Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

Shape-Informed Clustering of Multi-Dimensional Functional Data via Deep Functional Autoencoders

Samuel V. Singh[1], Shirley Coyle[2], Mimi Zhang[1]
[1]School of Computer Science and Statistics, Trinity College Dublin
[2]School of Electronic Engineering, Dublin City University

NEURAL INFORMATION PROCESSING SYSTEMS
Taighde Éireann Research Ireland
d-real SFI centre for research training in digitally-enhanced reality

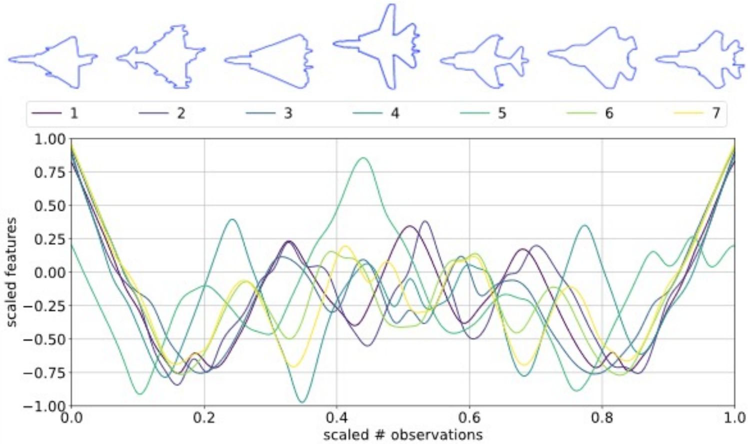
Introduction

Motivation and background

What are Functional Data (FD)?

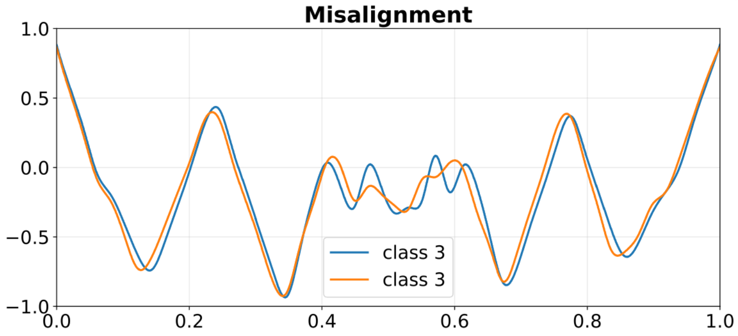
Why is clustering FD challenging?

fPCA or pairwise (dis)similarity measure + clustering algorithm



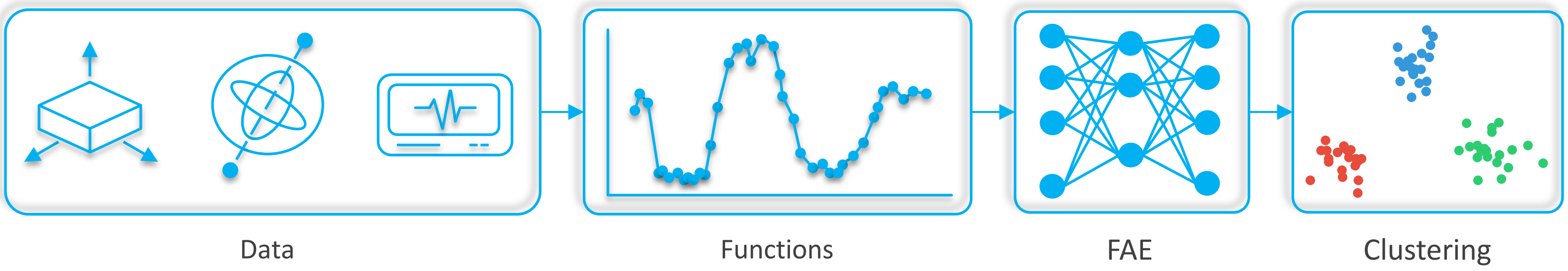
Key problems: high-dimensional, nonlinear, or misaligned in phase

Motivation: deep learning to model nonlinear relationships and incorporated shape-informed clustering



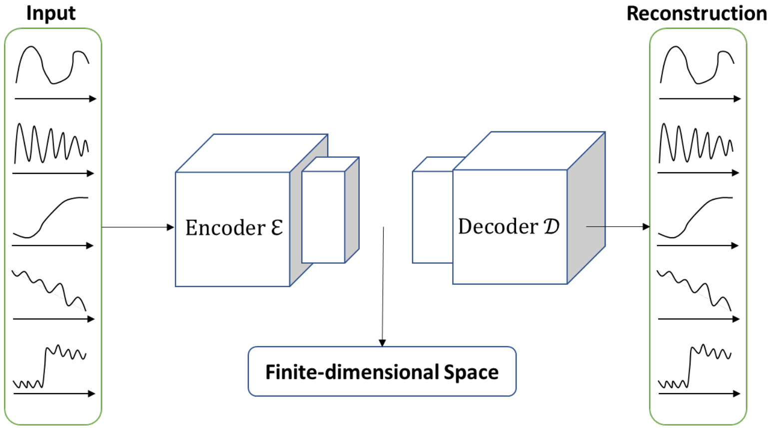
Introducing FAEclust

Functional AutoEncoder for Clustering



FAEclust

- encoder and decoder are both universal approximators
- joint clustering scheme
- shape-informed clustering, robust to phase variation



FAEclust Architecture

Encoder–Decoder

Encoder $\mathcal{E}: \ \mathcal{H}(\mathcal{T}, \mathbb{R}^{\mathrm{p}}) \to \mathbb{R}^{\mathrm{s}}$

$$\boldsymbol{x}^{(1)} = a\left(\int_{\mathcal{T}} \boldsymbol{W}^{(1)}(t)\boldsymbol{y}(t)dt + \boldsymbol{b}\right)$$

$$\boldsymbol{x} = \mathrm{MLP}(\boldsymbol{x}^{(1)})$$

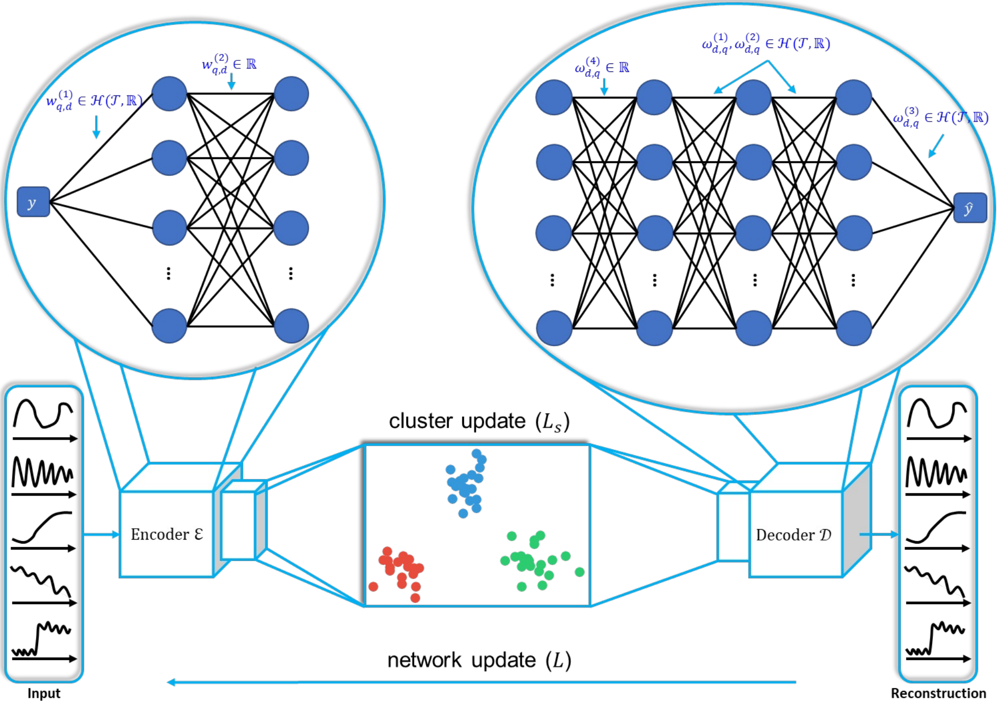
Decoder $\mathcal{D}: \ \mathbb{R}^{\mathrm{s}} \to \mathcal{H}(\mathcal{T}, \mathbb{R}^{\mathrm{p}})$

$$\widehat{\boldsymbol{x}}^{(1)} = \mathrm{MLP}(\boldsymbol{x})$$

$$\widehat{\boldsymbol{y}}^{(1)}(t) = a\left(\boldsymbol{\mathcal{W}}^{(1)}(t)\widehat{\boldsymbol{x}}^{(1)} + \boldsymbol{b}_1(t)\right)$$

$$\widehat{\boldsymbol{y}}^{(2)}(t) = a\left(\boldsymbol{\mathcal{W}}^{(2)}(t)\widehat{\boldsymbol{y}}^{(1)}(t) + \boldsymbol{b}_2(t)\right)$$

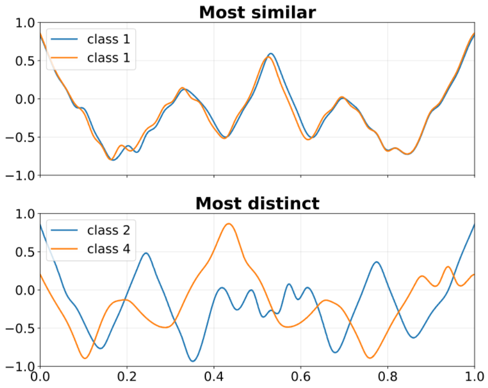
$$\widehat{\boldsymbol{y}}(t) = \boldsymbol{\mathcal{W}}^{(3)}(t)\widehat{\boldsymbol{y}}^{(2)}(t)$$

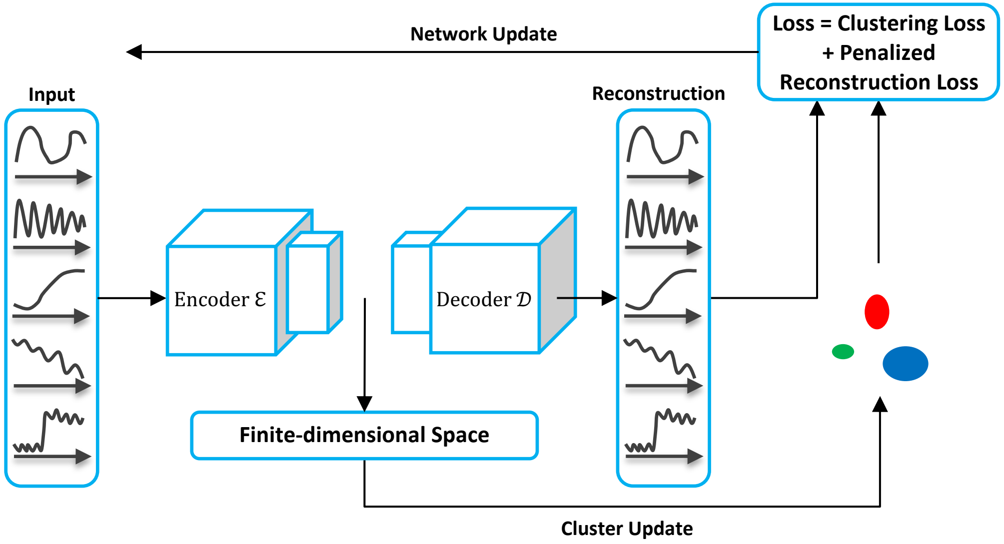


Joint Training & Shape-Informed Clustering

Network training: Forward Phase and Backward Phase

1. **Forward (cluster update):** via convex clustering, where the similarity measure depends on the elastic distance.
2. **Backward (network update):** minimize an integrated objective function L.





$$L = L_r + \lambda_w L_w + \lambda_c L_c$$

Experimental Setup (Data & Baselines)

Euclidean and Manifold-Valued FD Datasets

Baseline methods: FNN (Functional Neural Net), FAE (Functional AutoEncoder), VANO (Variational Autoencoding Neural Operator), funHDDC, funclust, FADPclust(FADP1/FADP2).

Euclidean FD: 17 UEA/UCR datasets

Manifold-valued FD: hypersphere, hyperbolic space, and Swiss-roll manifold, plus trajectories from the Lorenz attractor and a pendulum

Evaluation metrics: Adjusted Mutual Information (AMI), values near 1.0 indicate perfect clustering.

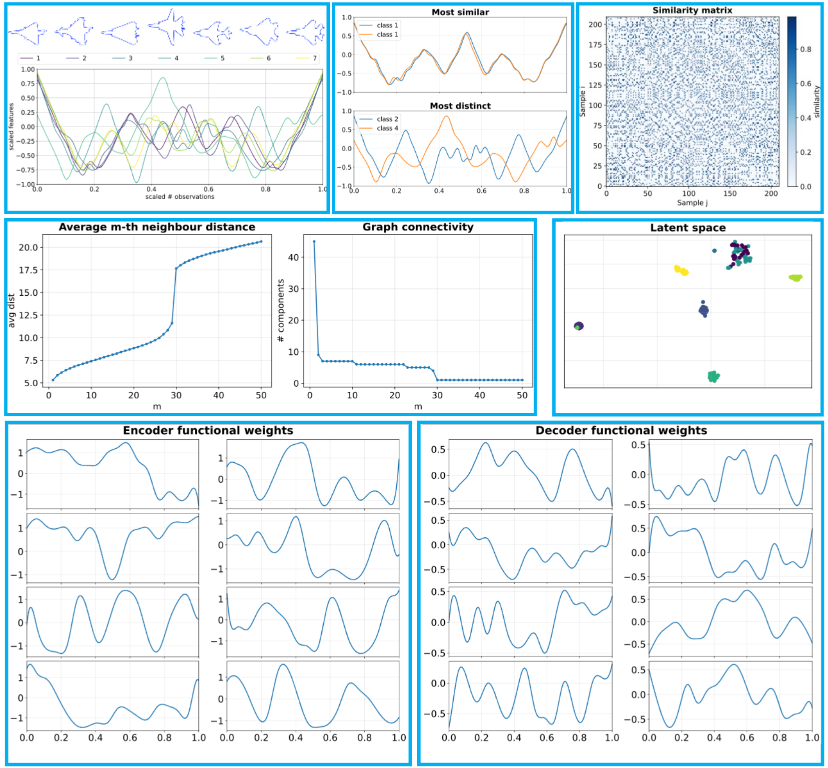
Datasets	funHDDC	funclust	FADP1	FADP2	FNN	FAE	VANO	FAEclust
BirdChicken	0.055	0.080	0.019	0.055	0.290	0.259	0.302	**0.339**
CBF	0.362	0.066	0.435	0.318	0.363	0.370	**0.743**	0.724
Chinatown	0.147	0.147	0.246	0.055	0.236	0.110	0.339	**0.343**
DSR	0.786	0.017	0.692	0.876	0.679	0.645	0.713	**0.887**
ECG200	0.173	0.101	0.201	0.143	0.214	0.213	0.217	**0.261**
Fungi	0.773	0.186	0.477	0.501	0.244	0.624	0.798	**0.925**
Plane	0.819	0.013	0.725	0.741	0.841	0.825	0.846	**0.907**
Rock	0.373	0.228	0.216	0.335	0.184	0.089	0.355	**0.447**
Symbols	0.767	0.001	0.435	0.712	0.748	0.800	0.817	**0.824**
Blink	0.410	0.048	0.189	0.177	0.453	0.506	0.522	**0.633**
BM	0.377	0.031	0.191	0.422	0.401	**0.676**	0.592	0.539
EOS	0.209	0.018	0.104	0.102	0.152	0.206	0.180	**0.266**
Epilepsy	0.143	0.028	0.077	0.225	0.274	0.209	0.297	**0.485**
ERing	0.735	0.012	0.288	0.714	0.643	**0.743**	0.733	0.664
FM	0.001	0.001	0.002	0.002	0.174	0.138	0.174	**0.228**
JV	0.840	0.069	0.294	0.466	0.236	0.854	**0.899**	0.893
SWJ	0.268	0.040	0.248	0.046	0.174	0.170	**0.344**	0.324
Hypersphere	0.016	0.478	0.137	0.067	0.089	0.307	0.443	**0.737**
Hyperbolic	0.005	0.013	0.001	0.001	0.004	0.047	0.410	**0.798**
Swiss roll	0.127	0.114	0.382	0.189	0.016	0.125	0.242	**0.432**
Lorenz	0.109	0.389	0.092	0.144	0.023	0.246	0.251	**0.457**
Pendulum	0.887	0.376	0.797	0.808	0.253	0.794	0.905	**0.986**

Results and Conclusion

Contributions & Takeaways

- Framework that unifies deep functional representation learning with clustering
- Shape-informed clustering objective
- Universal approximation and stability
- Empirical evidence through
  - Euclidean
  - Manifold
- Time warped scenarios

Limitation: slightly higher runtime



Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

Thank You

Scan to access full paper and code:

NEURAL INFORMATION PROCESSING SYSTEMS

Taighde Éireann Research Ireland

d· real

SFI centre for research training in digitally-enhanced reality