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Learning Mixtures of Gaussian Processes through Random Projection

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Functional Data

and

Functional Data Cluster Analysis

Examples of Functional Data

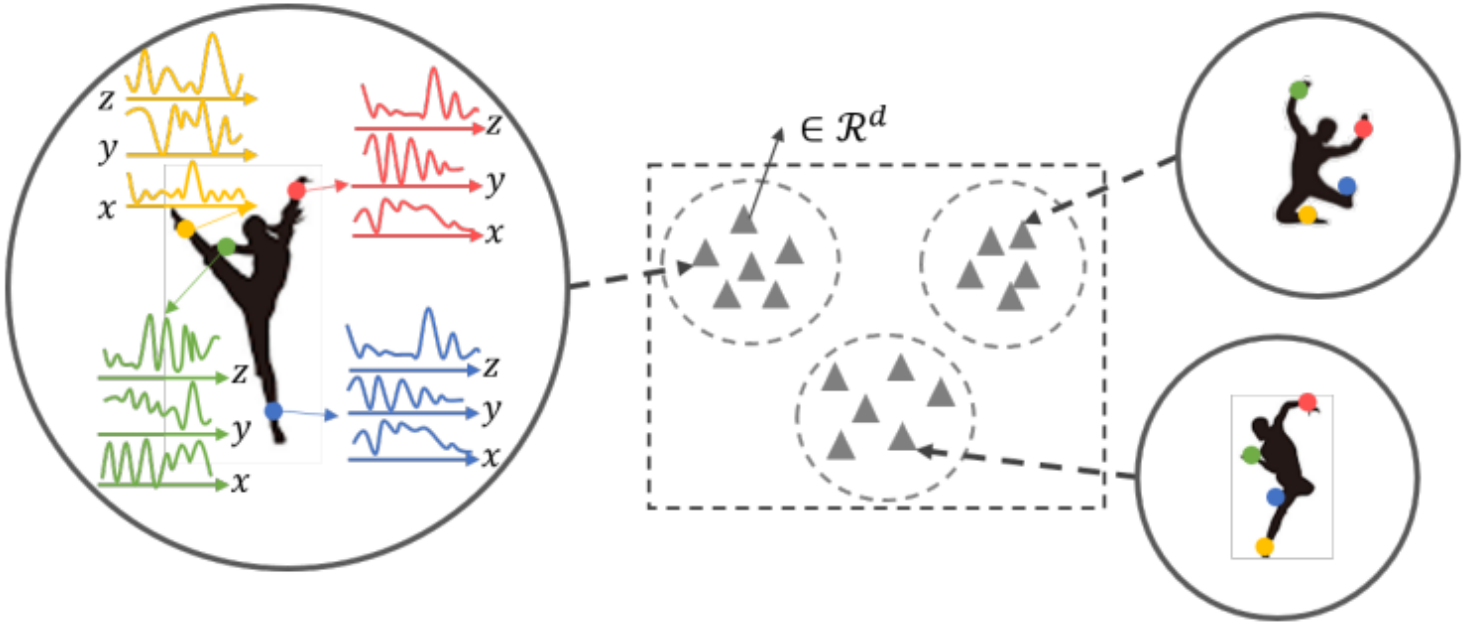
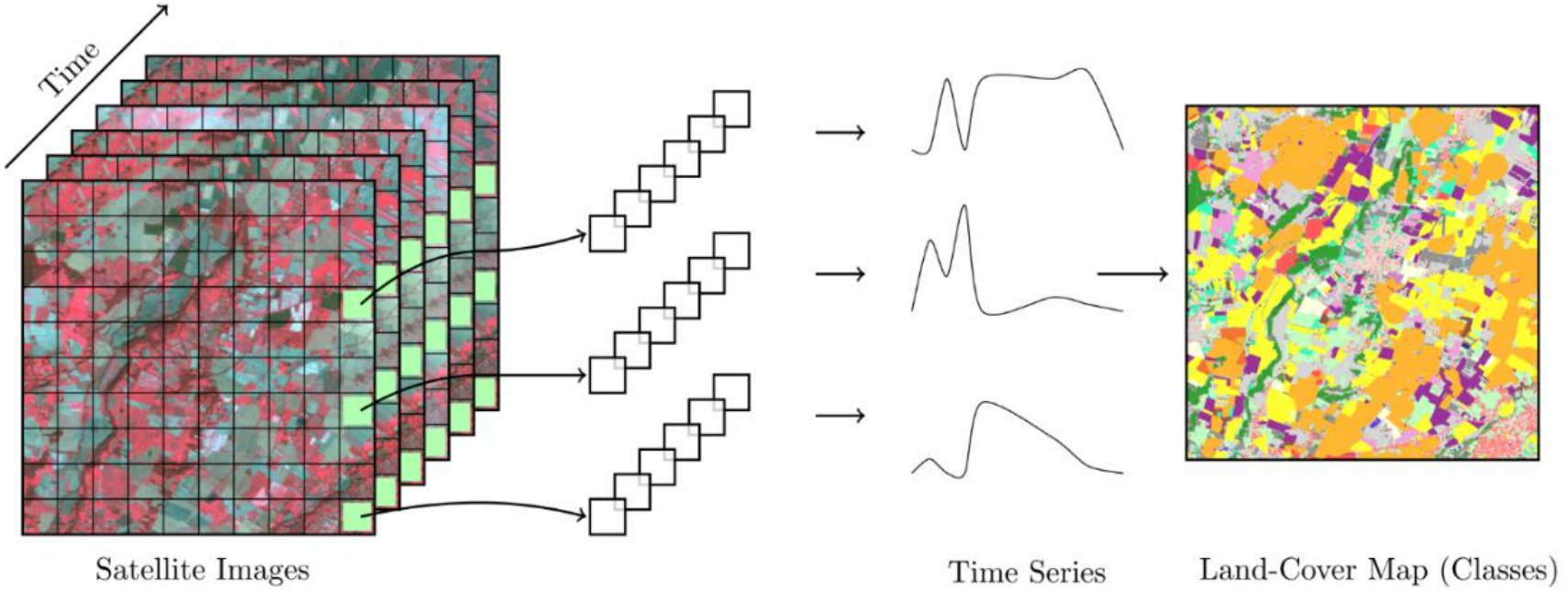


Image source [2]

Examples of Functional Data



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Examples of Functional Data

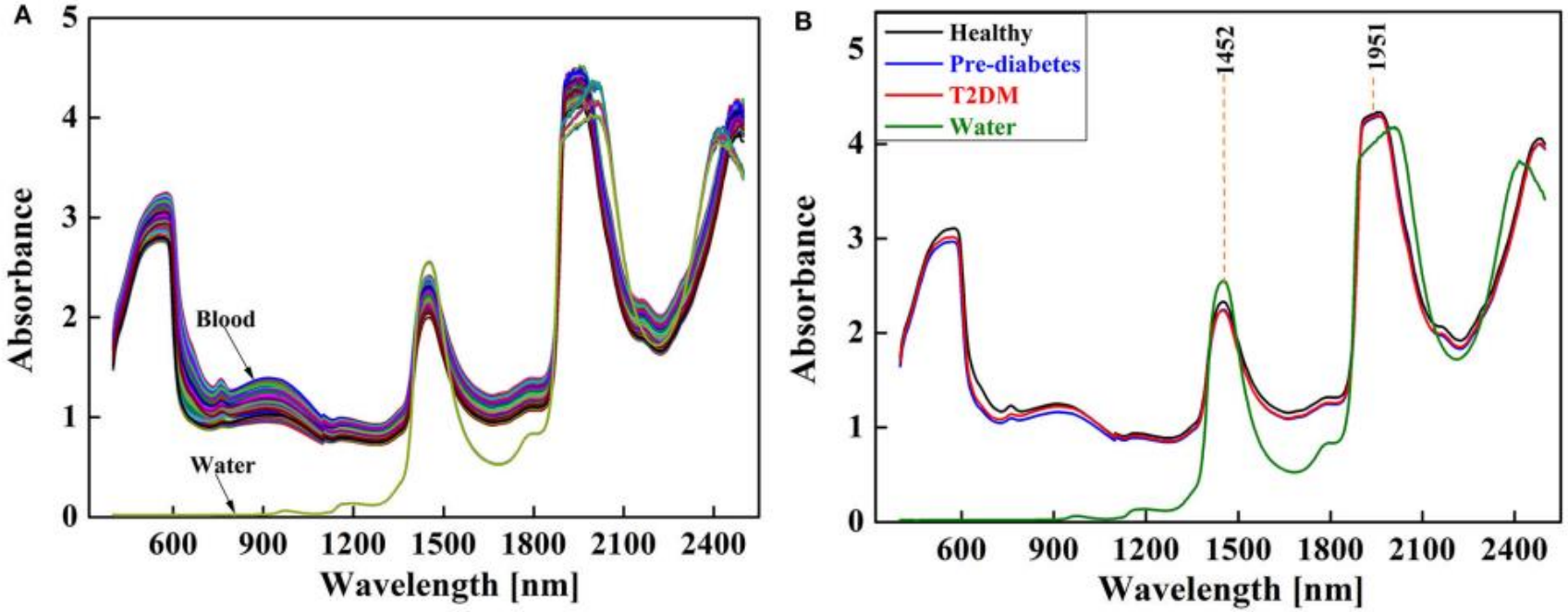


Image source [4]

Reasons for Considering Functional Data

Functional data analysis is about curves, surfaces or anything varying over a continuum.

- **It is more natural to think through modelling problems in a functional form.**
- **The functional form informs us the values of f(t) for t at nearby locations, its derivatives, resilient to noise contamination.**
- **The focus is on analysing relations among the random elements, rather than properties of individual random elements.**

Examples of Functional Data Clustering

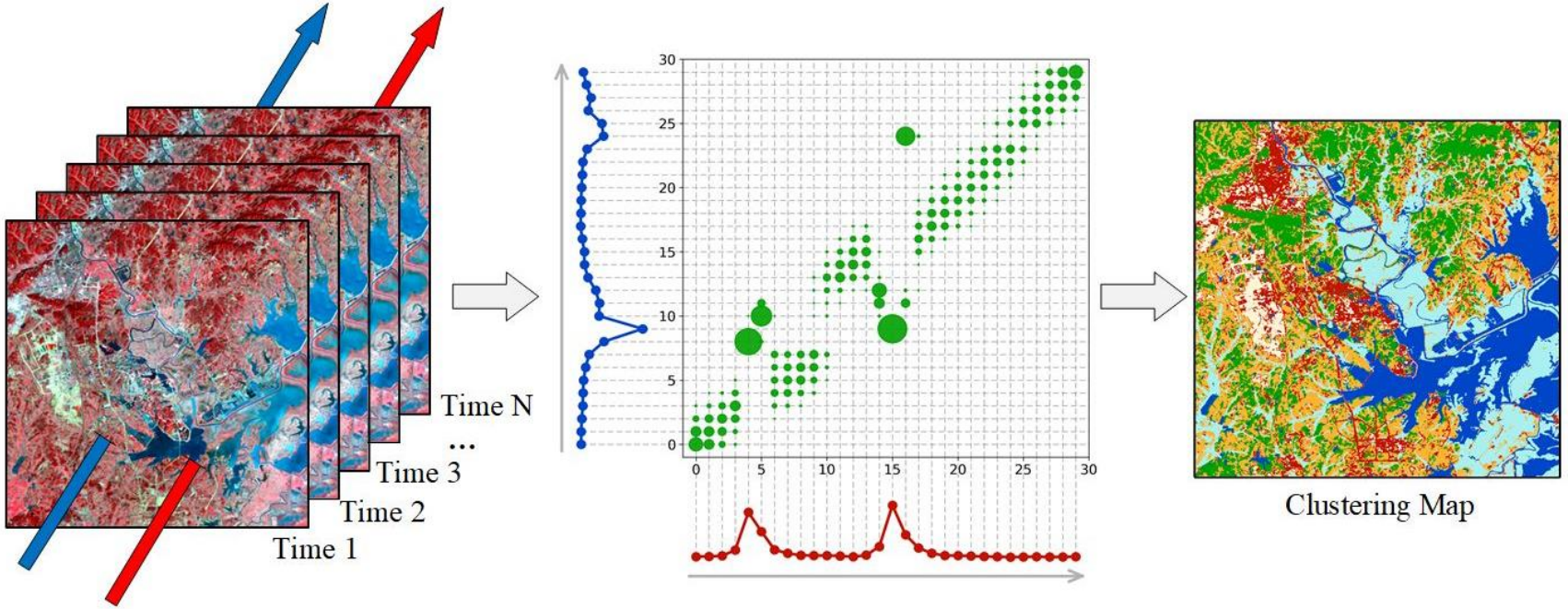


Image source [5]

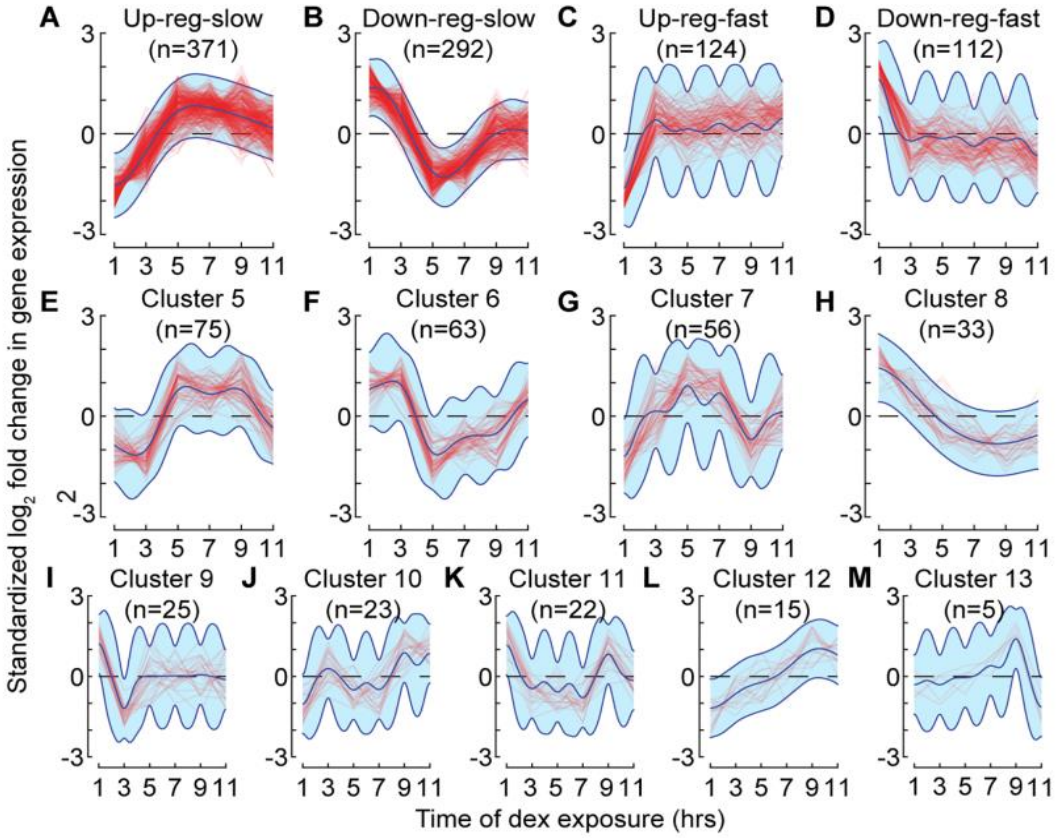
land cover mapping

Examples of Functional Data Clustering

RNA-seq data were generated from a human cell line at 1, 3, 5, 7, 9, and 11 hours after treatment with the synthetic gluco-corticoid (GC) dex.

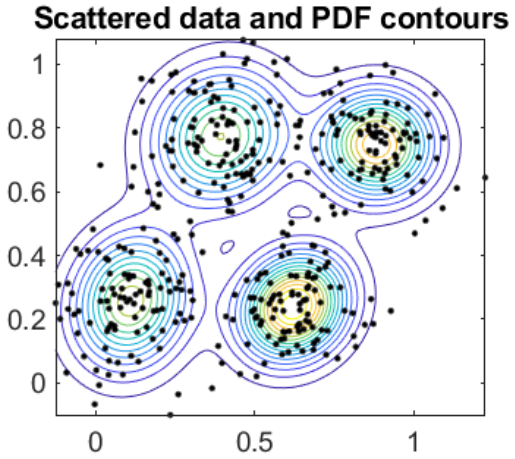
Clustering methods partition time series gene expression data into disjoint clusters based on the similarity of expression response.

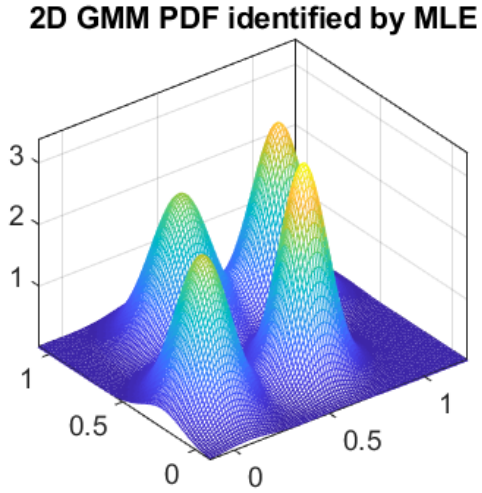
Image source [6]



Gaussian Process (GP) Mixture

Gaussian Mixture Model (GMM)





$$X \sim \sum_{k=1}^{K} \pi_k N(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) .$$

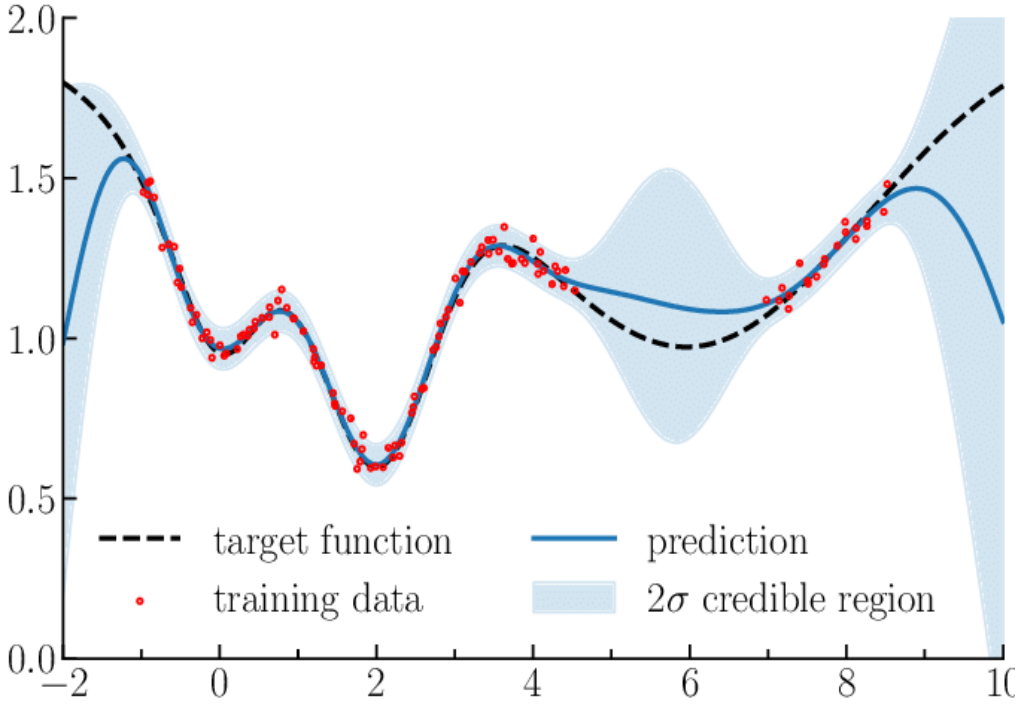
Clustering is done by assigning each $\boldsymbol{x}_i$ to the mixture component (i.e., cluster) to which it is most likely to belong a posteriori.

Gaussian Process (GP)

A Gaussian process $GP(\mu, \Sigma)$ is a stochastic process:

$X \sim GP(\mu, \Sigma)$, then $\forall\, \boldsymbol{t} = (t_1, \ldots, t_m)^T$,

$$X(\boldsymbol{t}) \sim N\big(\mu(\boldsymbol{t}), \Sigma(\boldsymbol{t}, \boldsymbol{t})\big).$$



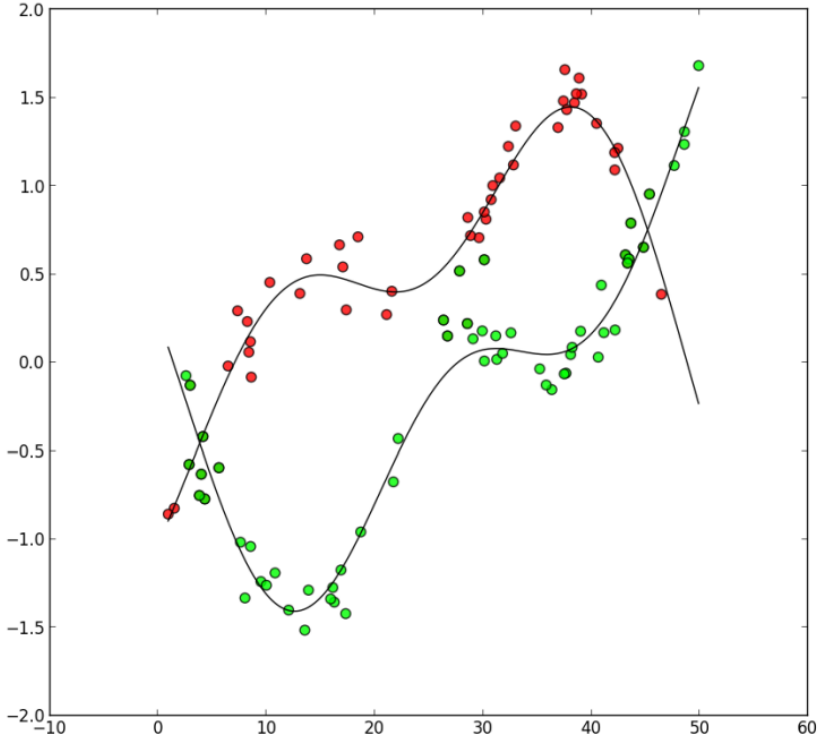
Gaussian Process (GP) Mixture

$$\{(x_i, z_i): i = 1, \dots, n\} \sim_{iid} (X, Z)$$

$$\Pr(Z = k) = \pi_k$$

$$[X|Z = k] = X_k \sim GP(\mu_k, \Sigma_k)$$

$$x_i(\boldsymbol{t}) \sim \sum_{k=1}^{K} \pi_k N\left(\mu_k(\boldsymbol{t}), \Sigma_k(\boldsymbol{t}, \boldsymbol{t})\right)$$



From

GP Mixture

to

Univariate Gaussian Mixture Model

Projecting onto One Dimension

Gaussian Random Variable	Gaussian Random Function
$[X\|Z=k]=X_k\sim N(\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)$: $\boldsymbol{\Sigma}_k=\sum_{r=1}^{\infty}\lambda_{kr}\boldsymbol{b}_{kr}\boldsymbol{b}_{kr}^T$.	$[X\|Z=k]=X_k\sim GP(\mu_k,\Sigma_k)$: $\Sigma_k(s,t)=\sum_{r=1}^{\infty}\lambda_{kr}b_{kr}(s)b_{kr}(t)$.
$\forall\,\boldsymbol{y}\in\mathbb{R}^p$, $\langle X_k,\boldsymbol{y}\rangle\sim N\left(\langle\boldsymbol{\mu}_k,\boldsymbol{y}\rangle,\sum_{r=1}^{\infty}\lambda_{kr}\langle\boldsymbol{b}_{kr},\boldsymbol{y}\rangle^2\right)$.	$\forall\,y\in\mathcal{H}(T,\mathbb{R})$, $\langle X_k,y\rangle\sim N\left(\langle\mu_k,y\rangle,\sum_{r=1}^{\infty}\lambda_{kr}\langle b_{kr},y\rangle^2\right)$.
$\langle X,\boldsymbol{y}\rangle\sim\sum_{k=1}^{K}\pi_k N(\langle\boldsymbol{\mu}_k,\boldsymbol{y}\rangle,\sum_{r=1}^{\infty}\lambda_{kr}\langle\boldsymbol{b}_{kr},\boldsymbol{y}\rangle^2)$	$\langle X,y\rangle\sim\sum_{k=1}^{K}\pi_k N(\langle\mu_k,y\rangle,\sum_{r=1}^{\infty}\lambda_{kr}\langle b_{kr},y\rangle^2)$

How to generate the projection function y?

Fixed:

- wavelets
- B-splines
- Fourier
- $\{b_1, \ldots, b_m\}$ from $\Sigma(s,t) = \sum_{r=1}^{\infty} \lambda_r b_r(s) b_r(t)$

Random:

- Ornstein-Uhlenbeck process
- $y(t) = \sum_{r=1}^{m} a_r b_r(t)$ where $a_r \sim N(0, \lambda_r)$

The GPmix Algorithm

Input: The raw data $\mathcal{D} = \{y_i(t_i)\}_{i=1}^n$, the projection functions $\{\beta_v\}_{v=1}^V$, and the number of clusters K.

Output: The learned cluster labels $\{z_i\}_{i=1}^n$.

1: Estimate the population mean function μ and the n sample functions $\{x_i\}_{i=1}^n$.

2: **for** $v = 1, \ldots, V$ **do**

3: Calculate the n projection coefficients:

$$\alpha_{iv} = \langle x_i - \mu, \beta_v \rangle, \quad 1 \le i \le n.$$

4: Train a univariate GMM from the data $\{\alpha_{iv}\}_{i=1}^n$, denoted by $\sum_{k=1}^K \pi_{vk}\phi(\alpha; u_{vk}, \sigma_{vk}^2)$.

5: Obtain the cluster membership matrix $\mathbf{M}_v$:

$$m_{ik}^v = \frac{\pi_{vk}\phi(\alpha_{iv}; u_{vk}, \sigma_{vk}^2)}{\sum_{j=1}^K \pi_{vj}\phi(\alpha_{iv}; u_{vj}, \sigma_{vj}^2)}, \quad 1 \le i \le n,\ 1 \le k \le K.$$

6: Construct a binary membership indicator matrix $\mathbf{B}_v$:

$$b_{ik}^v = \begin{cases} 1, & \text{if } k = \arg\max_{1 \le j \le K}\{m_{ij}^v\}; \\ 0, & \text{otherwise.} \end{cases}$$

7: Calculate the weight $w_v (> 0)$: $\sum_{v=1}^V w_v = 1$.

8: **end for**

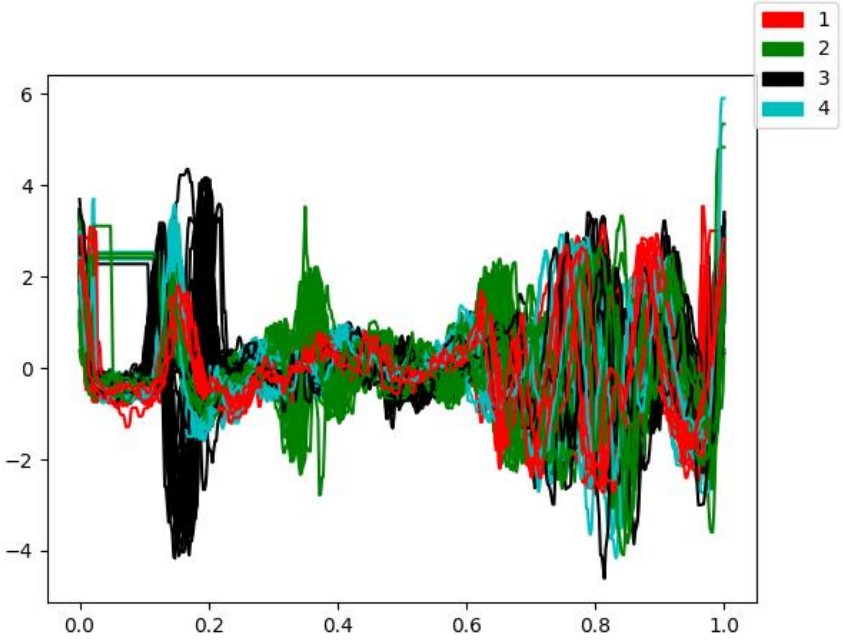
9: Apply a multivariate clustering method on the affinity matrix $\mathbf{A} = \sum_{v=1}^V w_v \mathbf{B}_v \mathbf{B}_v^T$ and return the identified cluster labels $\{z_i\}_{i=1}^n$.

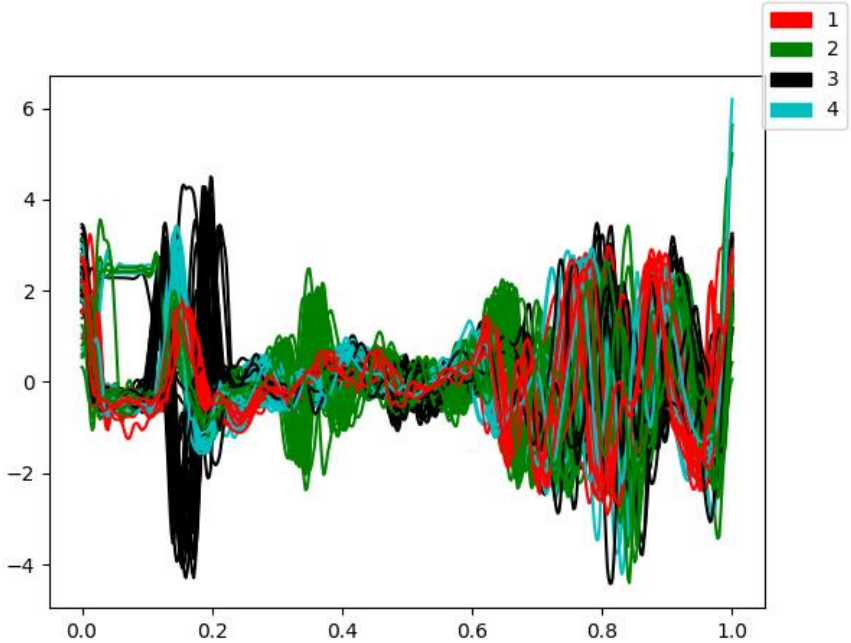
from raw data to smooth functions

projecting functional data & learning a univariate GMM from the projection coefficients

extracting a consensus clustering from the multiple GMMs

Algorithm - Smooth

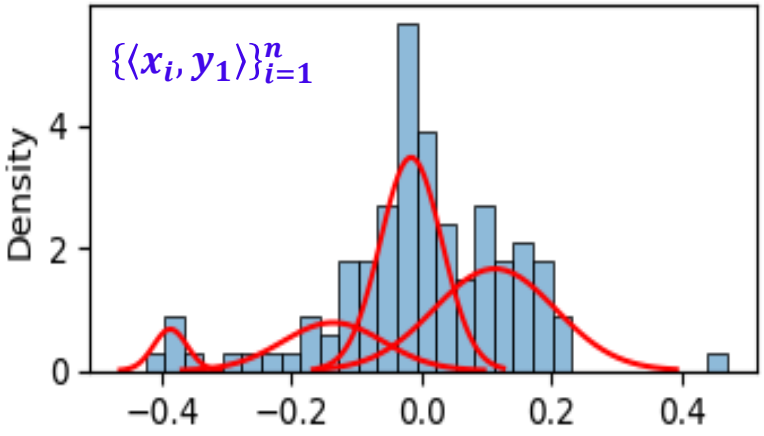




FaceFour from UEA & UCR Time Series Classification Repository.

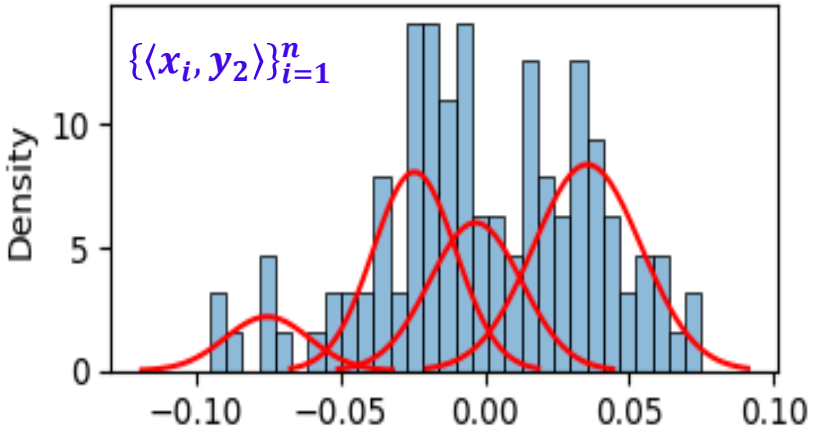
Algorithm - Projection

Projection function y_1 (wavelet: sym17)



Univariate GMM $\sum_{k=1}^{4} \pi_k N(u_{1k}, \sigma_{1k}^2)$

Projection function y_2 (wavelet: sym17)



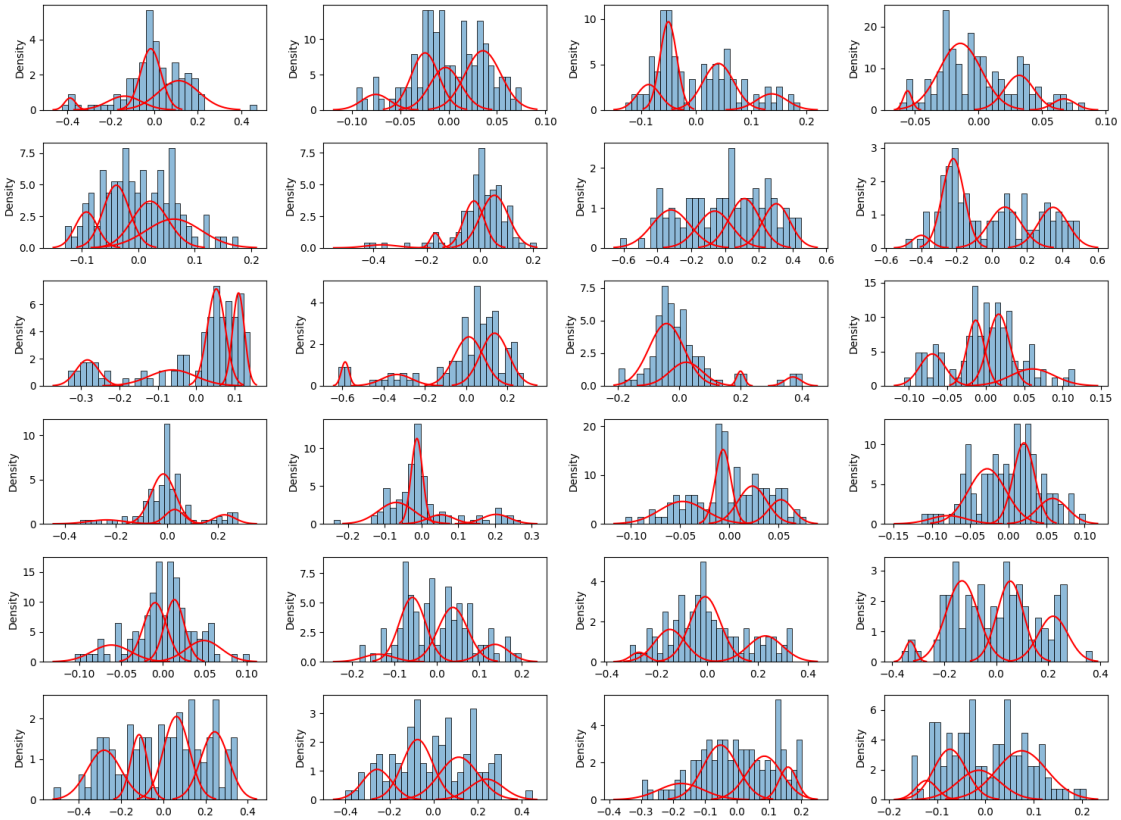
Univariate GMM $\sum_{k=1}^{4} \pi_k N(u_{2k}, \sigma_{2k}^2)$

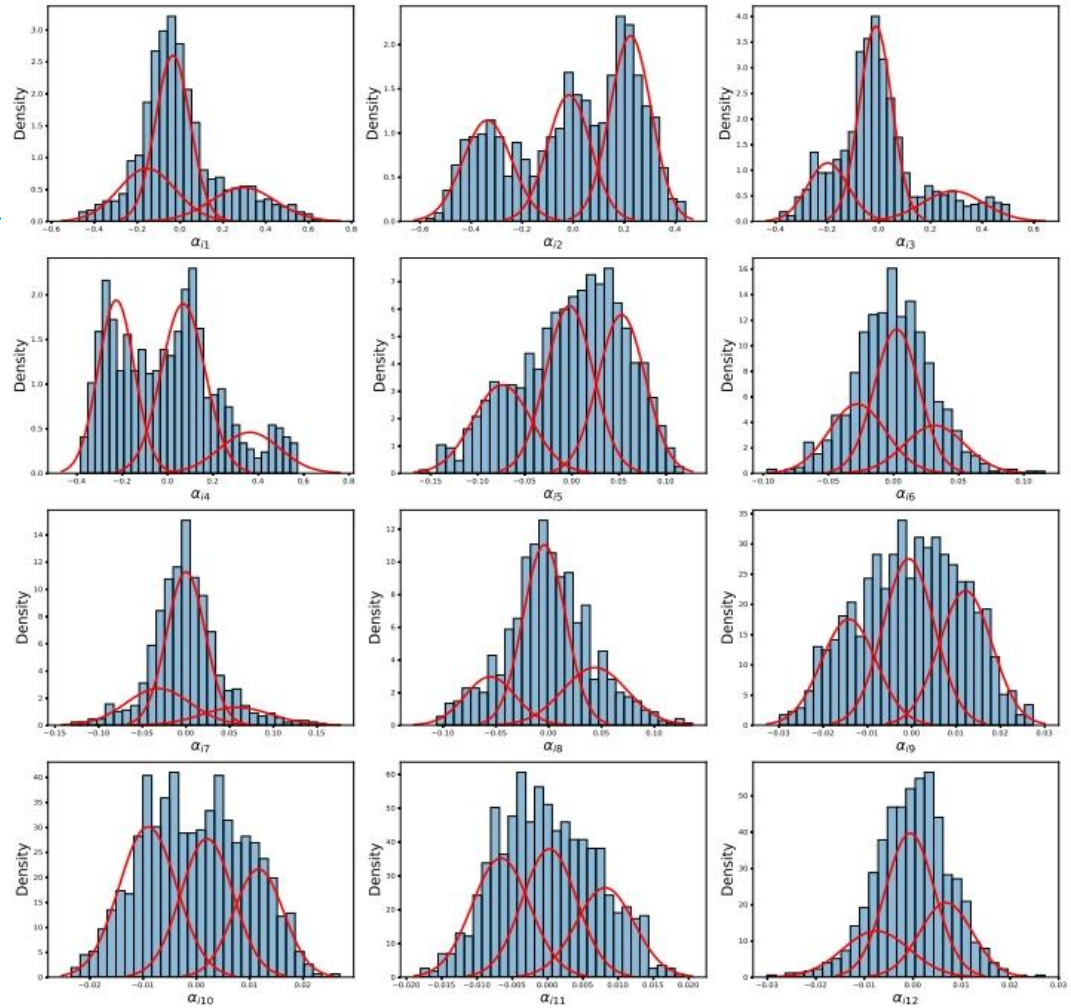
Algorithm - Ensemble

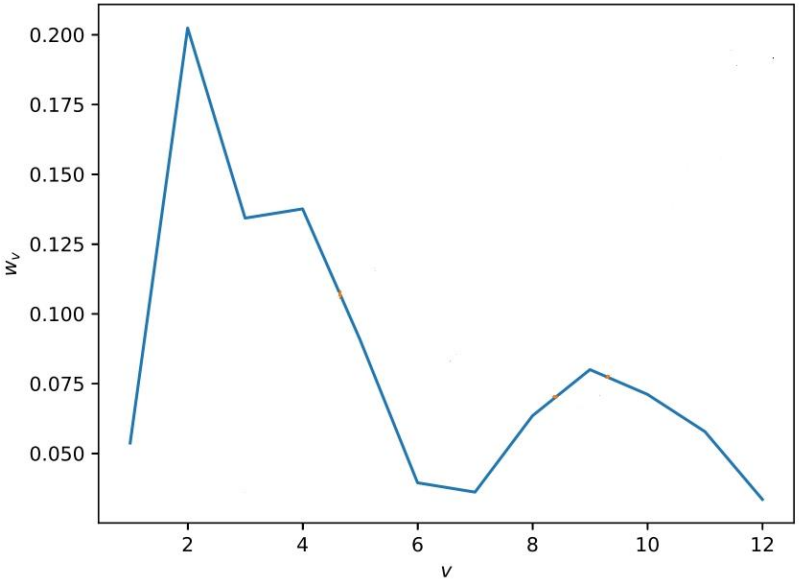
Perform cluster analysis on

$$A = \sum_{r=1}^{m} w_r B_r B_r^T,$$

- B_r is the membership indicator matrix obtained from r-th GMM.
- w_r is a data-driven weight on the r-th GMM.







Base clustering weights W_r, calculated according to the overlapping degree of mixture components.

Theoretical Analysis

Conditions for the identifiability of GP mixtures.

The probability that a 1-dimensional random projection achieves a separation of ϵ or higher among the mixture components.

Sample complexity and computational complexity of the learning problem are in every way polynomial.

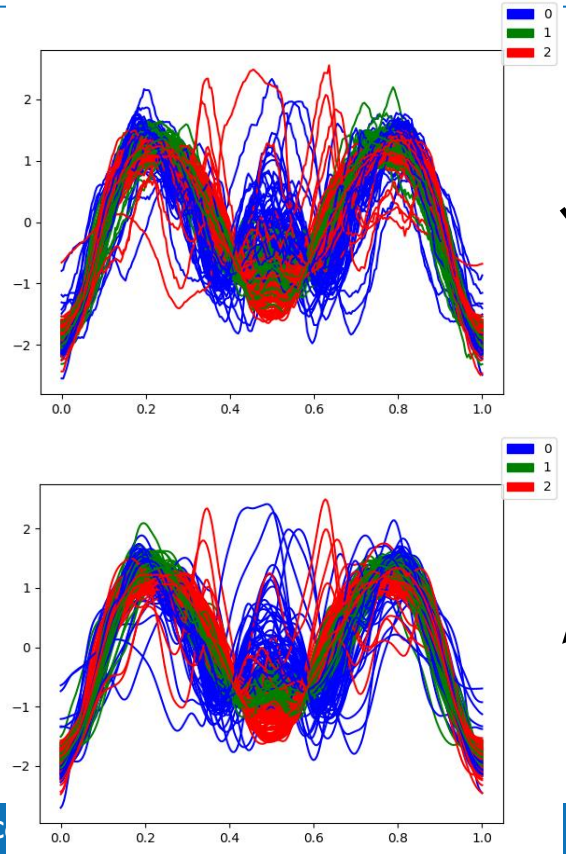
Experimental Results

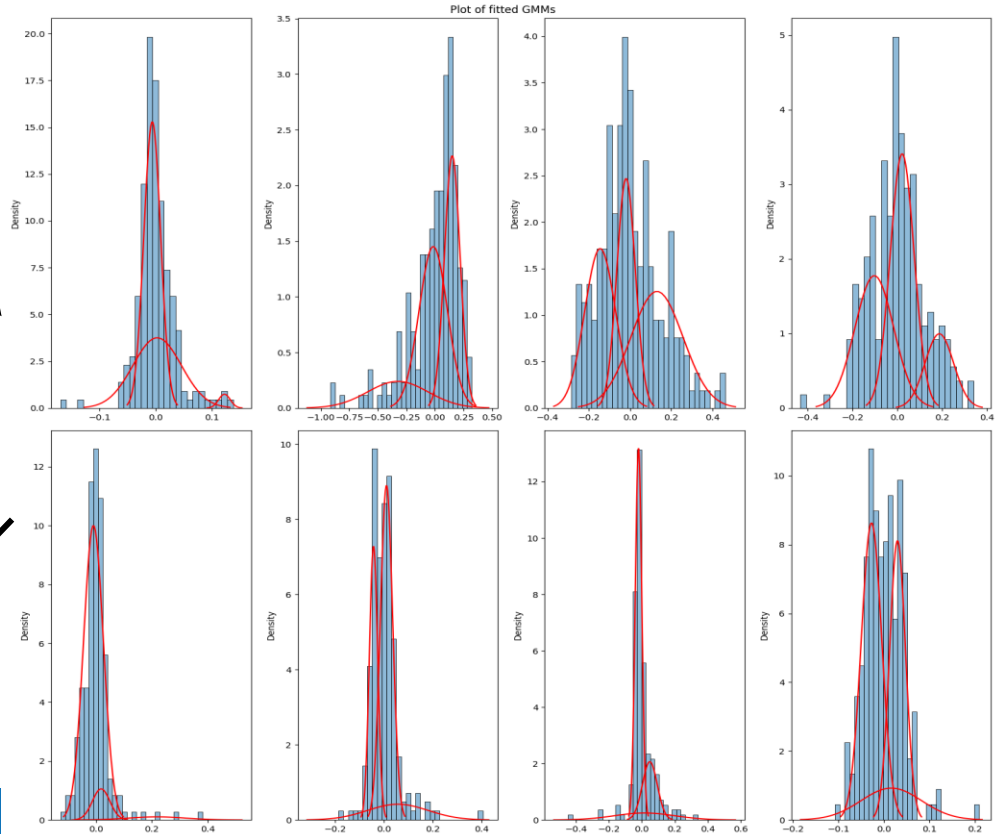
Real Data Analysis

ArrowHead

wavelet: db10

AMI: 0.37
ARI: 0.36
CCA: 0.67



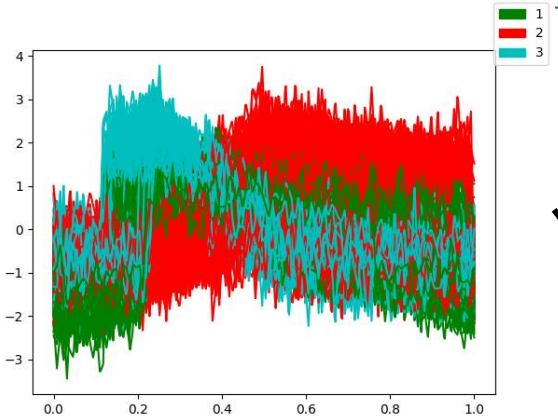


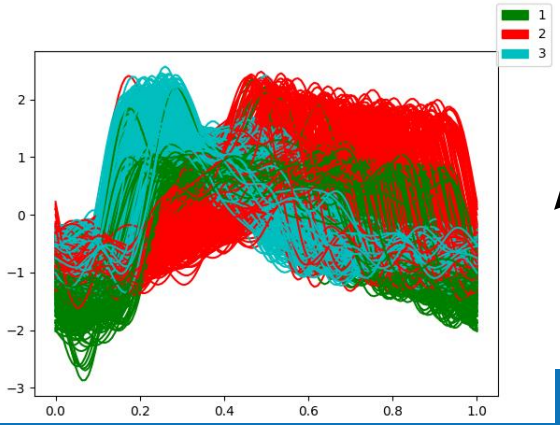
Real Data Analysis

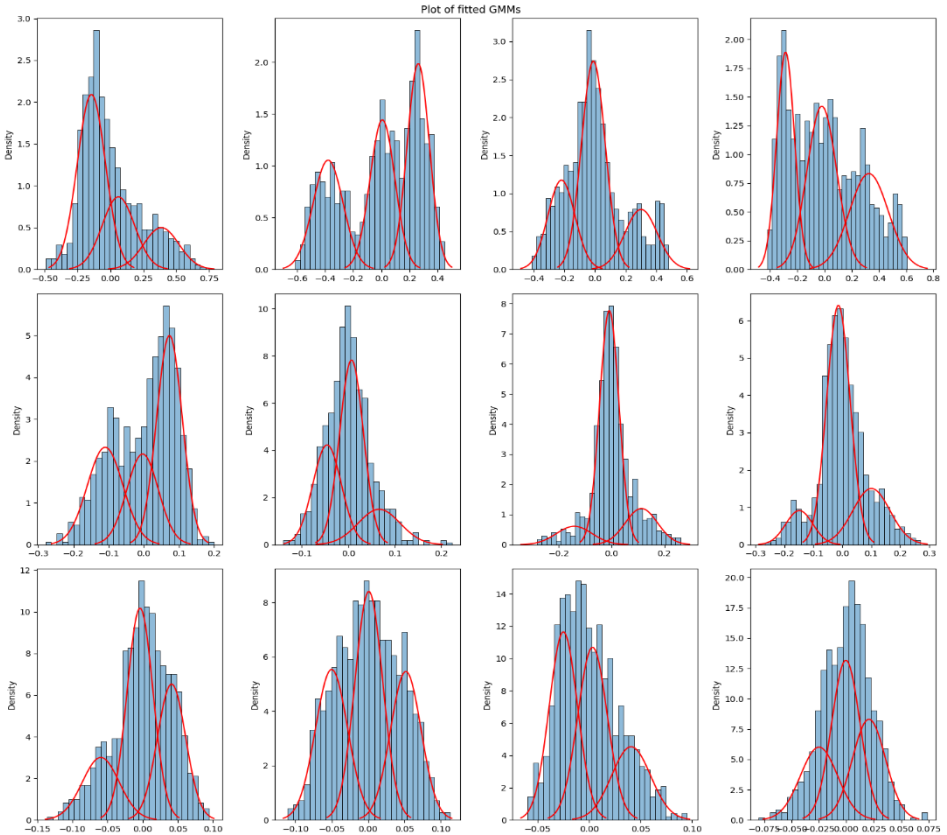
CBF

wavelet: Haar

AMI: 0.84
ARI: 0.87
CCA: 0.89







Real Data Analysis

Data	Projection Function	No. Projections	AMI	ARI	CCA
FaceFour	wavelet: bior2.4	64	0.77	0.76	0.86
ECG200	wavelet: Haar	6	0.37	0.38	0.83
CBF	wavelet: Haar	14	0.84	0.87	0.89
Symbols	Fourier	16	0.75	0.66	0.69
Meat	wavelet: bior2.4	10	0.70	0.69	0.84
Diatom Size Reduction	OU	32	0.94	0.95	0.98
Trace	wavelet: db35	8	0.49	0.43	0.68
ArrowHead	wavelet: db10	8	0.37	0.36	0.67
GunPoint	wavelet: bior2.4	6	0.34	0.25	0.75

Real Data Analysis

Benchmarking with:

funFEM
funHDDC
Funclust (from Funclustering)
FClust (from fdapace)
kmeans_align (from fdasrvf)
FADPclust

DATA	GPMIX	FEM	HDD	CLU	FC	KM	ADP
AH	**0.37**	0.25	0.22	0.05	0.24	0.28	0.19
	0.36	0.29	0.21	0.01	0.25	0.26	0.18
BC	**0.24**	0.03	0.06	0.22	0.08	0.10	0.08
	0.29	0.04	0.07	0.15	0.10	0.10	0.10
CBF	**0.84**	0.37	0.47	0.01	0.53	0.34	0.40
	0.87	0.35	0.44	0.00	0.44	0.31	0.31
DSR	**0.94**	0.79	0.82	0.00	0.83	0.72	0.78
	0.95	0.83	0.86	0.01	0.86	0.73	0.82
ECG	**0.37**	0.15	0.17	0.03	0.37	0.17	0.07
	0.38	0.26	0.28	0.03	0.37	0.28	0.14
FF	**0.77**	0.47	0.40	0.06	0.56	0.50	0.44
	0.76	0.41	0.36	0.08	0.54	0.45	0.32
GUP	**0.34**	0.00	0.00	0.02	0.00	0.15	0.01
	0.25	0.00	0.00	0.02	0.00	0.07	0.01
MEAT	0.70	**0.93**	0.54	0.36	0.54	0.66	0.72
	0.69	**0.95**	0.44	0.37	0.49	0.69	0.69
SB	**0.32**	0.08	0.00	0.03	0.12	0.07	0.03
	0.30	0.00	0.00	0.03	0.04	0.07	0.05
SYM	0.75	0.63	0.77	0.00	**0.85**	0.69	0.37
	0.66	0.53	0.67	0.00	**0.80**	0.62	0.30

Ref

[1] E. Akeweje and M. Zhang. *Learning Mixtures of Gaussian Processes through Random Projection*. In 41st International Conference on Machine Learning (ICML 2024), Vienna, Austria, 2024.

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