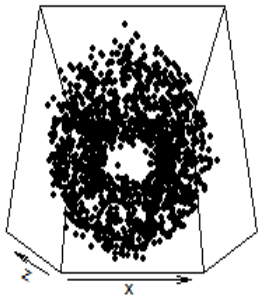
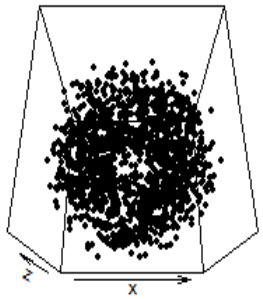
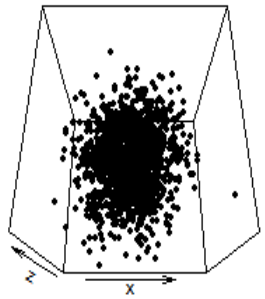
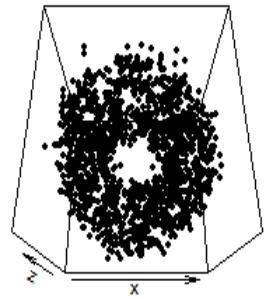
- Let's see how it works in practice!

Predictive samples









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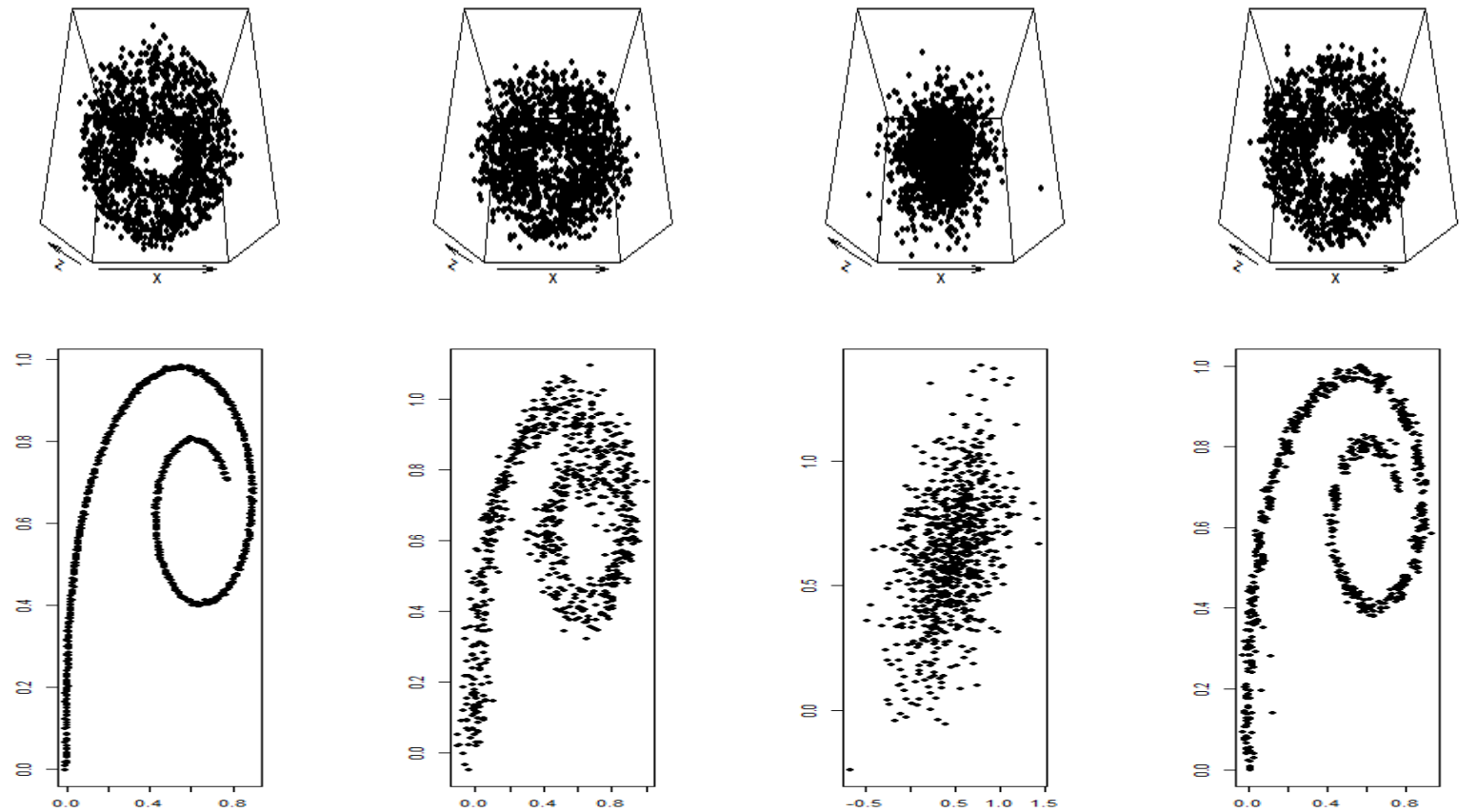
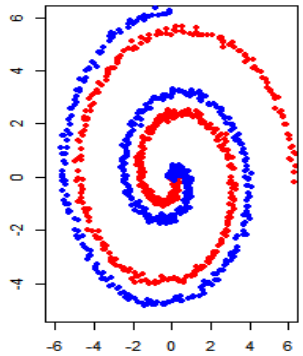


(a) Observations (b) KDE (c) DPMG (d) DPMFG

Two Spiral - Density based classification



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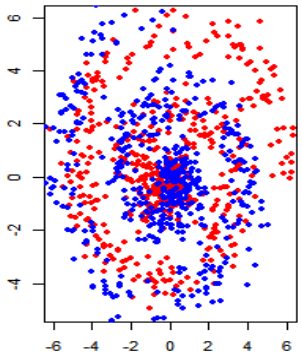

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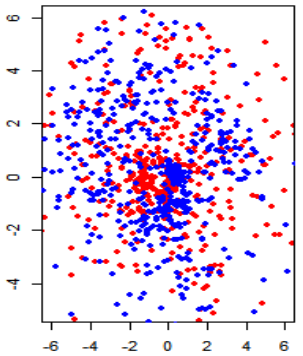

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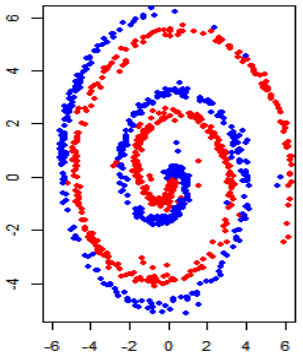

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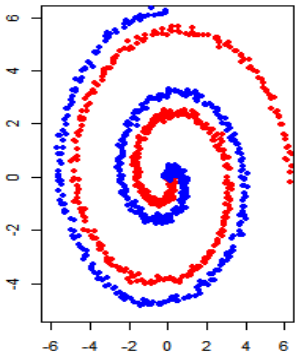

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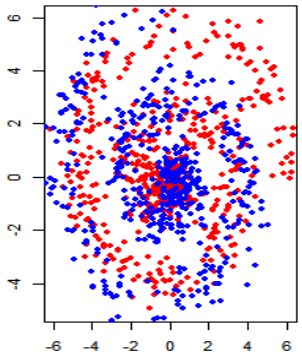

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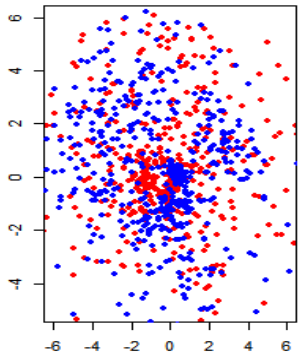

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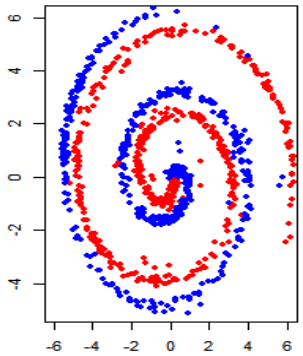

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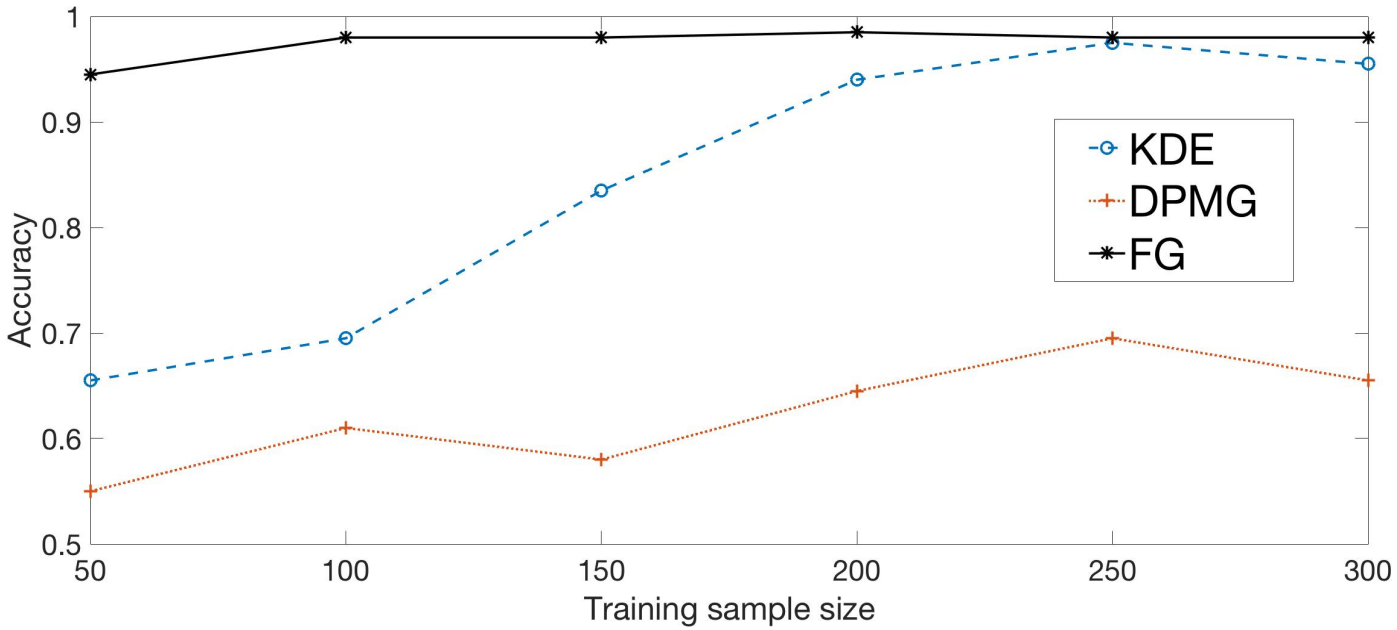
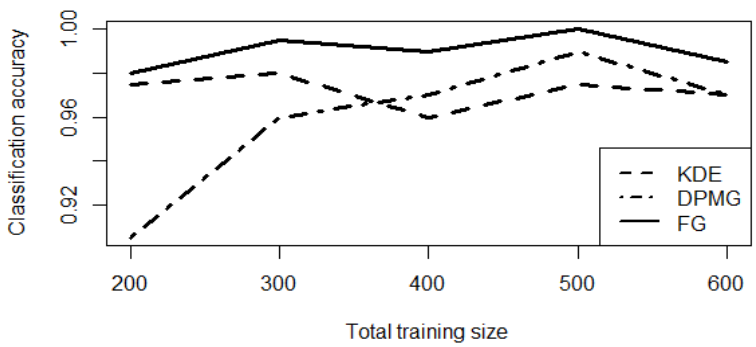
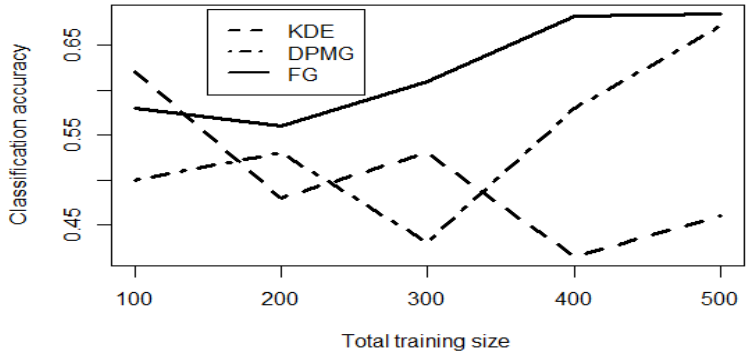


Galaxy Zoo and Balance scale datasets





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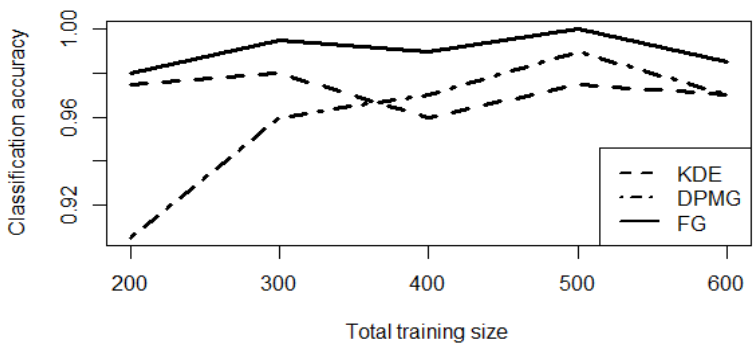

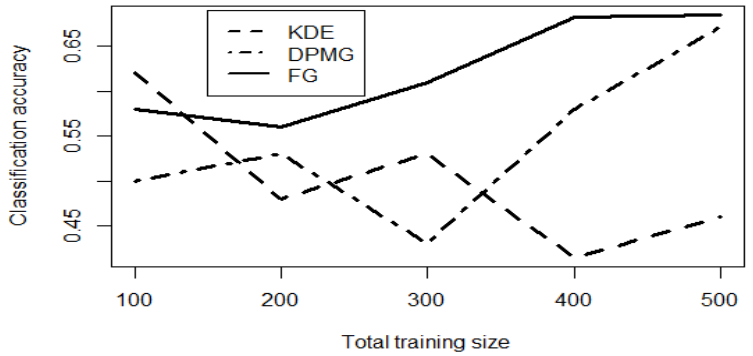

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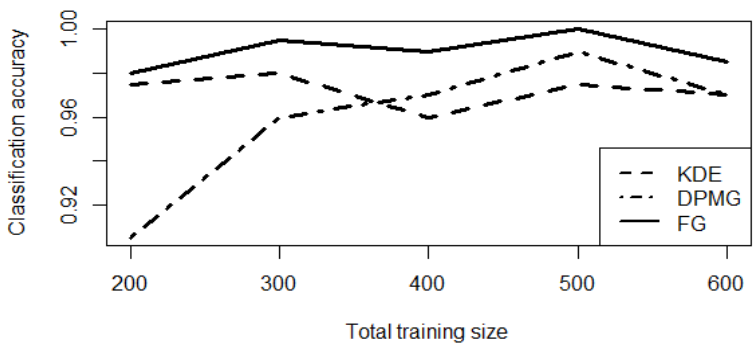

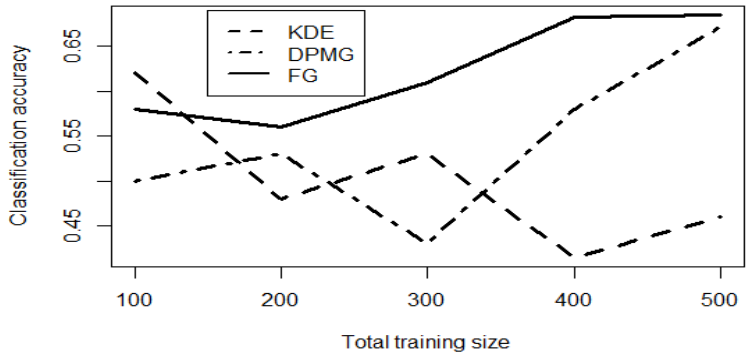

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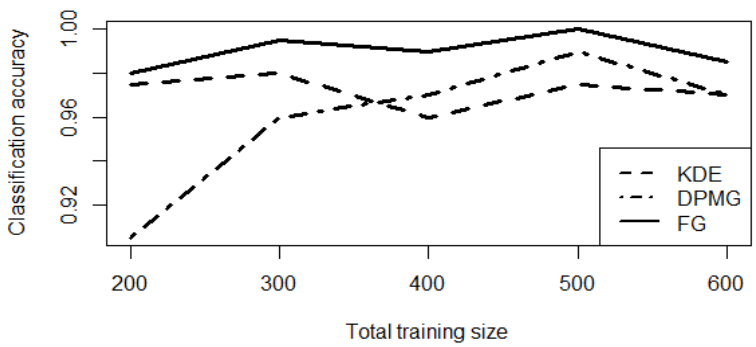

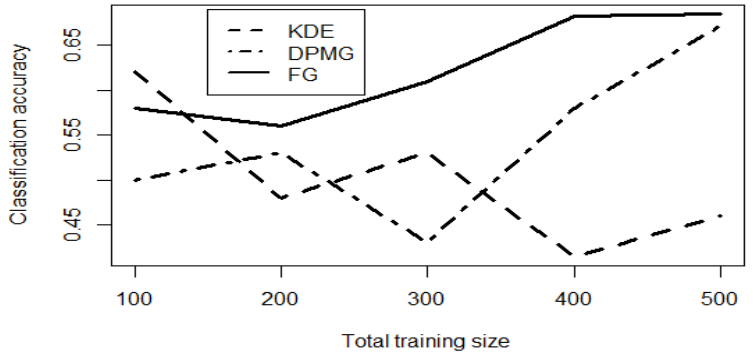

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- Gesture phase data: 32 features from 7 videos of people gesticulating, aimed at studying gesture phase segmentation. FG had much better classification accuracy (results in paper)

Density estimation

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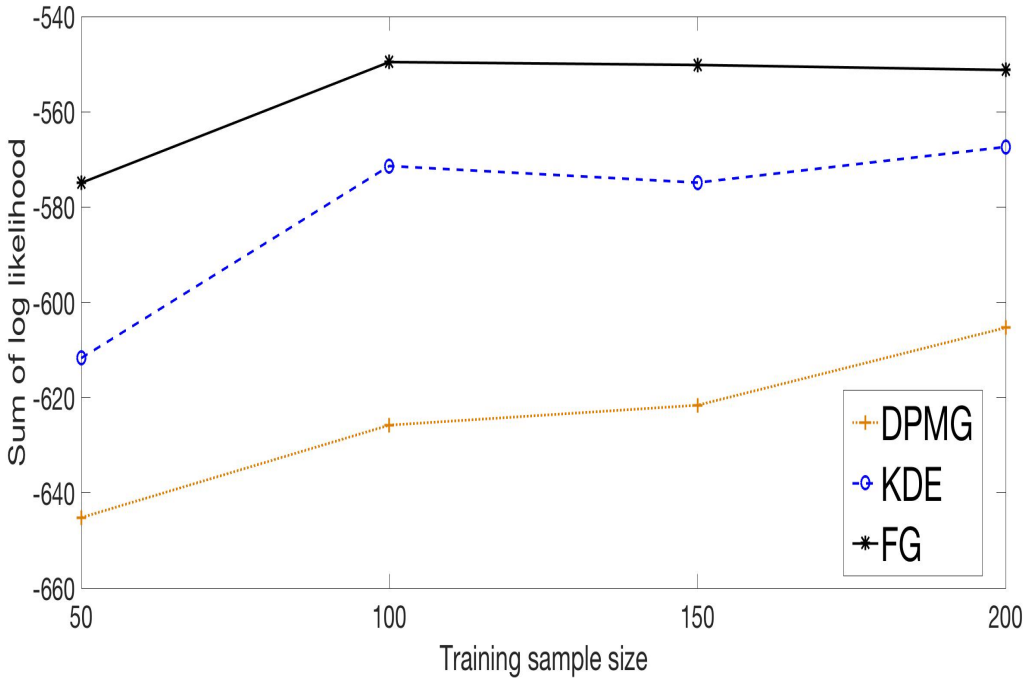
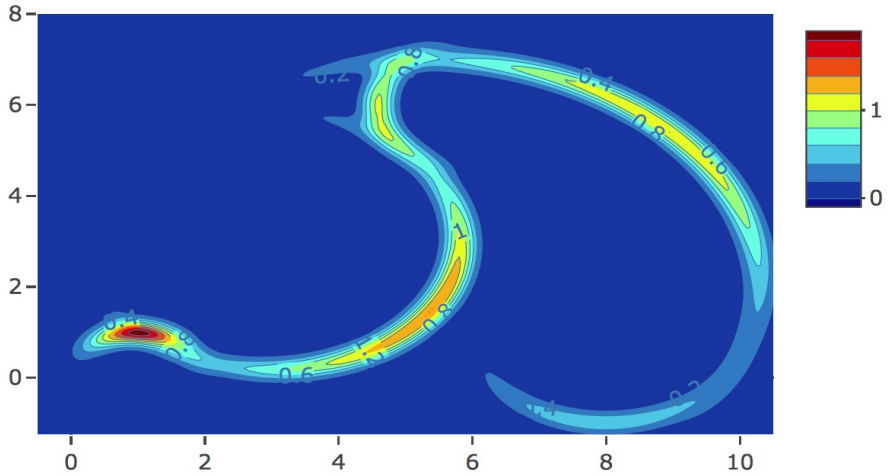


Sum of log likelihood for the Balance scale.

FG mixtures - comments & where to go now?



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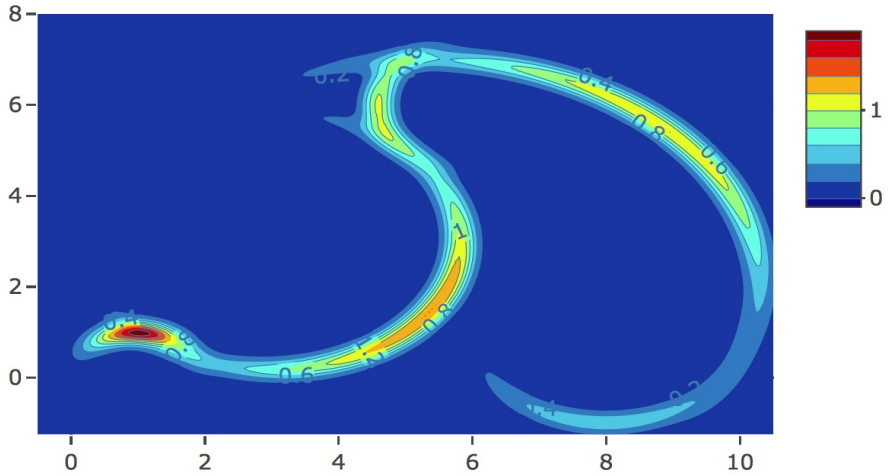

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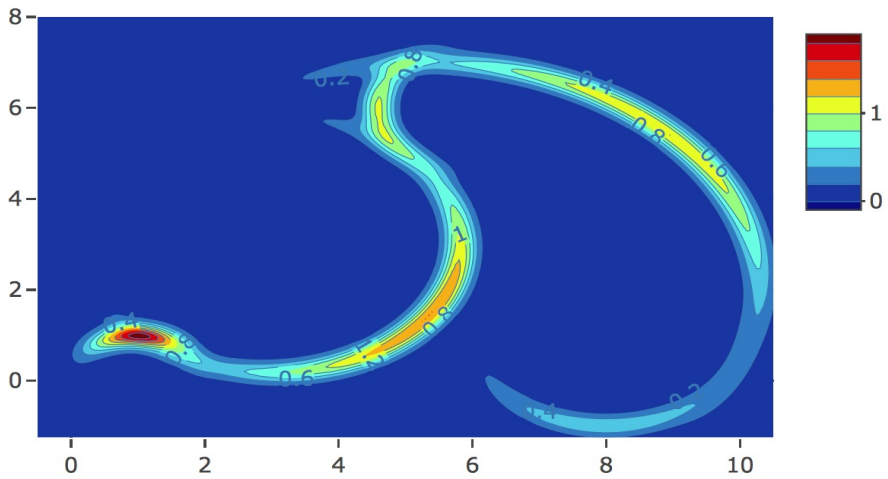

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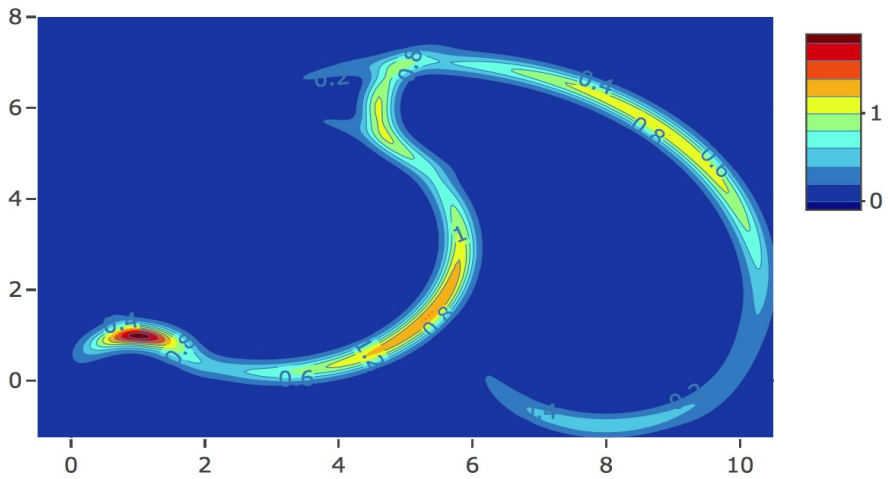

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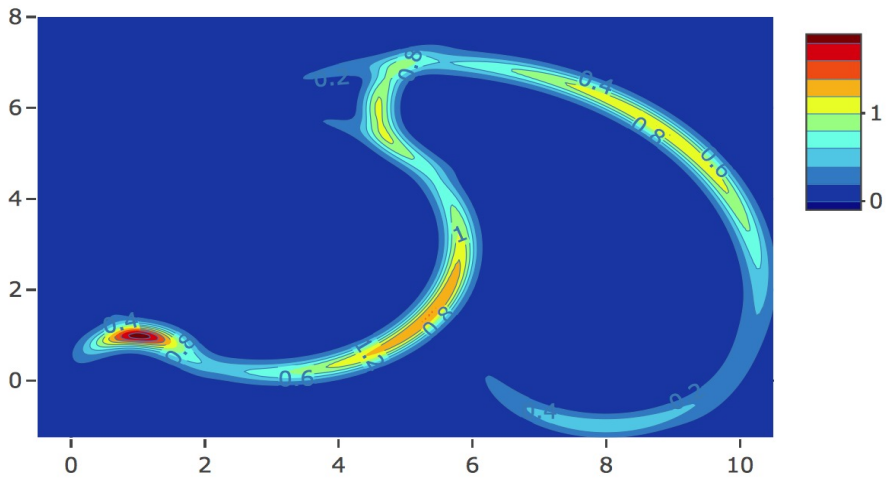

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- In the remainder, I will discuss two additional methods inspired by spherelets - for classification & distance estimation

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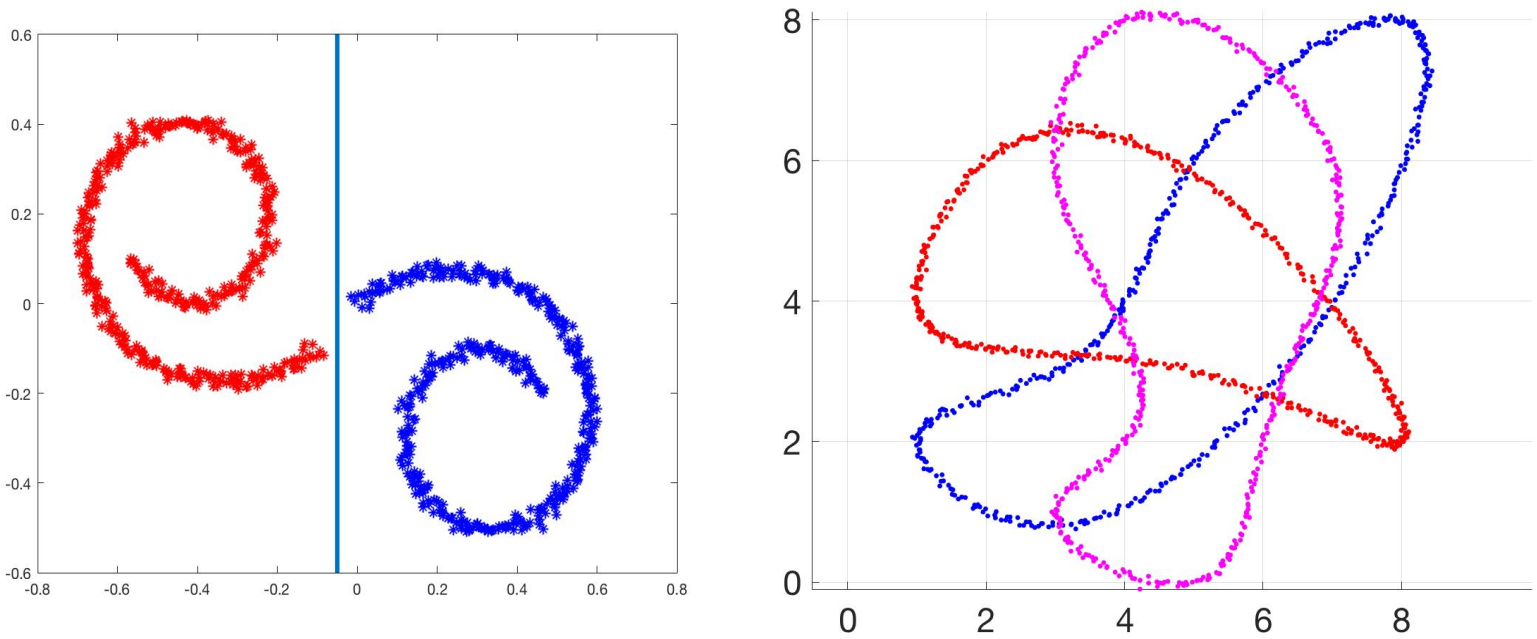

Separable and inseparable cases.

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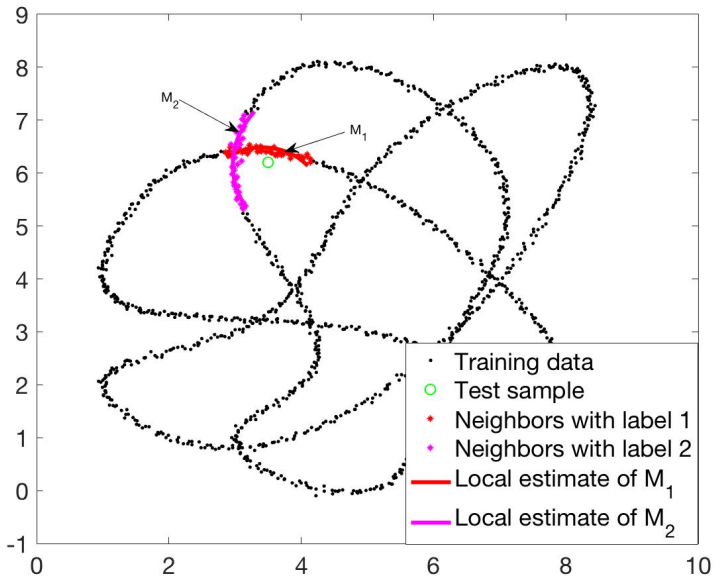

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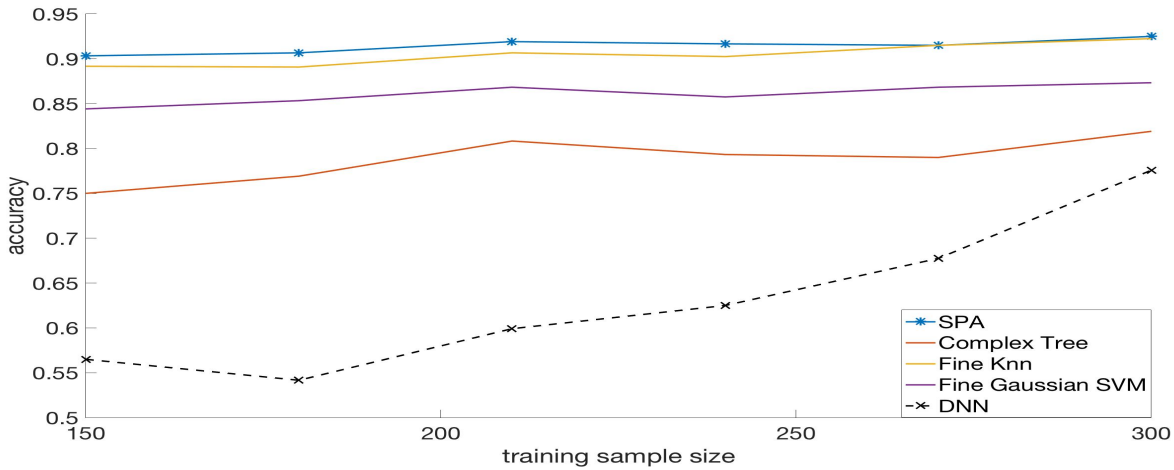

Funky curves data, sample size v.s. accuracy plot

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Theorem (Li, D., 19')

Let $\delta > 0$ and $B_\delta(M) := \{x \mid d(x, M) < \delta\}$, then $\lim_{n\to\infty} \mathbb{P}(y \neq \widehat{y}_n)$ is upper bounded by

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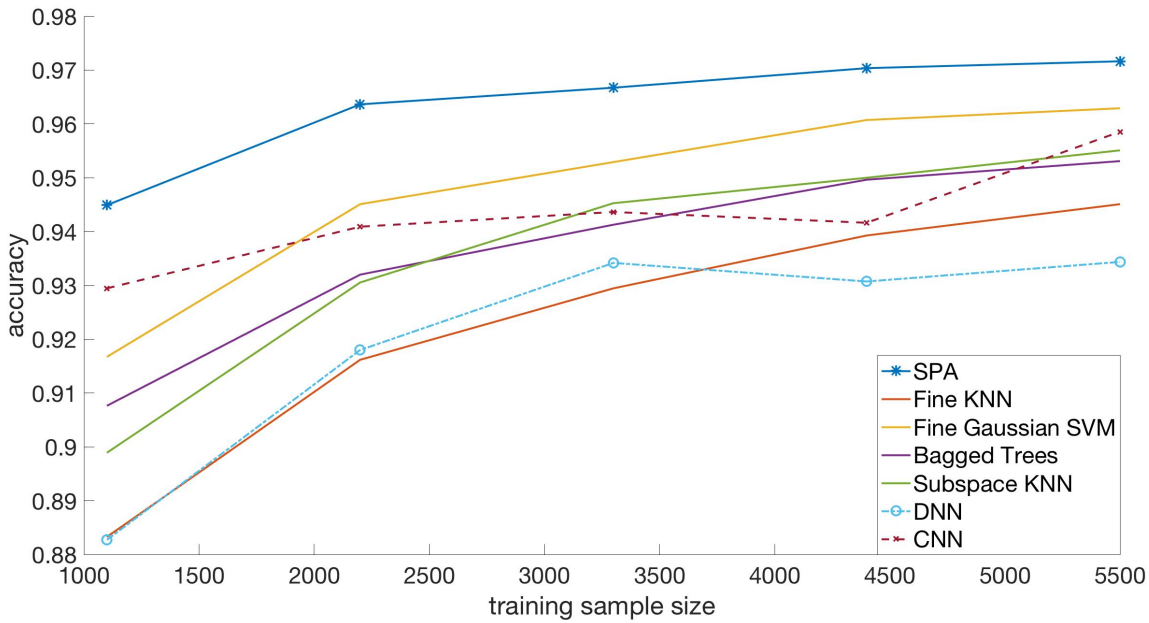

USPS hand written digits data set

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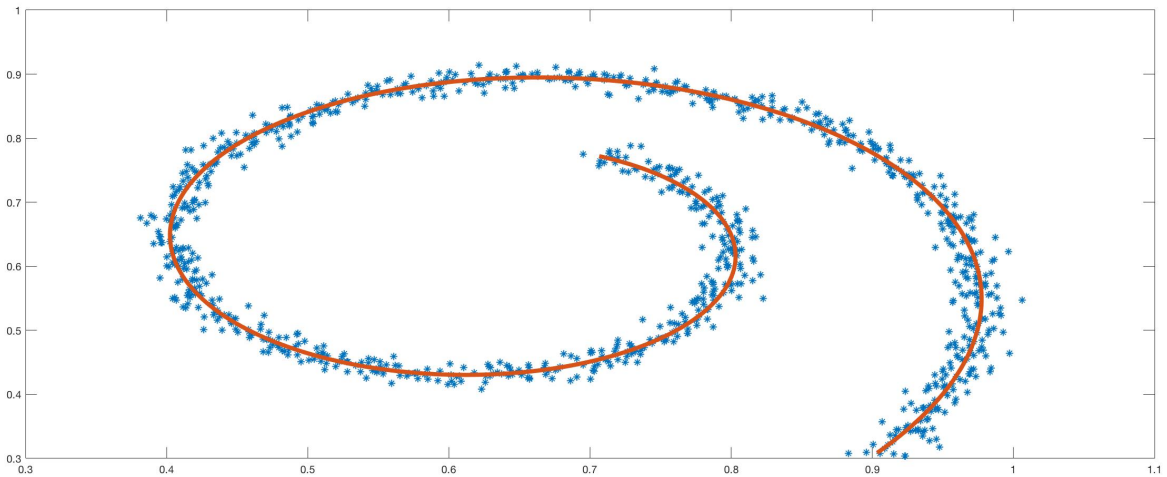

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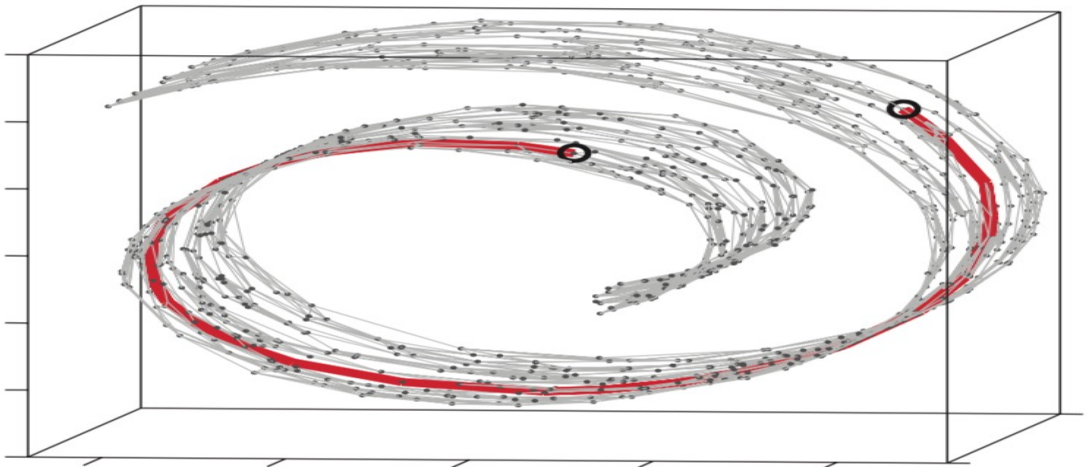

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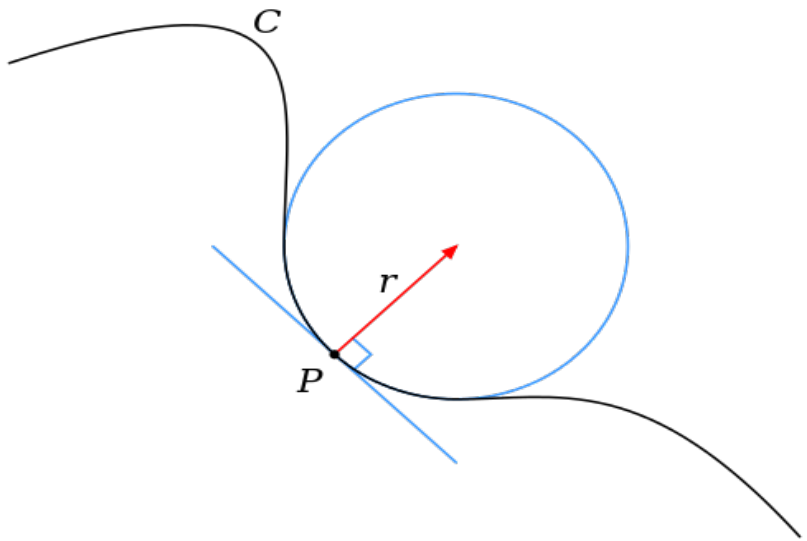

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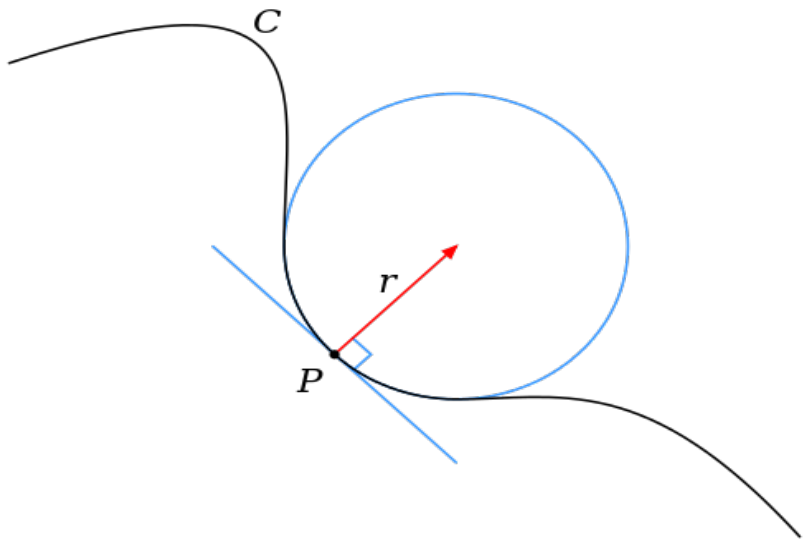

- Let $\hat{x}, \hat{y} \in S(c, r)$ be the projection of $x, y \in M$ to the "best" sphere $S(c, r)$ and estimate $d_M(x, y)$ by the spherical distance $d_S(\hat{x}, \hat{y})$.

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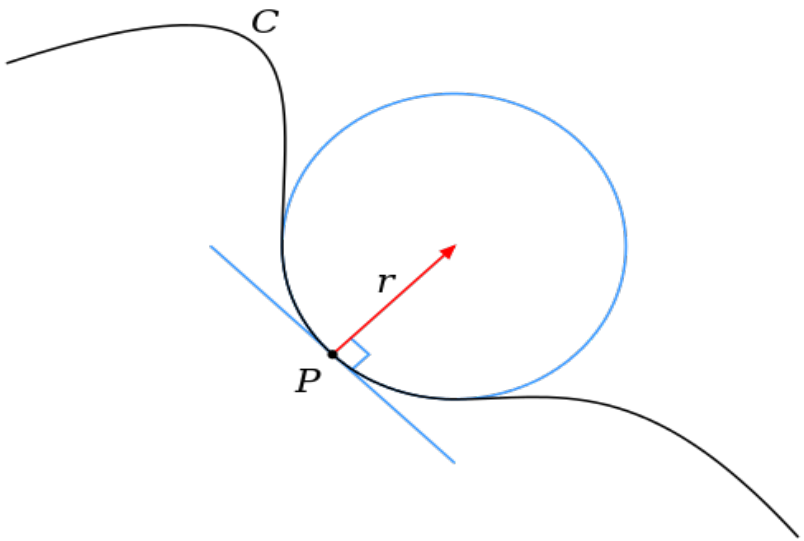
- On a sphere centered at c with radius r, geodesic distance: $d_S(x, y) = r \arccos\left(\frac{(x-c)^\top (y-c)}{r^2}\right)$.



- Let $\widehat{x}, \widehat{y} \in S(c, r)$ be the projection of $x, y \in M$ to the "best" sphere $S(c, r)$ and estimate $d_M(x, y)$ by the spherical distance $d_S(\widehat{x}, \widehat{y})$.
- The error is in general smaller than the Euclidean estimation.

Local error

Theorem (Li, D., 19')

Let γ be a curve and $d_M(x, y) = s$ for $x, y \in \gamma$. Then

$$\|x - y\| = s + O(s^3), \quad d_S(x, y) = s + O(s^4).$$

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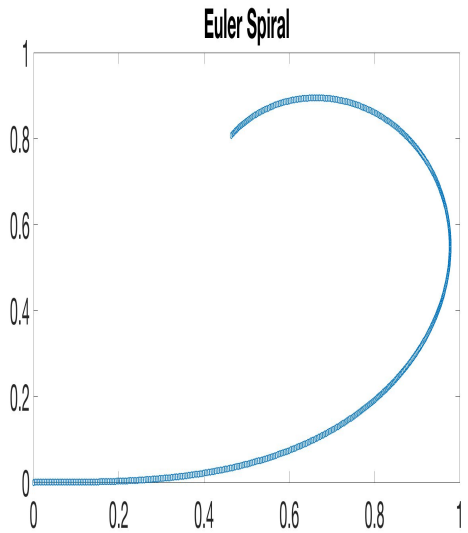

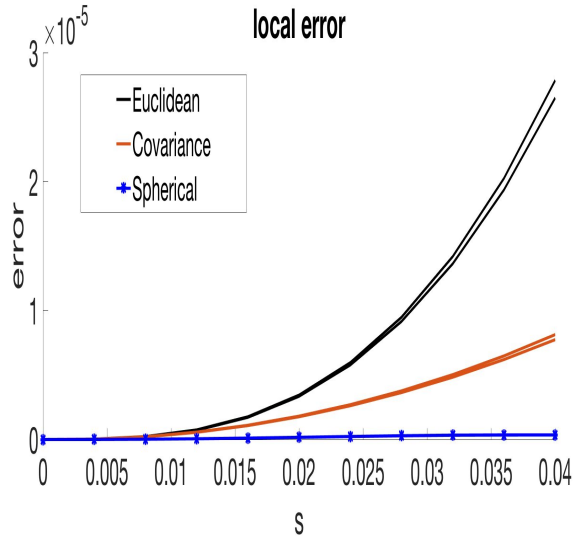

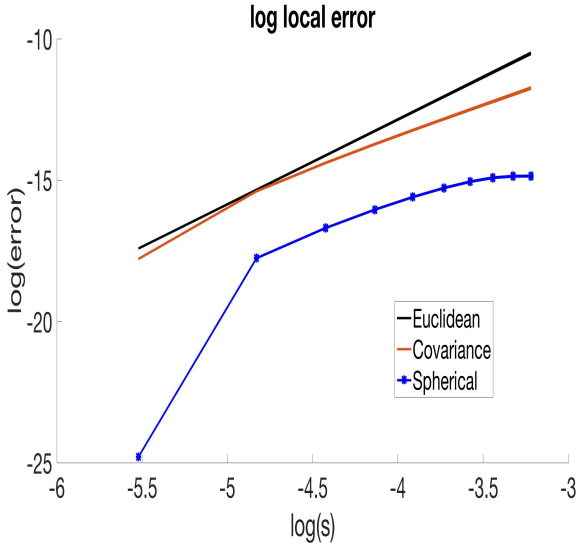

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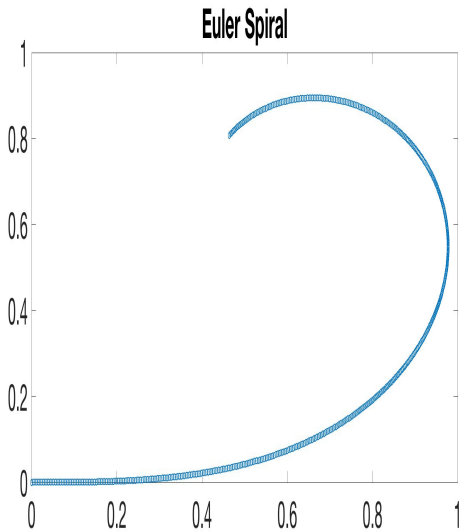

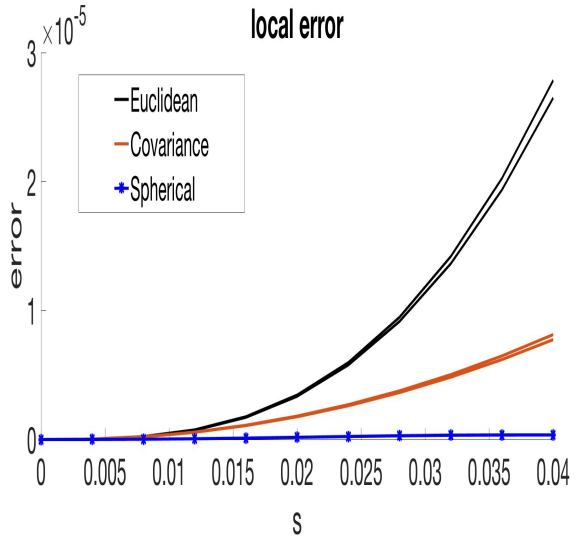

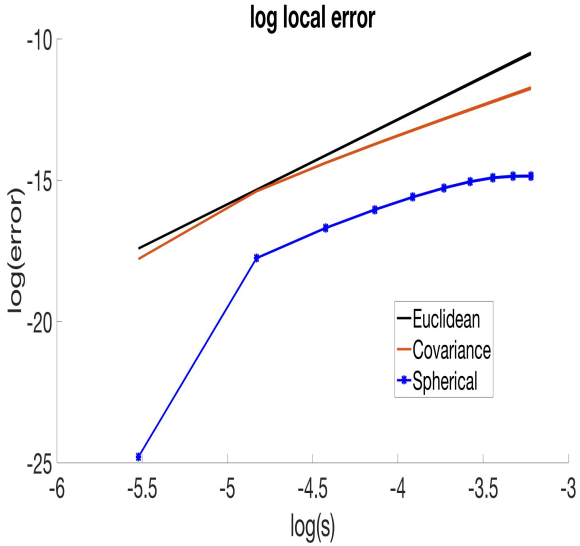

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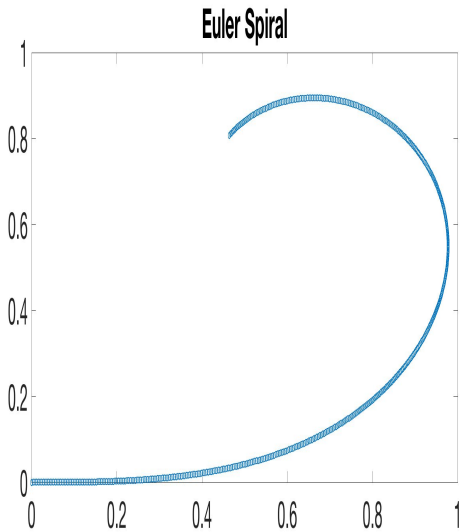

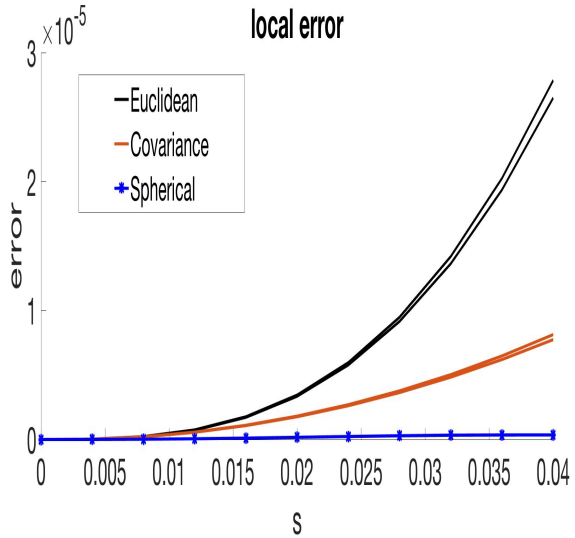

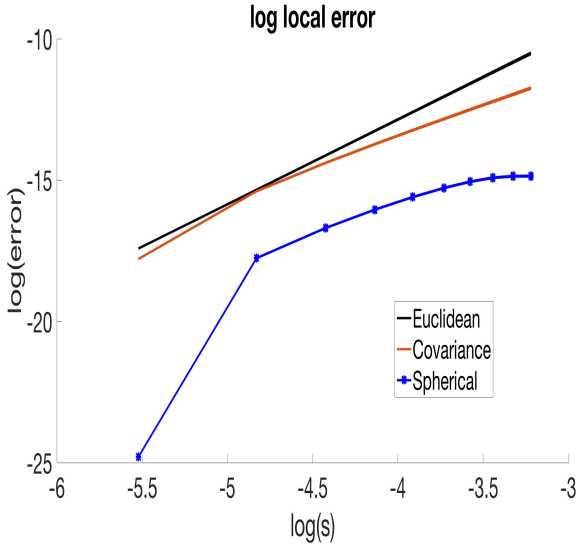

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- Simulation results match our theory.

Clustering

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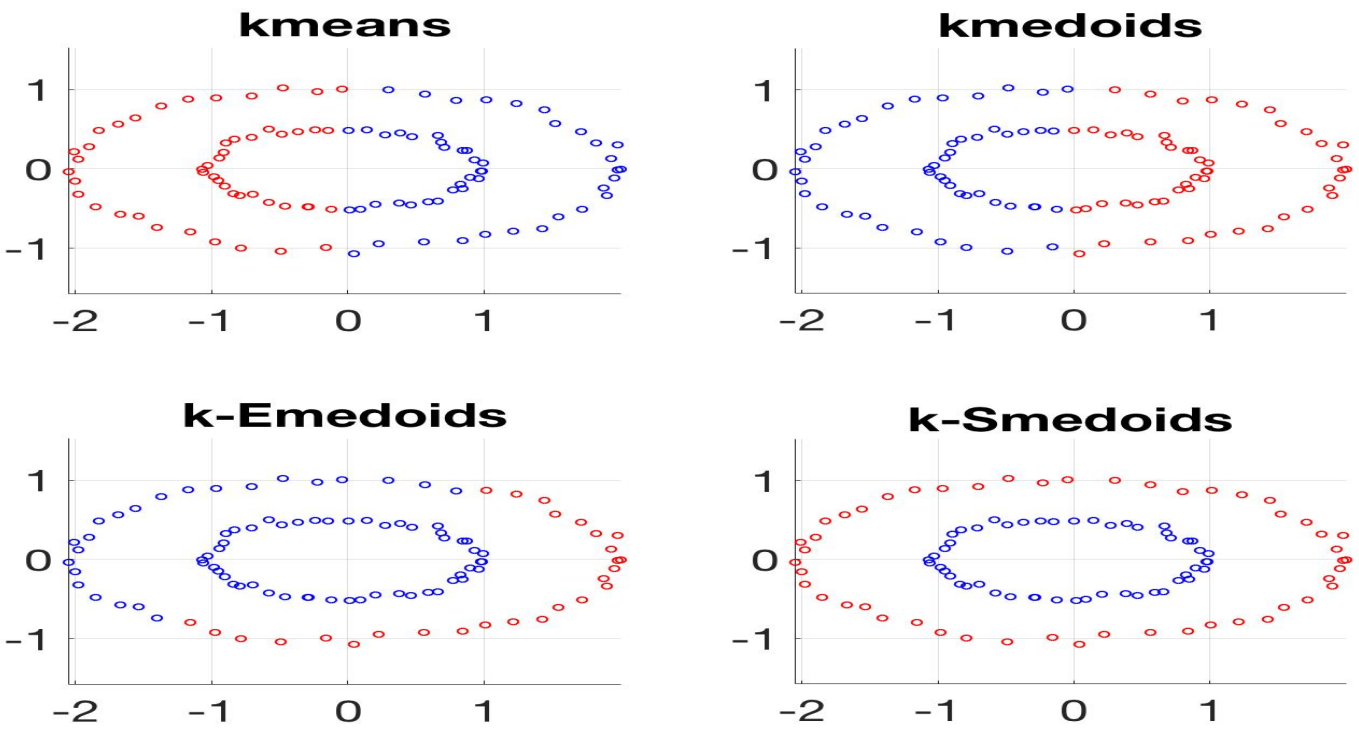

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Table: Clustering performance for Galaxy Zoo

	k-medoids	k-Emedoids	k-Smedoids
ARI	0.744	0.805	**0.954**
MIBS	0.6402	0.702	**0.900**
HOM	0.712	0.763	**0.919**
COM	0.641	0.702	**0.900**
VM	0.674	0.731	**0.909**
FMS	0.899	0.923	**0.983**

Galaxy Zoo

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Table: Clustering performance for Banknote

	k-medoids	k-Emedoids	k-Smedoids
ARI	0.059	0.004	**0.452**
MIBS	0.041	0.008	**0.439**
HOM	0.0416	0.009	**0.439**
COM	0.041	0.138	**0.508**
VM	0.0415	0.0163	**0.471**
FMS	0.533	0.707	**0.754**

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  - To address data not in $\mathbb{R}^p$, like categorical data or functional data.

Key References

- D. Li, M. Mukhopadhyay and D. Dunson, Efficient Manifold and Subspace Approximations with Spherelets, arXiv: 1706.08263, 2018.
- M. Mukhopadhyay, D. Li and D. Dunson, Estimating densities with nonlinear support using Fisher-Gaussian kernels, arXiv:1907.05918, 2019.
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Brilliant collaborators who did everything important