Enhanced Mode Clustering

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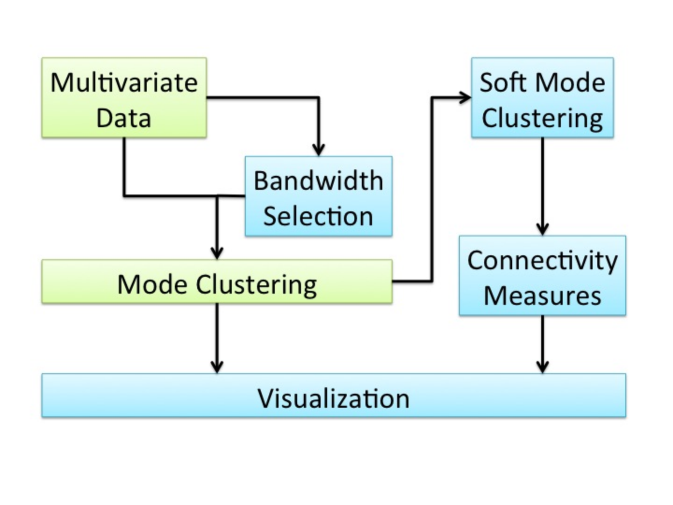
Outline

- Introduction
- Proposed Methods:
  - Soft Mode Clustering
  - Connectivity Measures
  - Bandwidth Selection
  - Visualizations
- Data Analysis
- Conclusion

Outline for the Proposed Methods



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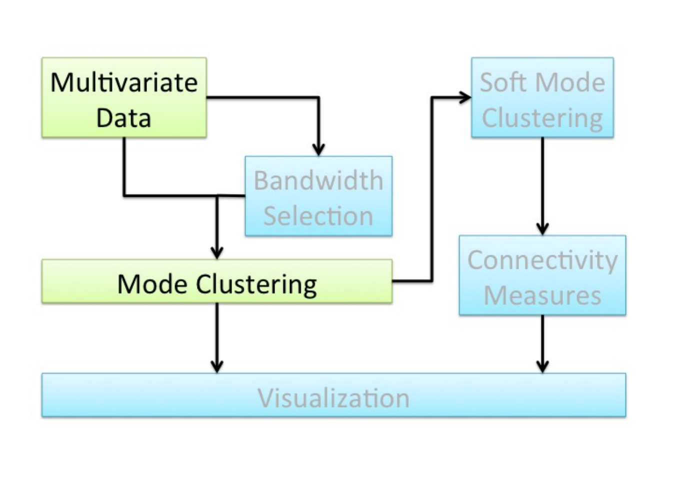

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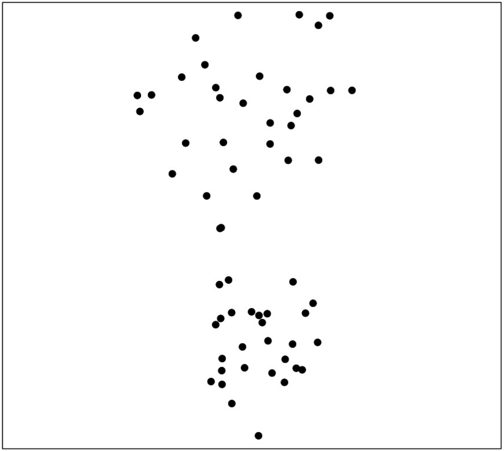

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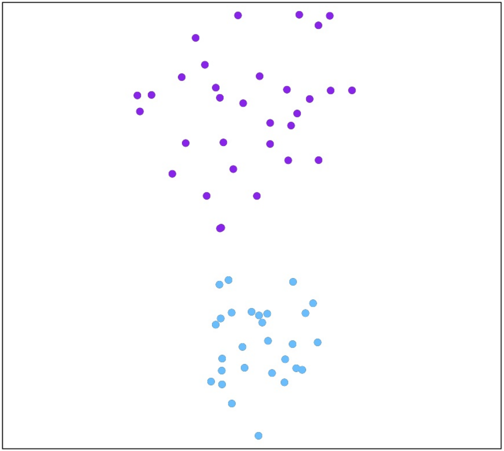

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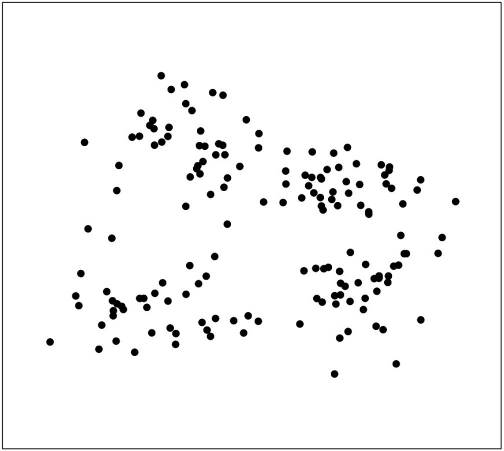

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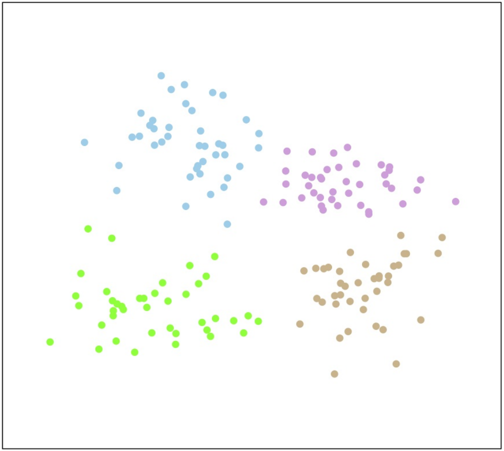

Density Mode Clustering: A Population Level Clustering

- Let $p : \mathbb{R}^d \mapsto \mathbb{R}$ be a density function.
- The gradient $g(x) = \nabla p(x)$ and the Hessian $H(x) = \nabla\nabla p(x)$.

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- We denote $\mathcal{M} = \{m_1, \cdots, m_k\}$.

Density Mode Clustering: An Example

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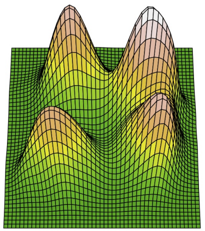

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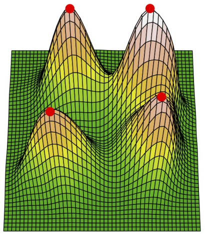

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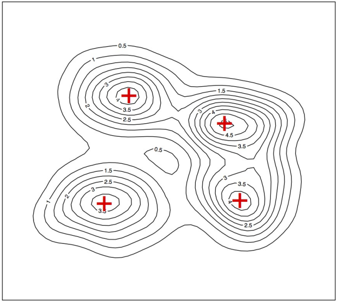

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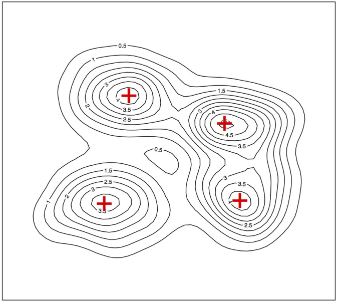

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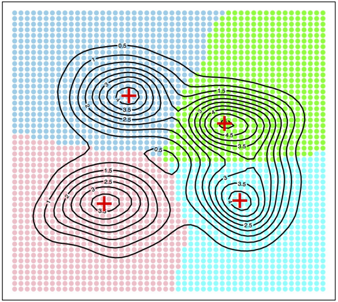

Density Mode Clustering: Based on the KDE

- The kernel density estimator (KDE):

$$\widehat{p}_n(x) = \frac{1}{nh^d} \sum_{i=1}^{n} K\left(\frac{x - X_i}{h}\right).$$

- The gradient:

$$\widehat{g}_n(x) = \nabla \widehat{p}_n(x) = \frac{1}{nh^d} \sum_{i=1}^{n} \nabla K\left(\frac{x - X_i}{h}\right).$$

- Clustering: Based on the gradient of $\widehat{g}_n(x)$.
- Algorithm: The mean shift algorithm [Fukunaga1975, Cheng1995, Comaniciu2002].

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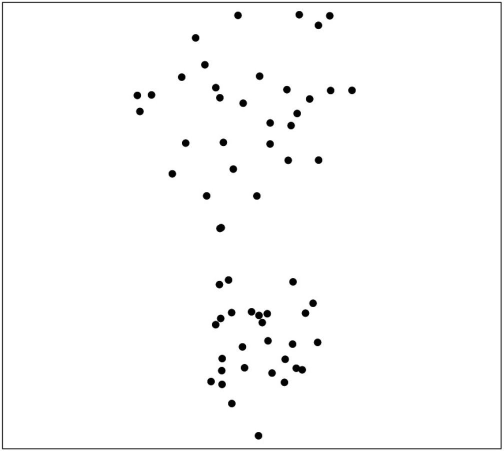

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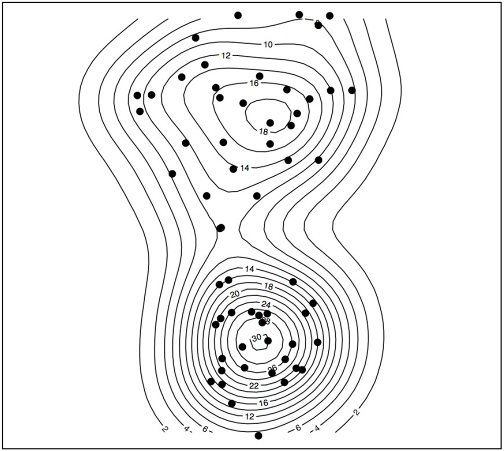

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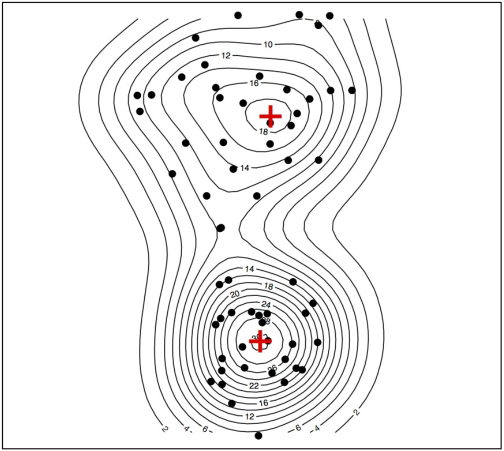

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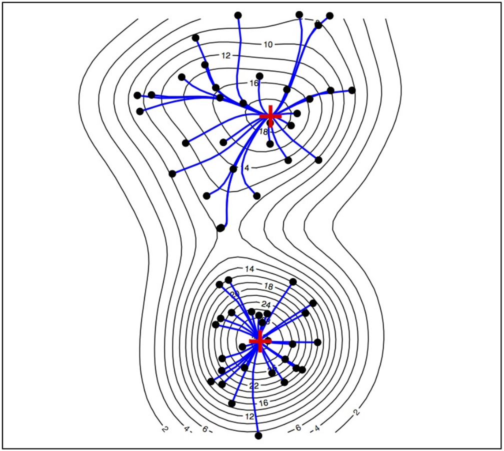

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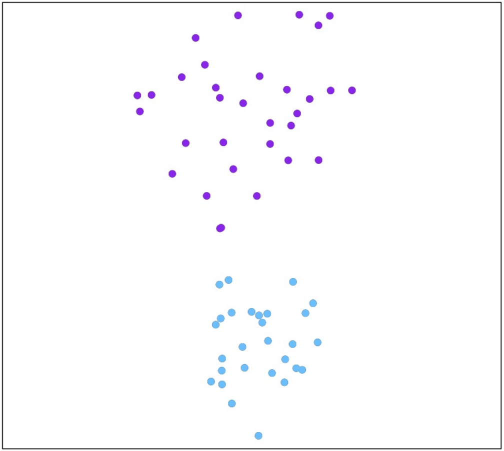

Conventions on Notations

- True local modes

$$\mathcal{M} = \{m_1, \cdots, m_k\}.$$

- Estimated local modes

$$\widehat{\mathcal{M}}_n = \{\widehat{m}_1, \cdots, \widehat{m}_{\widehat{k}}\}.$$

- The cluster regions (also known as basins of attraction):

$$C_j = \{x : x \text{ being assigned to } m_j \text{ under } g\}.$$

- The estimated cluster regions:

$$\widehat{C}_j = \{x : x \text{ being assigned to } \widehat{m}_j \text{ under } \widehat{g}_n\}.$$

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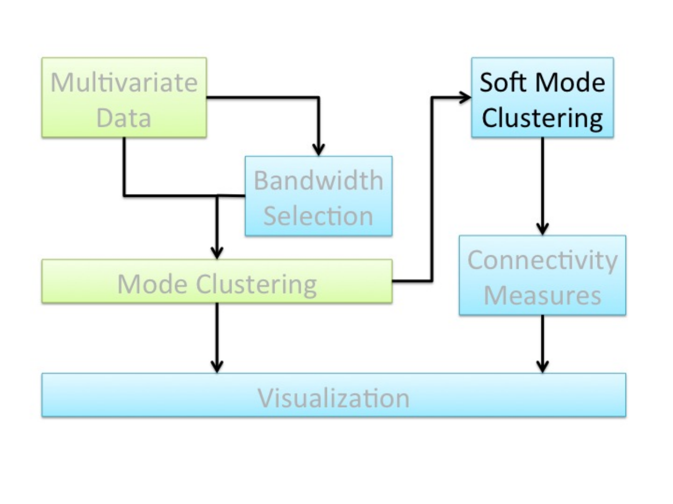

Basic Ideas for Soft Clustering

- Usual (Hard) clustering: assign each data to a cluster.
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  $\longrightarrow$ We have strong **confidence** that x is assinged to cluster 2

Soft Mixture Clustering

- A common soft clustering method: mixture model.
- $p(x) = \pi p_1(x) + (1-\pi)p_2(x)$
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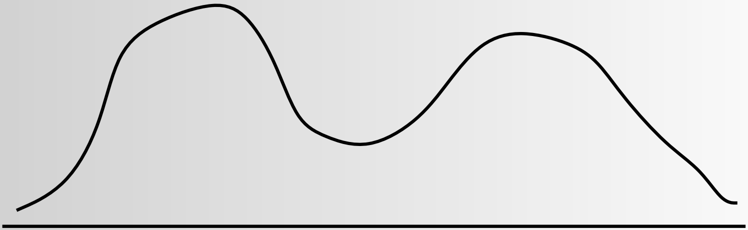

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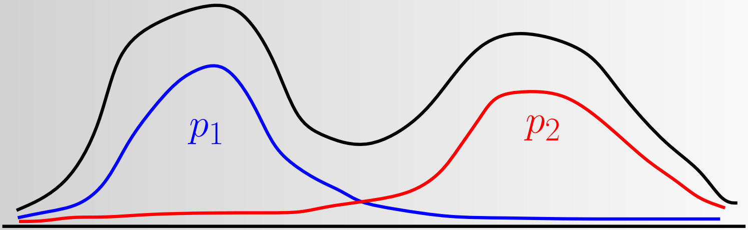

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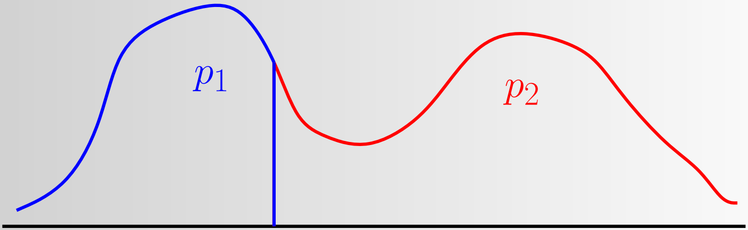


Basic Ideas for Soft Mode Clustering

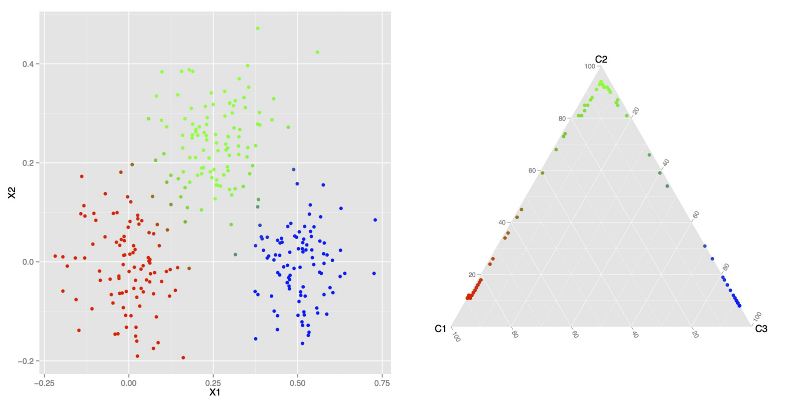
- In mode clustering, we have fixed local modes $\widehat{m}_1, \cdots, \widehat{m}_{\widehat{k}}$.
- All we need is to construct the **soft assignment vector** $a(x)$.

Soft Mode Clustering: The Bootstrap

1. Given data points $X_1, \cdots, X_n$, we find the local modes.
2. For each $x \in \mathbb{R}$, perform the bootstrap and redo the mode clusteirng.
3. Construct the soft assignment vector $a(x) = \left(a_1, \cdots, a_{\widehat{k}}(x)\right)$ where

$$a_\ell(x) = \text{ fraction of } x \text{ being assigned to cluster } \ell.$$

The Bootstrap: Example



Soft Mode Clustering: The Hitting Probability

- We define a diffusion between local modes and data points.
- $\widehat{k} + n$ states: $\widehat{m}_1, \cdots, \widehat{m}_{\widehat{k}}, X_1, \cdots, X_n$.

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- The transition probability between data points:

$$\mathbf{P}(X_i \to X_j) = \frac{K\left(\frac{X_i-X_j}{h}\right)}{\sum_{j=1}^{n} K\left(\frac{X_i-X_j}{h}\right) + \sum_{\ell=1}^{\widehat{k}} K\left(\frac{X_i-\widehat{m}_\ell}{h}\right)}.$$

- The transition probability to local modes:

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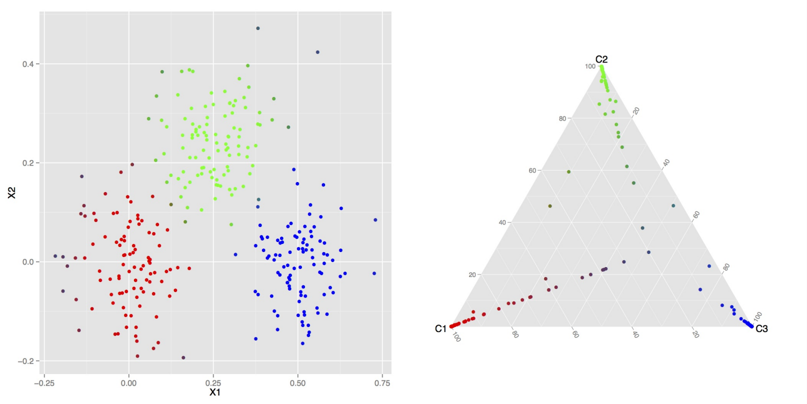
- Soft assignement vector:

$$a_\ell(X_i)=\mathbb{P}\left(\text{from } X_i \text{ and hits } \widehat{m}_\ell \text{ first}\right)$$

The Hitting Probability: Example



Soft Mode Clustering: The Level Set

- The third method is based on the level set.
- We create a distance $d_\ell(x)$ for each $\ell = 1, \cdots, k$.
- Transform the distance into soft assignment vector. e.g.

$$a_\ell(x) = \frac{\exp(-\beta_0 d_\ell(x))}{\sum_{j=1}^{k} \exp(-\beta_0 d_j(x))}.$$

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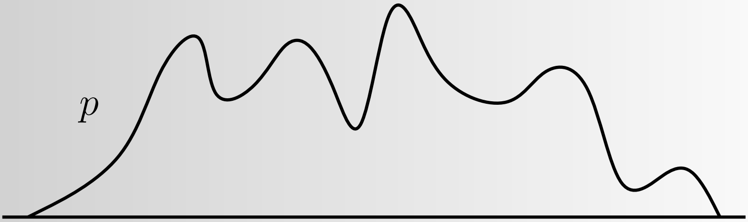

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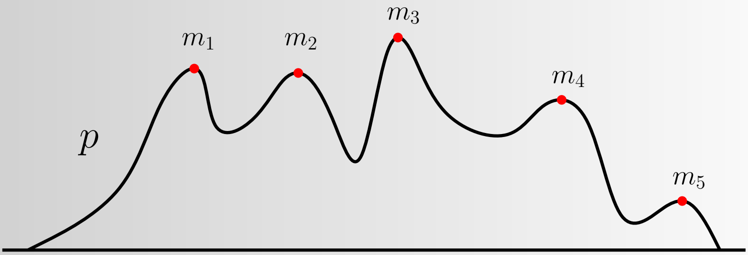

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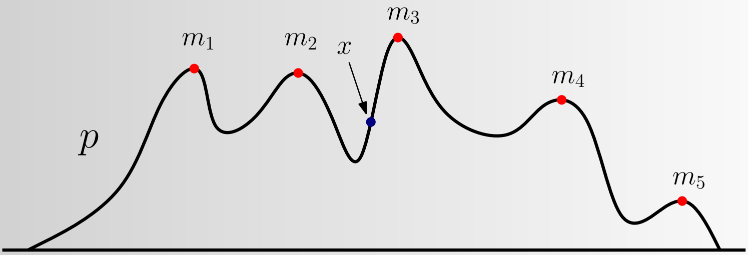

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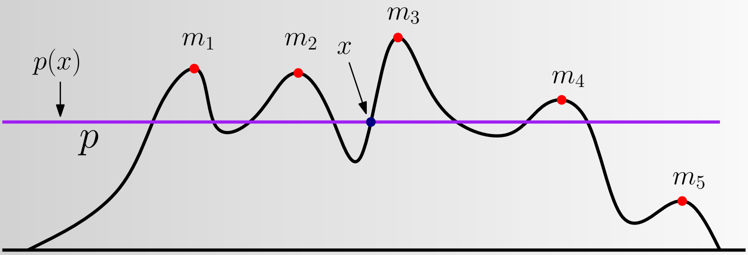

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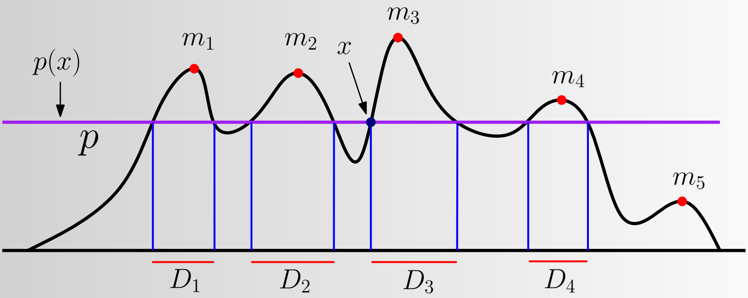

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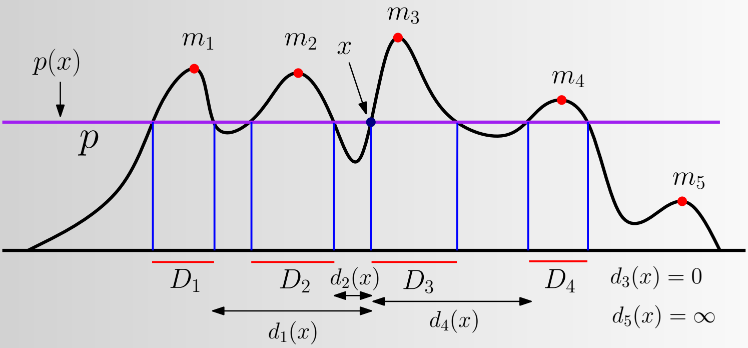

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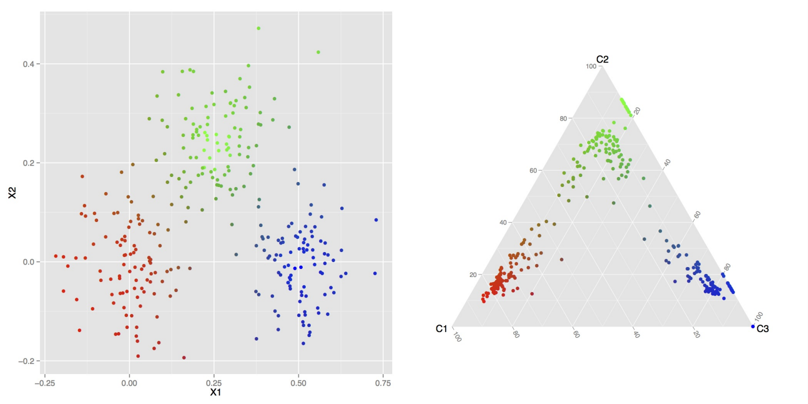

Soft Mode Clustering: Other Distance Methods

Other possible approaches:

- Diffusion distance
- Density integral distance

We need a conversion between distances $d_\ell(x)$ and soft assignment vector $a(x)$.

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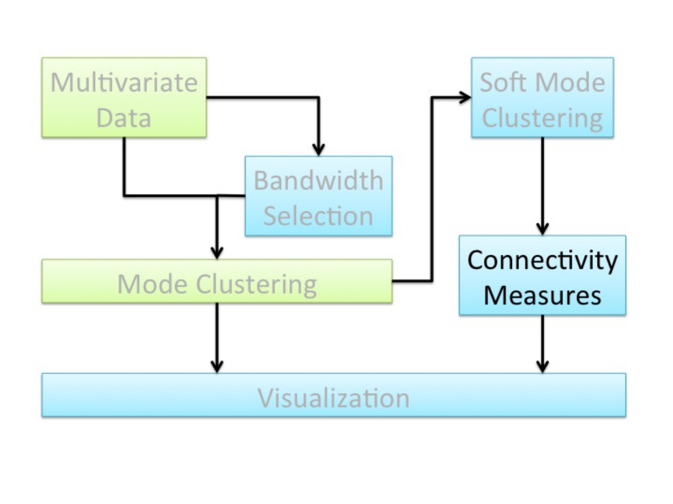
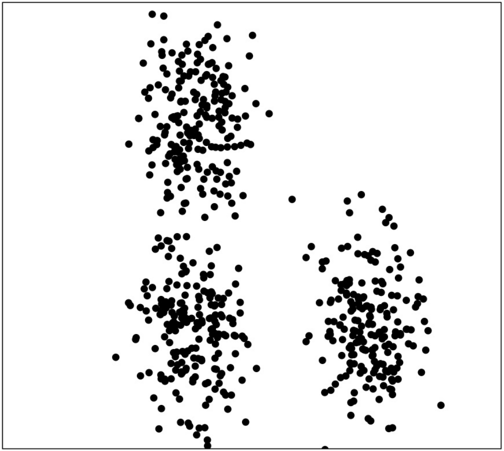


A Motivating Example



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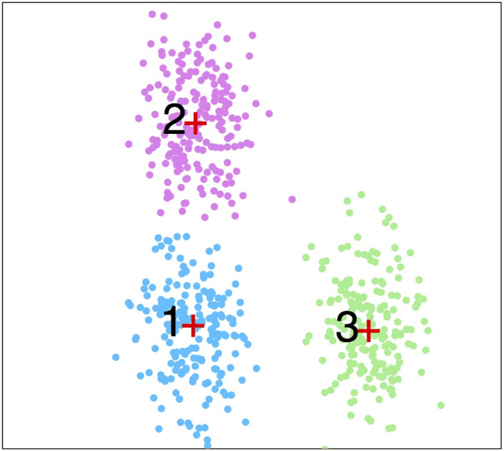

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- The quantity

$$\frac{1}{N_j}\sum_{i:X_i\in\widehat{C}_j} a_\ell(X_i)$$

  measures the confidence for cluster j being assigned to cluster ℓ; note N_j is the number of points in $\widehat{C}_j$.

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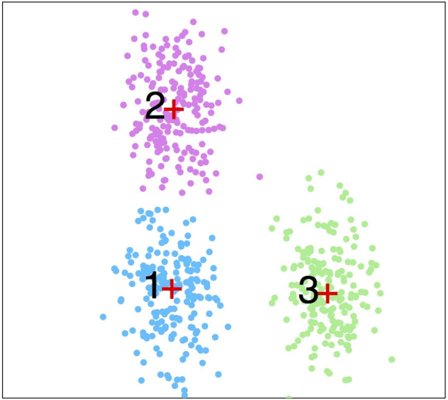
  measures the confidence for cluster j being assigned to cluster ℓ; note N_j is the number of points in $\widehat{C}_j$.
- We define the *connectivity measure* between cluster j,ℓ as

$$\Omega_{j\ell}=\frac{1}{2}\left(\frac{1}{N_j}\sum_{i:X_i\in\widehat{C}_j} a_\ell(X_i)+\frac{1}{N_\ell}\sum_{i:X_i\in\widehat{C}_\ell} a_j(X_i)\right).$$

Example for Connectivity Matrix



	1	2	3
1	–	0.27	0.21
2	0.27	–	0.12
3	0.21	0.12	–

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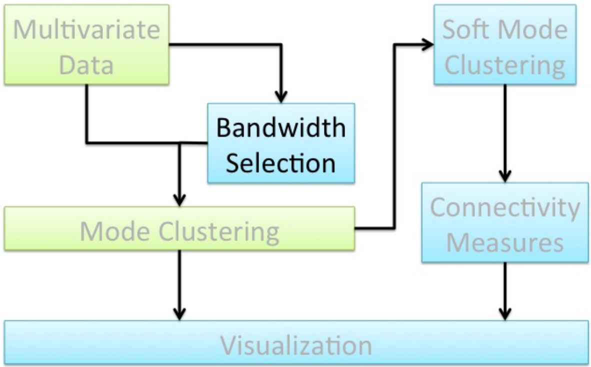

Optimality for Bandwidth

- Usually, we select smoothing bandwidth h according to minimize some loss function.
- Mean integrated square errors (MISE):

$$MISE(\widehat{p}_n) = \mathbb{E}\left(\int (\widehat{p}_n(x) - p(x))^2\, dx\right).$$

- L_∞ loss:

$$\|\widehat{p}_n - p\|_\infty = \sup_x |\widehat{p}_n(x) - p(x)|.$$

Optimality for Mode Clustering

For mode clustering, the important quantity is the gradient $g(x)$ and its estimator $\widehat{g}_n(x)$.

- MISE:

$$MISE(\widehat{g}_n) = \mathbb{E}\left(\int \|\widehat{g}_n(x) - g(x)\|_2^2\, dx\right).$$

- L_∞ loss:

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- This suggests two different optimality criteria:

$$h_{MISE} = C_1\left(\frac{1}{n}\right)^{\frac{1}{d+6}} \qquad h_{L_\infty} = C_2\left(\frac{\log n}{n}\right)^{\frac{1}{d+6}}$$

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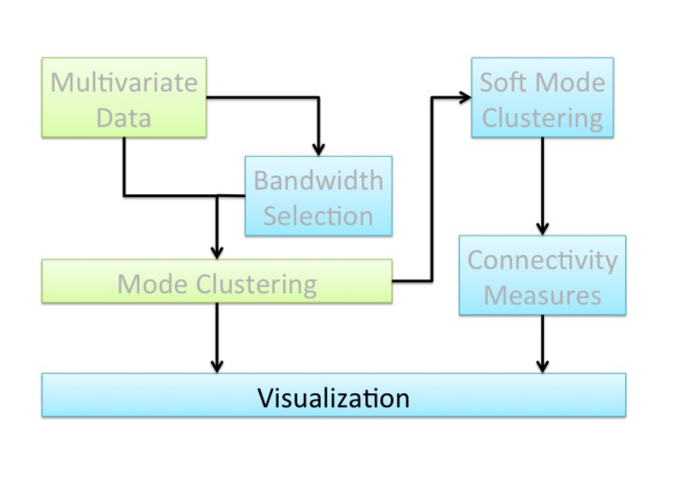
$$h_{MISE} = C_1 \left(\frac{1}{n}\right)^{\frac{1}{d+6}} \qquad h_{L_\infty} = C_2 \left(\frac{\log n}{n}\right)^{\frac{1}{d+6}}$$

- In practice, we use the normal reference rule [Sliverman1986, Chacon2011,13]:

$$h_{NR} = sd(\mathbb{X}) \times \left(\frac{4}{d+4}\right)^{\frac{1}{d+6}} \left(\frac{1}{n}\right)^{\frac{1}{d+6}}.$$

Outline for the Proposed Methods



Multidimensional Scaling (MDS): An Introduction

- Input: $X_1, \cdots, X_n \in \mathbb{R}^d$.
- Output: $Z_1, \cdots, Z_n \in \mathbb{R}^r$ with $r < d$.
- Distance preserved:

$$\min \sum_{i \neq j} |d(X_i, X_j) - d(Z_i, Z_j)|$$

  for some distance function d.
- In practice, we use the classical scaling.

Two-Stage MDS

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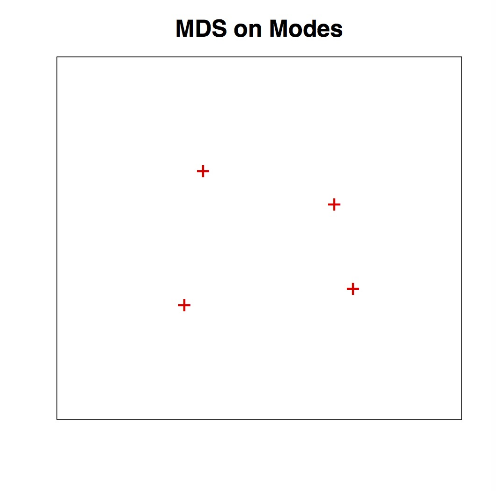

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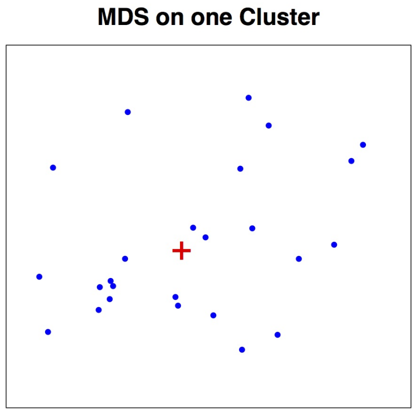

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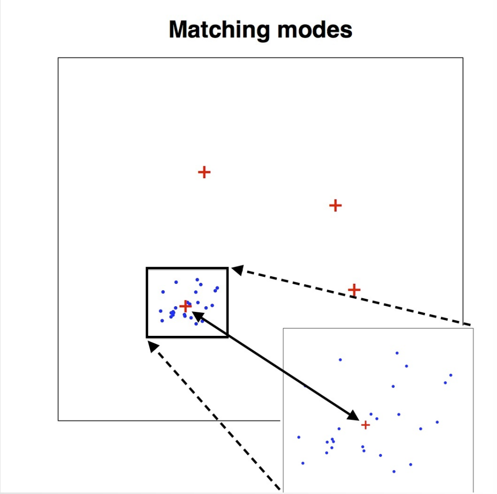

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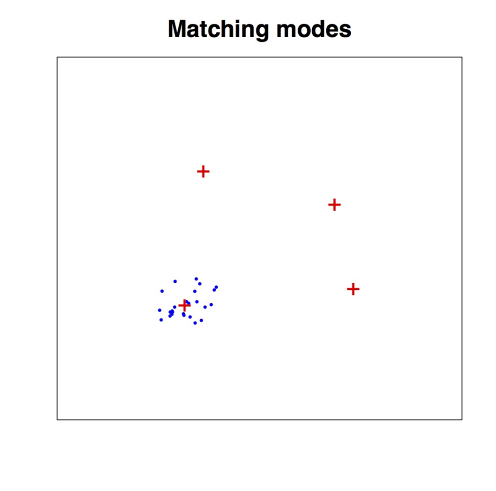

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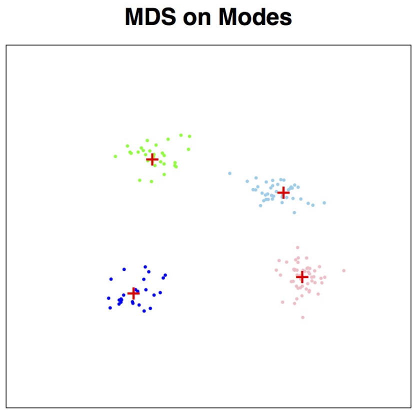
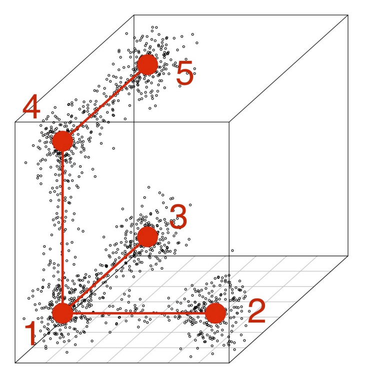


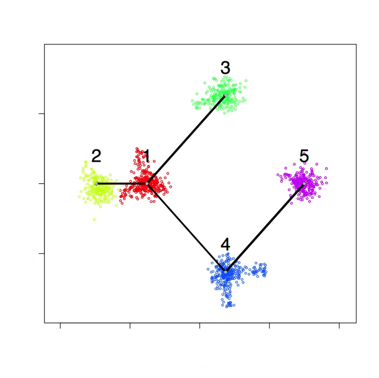
Outline

5-Cluster in d=6



- 5 clusters each with $n_C = 200$.
- 4 edges connecting clusters and each with $n_E = 100$.
- Embedding this structure in $d = 6$ and add Gaussian noise.

5-Cluster in d=6



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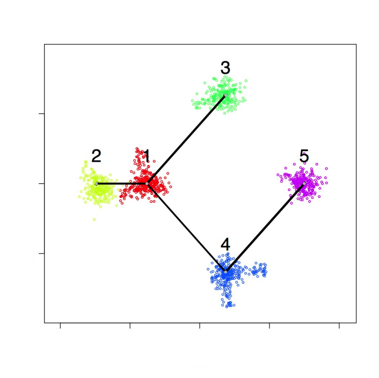


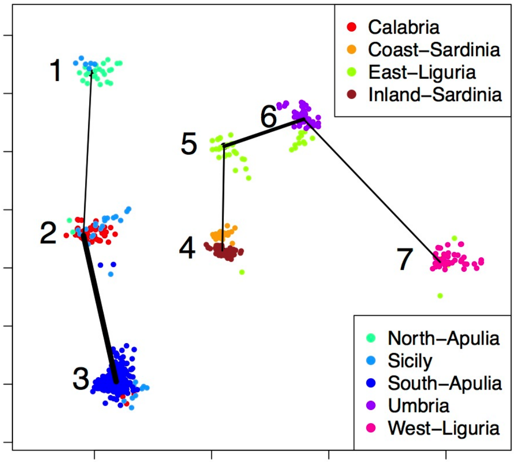
	1	2	3	4	5
1	–	0.17	0.19	0.15	0.05
2	0.17	–	0.05	0.04	0.01
3	0.19	0.05	–	0.05	0.01
4	0.15	0.04	0.05	–	0.20
5	0.05	0.01	0.01	0.20	–

The Olive Oil Data: Description

- A data consists of 572 olive oil sample produced in 9 different areas in Italy.
- We measure 8 different chemical contents for each oil.

	palmitic	palmitoleic	stearic	oleic	linoleic	linolenic	arachidic	eicosenoic
1	1088	73	224	7709	781	31	61	29
2	911	54	246	8113	549	31	63	29
3	966	57	240	7952	619	50	78	35
4	1051	67	259	7771	672	50	80	46
5	911	49	268	7924	678	51	70	44
6	1100	61	235	7728	734	39	64	35

The Olive Oil Data: Analysis



The Olive Oil Data: Analysis

	1	2	3	4	5	6	7
Calabria	0	51	5	0	0	0	0
Coast-Sardinia	0	0	0	33	0	0	0
East-Liguria	0	0	0	1	32	11	6
Inland-Sardinia	0	0	0	65	0	0	0
North-Apulia	23	2	0	0	0	0	0
Sicily	6	19	11	0	0	0	0
South-Apulia	0	2	204	0	0	0	0
Umbria	0	0	0	0	0	51	0
West-Liguria	0	0	0	0	0	0	50

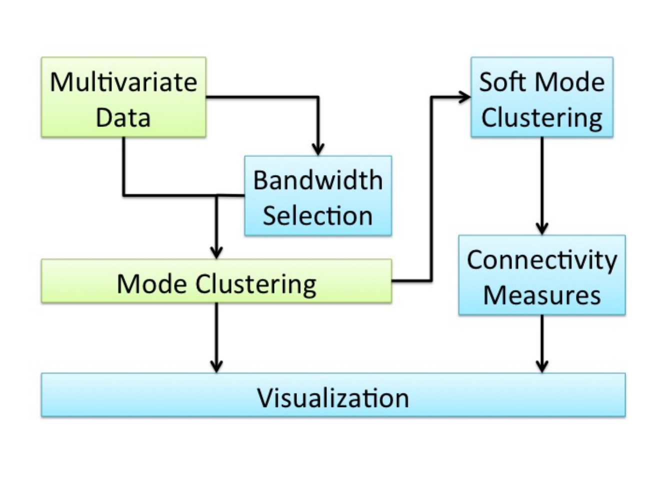
The Olive Oil Data: Analysis

	1	2	3	4	5	6	7
1	–	0.08	0.05	0.00	0.01	0.02	0.00
2	0.08	–	0.30	0.01	0.01	0.00	0.00
3	0.05	0.30	–	0.02	0.01	0.00	0.00
4	0.00	0.01	0.02	–	0.09	0.02	0.01
5	0.01	0.01	0.01	0.09	–	0.19	0.04
6	0.02	0.00	0.00	0.02	0.19	–	0.09
7	0.00	0.00	0.00	0.01	0.04	0.09	–

Outline

- Introduction
- Proposed Methods:
  - Soft Mode Clustering
  - Connectivity Measures
  - Bandwidth Selection
  - Visualizations
- Data Analysis
- Conclusion

Conclusion


Multivariate Data
Bandwidth Selection
Mode Clustering
Soft Mode Clustering
Connectivity Measures
Visualization

Thank you!

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The Classical Scaling

- Minimizing

$$\sum_{i \neq j} \left| \left(X_i - \bar{X}_n\right)^T \left(X_j - \bar{X}_n\right) - \left(Z_i - \bar{Z}_n\right)^T \left(Z_j - \bar{Z}_n\right) \right|$$

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- Analystical solution:

$$\mathbf{Z} = (Z_1, \cdots, Z_n)^T = \mathbf{V}_k \mathbf{D}_k,$$

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where $\mathbf{V}_k = [v_1, \cdots, v_k]$ and $\mathbf{D}_k = \mathrm{Diag}(\sqrt{(}\lambda_1), \cdots, \sqrt{\lambda_k})$ with (v_j, λ_j) being j-th eigenvector/value of a $n \times n$ matrix $\mathbf{S}$.

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