Scalable Gromov-Wasserstein based comparison of biological time series

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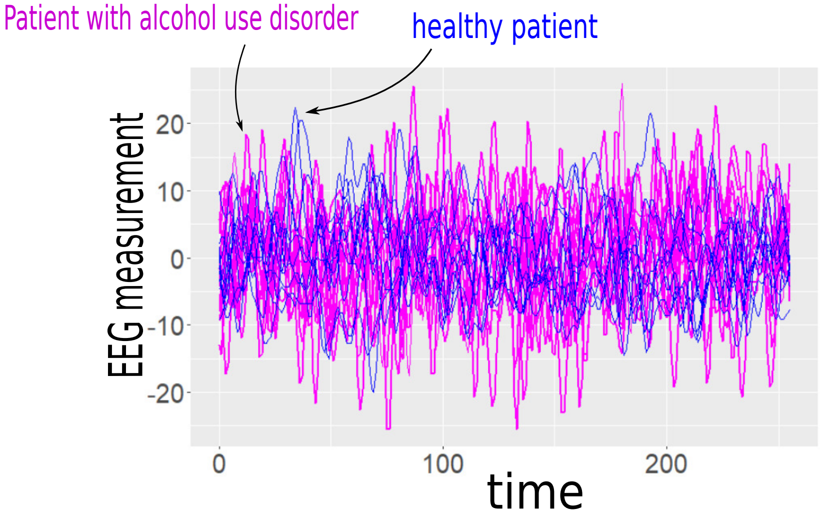
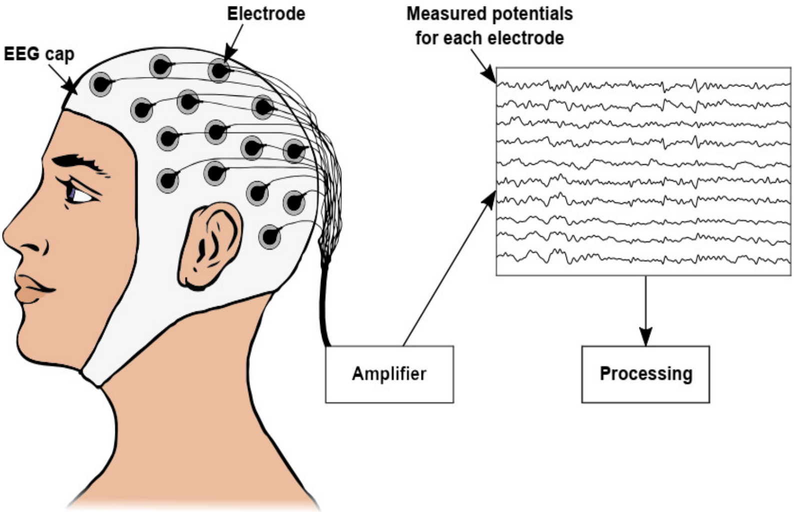
Paper: Kravtsova, McGee II, Dawes (2023), *Bull. Math. Biol.*

Motivating example:
Medical time series with two classes



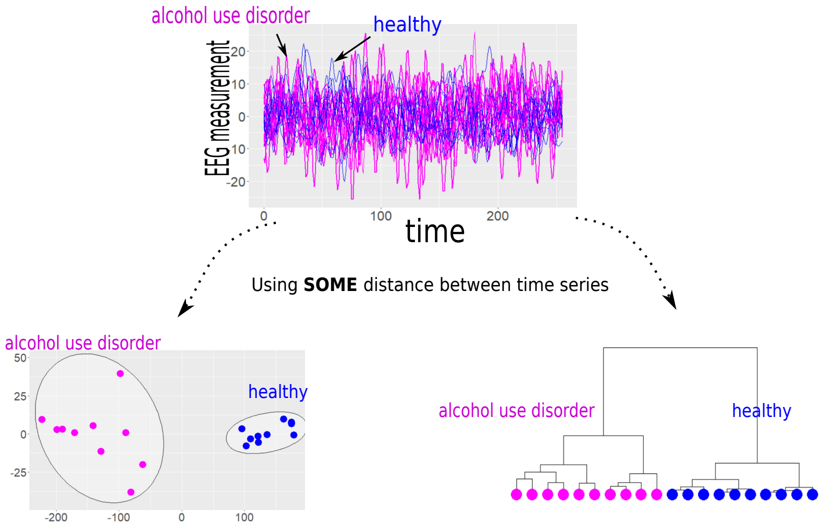
Dataset *smni9_eeg_data* from *UCI Machine Learning repository (Dua and Graph 2017)*

Motivating example: Electroencephalogram (EEG) process illustration

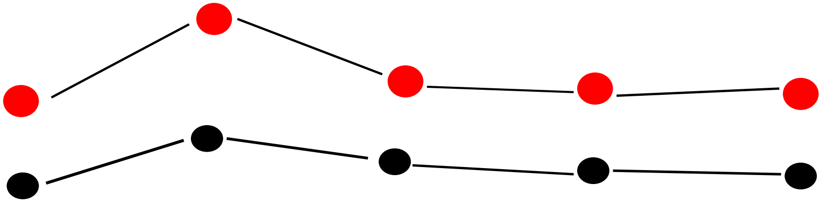


Picture from *Nagel 2019*

Motivating example:
Separate two classes (healthy vs. alcohol use disorder)

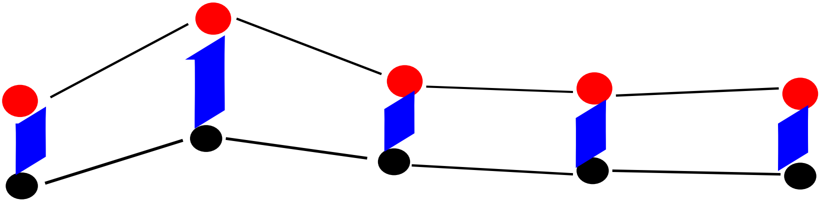


Distance between two trajectories



Distance between two trajectories

Euclidean



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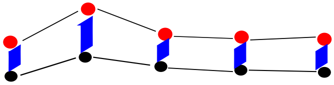

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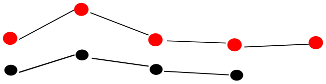

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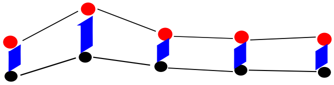
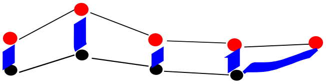
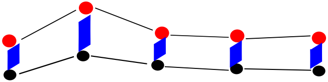


DTW



Distance between two trajectories

Euclidean



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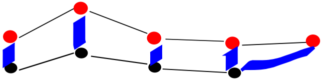

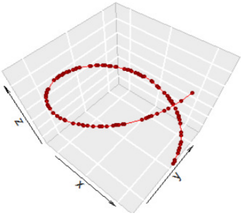

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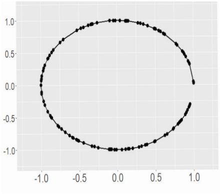

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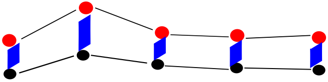

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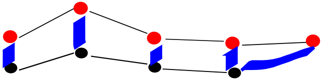

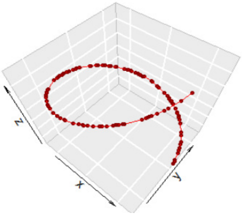

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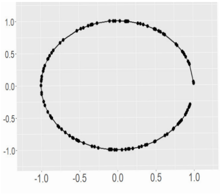

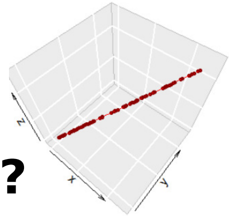

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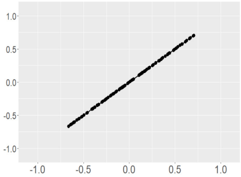
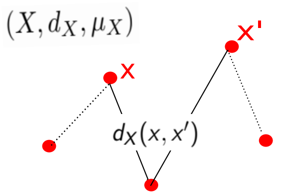
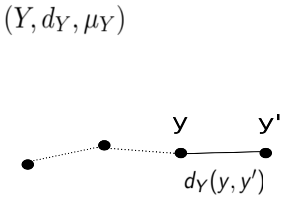


Define distance between time series based on Gromov-Wasserstein distance of *Mémoli 2011*

View two trajectories as metric measure spaces:



$\mu_X = (1/5, \ 1/5 \ \ 1/5 \ \ 1/5 \ \ 1/5)$



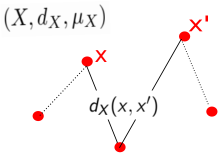
$\mu_Y = (1/4 \ \ 1/4 \ \ 1/4 \ \ 1/4)$

NOTE: Even if both trajectories lie in the same space (e.g. $\mathbb{R}^2$), this technique purposely ignores it

Define distance between time series based on Gromov-Wasserstein distance of *Mémoli 2011*

Mémoli 2011 defines the $p \in [1, \infty)$ **Gromov-Wasserstein distance** between metric measure spaces by

$$GW(X, Y) := \frac{1}{2} \inf_{\mu \in \mathcal{C}(\mu_X, \mu_Y)} \left(\int_{X \times Y} \int_{X \times Y} |d_X(x, x') - d_Y(y, y')|^p \, d\mu(x, y) d\mu(x', y') \right)^{1/p}$$



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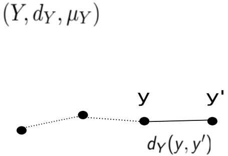


$\mu_Y = (1/4 \ \ 1/4 \ \ 1/4 \ \ 1/4)$

Note: Non-convex program

Define distance between time series based on Gromov-Wasserstein distance of *Mémoli 2011*

To overcome non-convexity issue, two main approaches exist:

1. Regularize *GW* objective (*Peyré, Cuturi, & Solomon 2016*)

   Disadvantages: Still non-convex

   Advantages: Convenient gradient descent (used in *Demetci et al. 2022* for bio application)

Define distance between time series based on Gromov-Wasserstein distance of *Mémoli 2011*

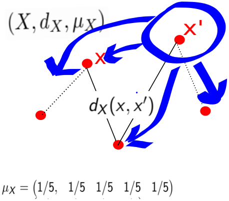
To overcome non-convexity issue, two main approaches exist:

2. Replace *GW* it's lower bounds (*Mémoli 2011*, *Chowdhury & Mémoli 2019*)

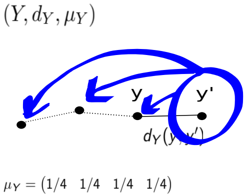
   Advantages: - Convex programs → can be solved exactly!
   - Amenable to statistical analysis (*Weitkamp et al. 2022*)

   Disadvantages: how far is given lower bound from actual *GW*?

Define distance between time series based on Gromov-Wasserstein distance of *Mémoli 2011*



Local distribution of distance at x':
distribution of $d_X(x', \cdot)$

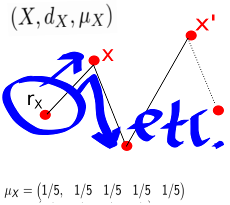


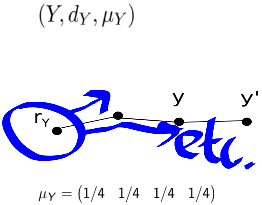
Local distribution of distance at y':
distribution of $d_Y(y', \cdot)$

The Third Lower Bound (*Mémoli 2011*, *Chowdhury & Mémoli 2019*) would compare **ALL** local distributions

Define distance between time series based on Gromov-Wasserstein distance of *Mémoli 2011*

We propose to pick **ONE** particular local distribution:
local distribution at the start of the trajectory





Our program reads: for any $p \in [1, \infty)$,

$$GW_\tau(X, Y) := \inf_{\mu \in \mathcal{C}(\mu_X, \mu_Y)} \left(\int_{X \times Y} |d_X(r_X, x) - d_Y(r_Y, y)|^p \, d\mu(x, y) \right)^{1/p}$$

Properties of GW_τ distance between time series

The object

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satisfies:

1. GW_τ is an upper bound of GW.
   Open question: $TLB \leq GW \leq GW_\tau$

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4. Similar construction is defined for graphs in *Le, Ho, & Yamada 2022*

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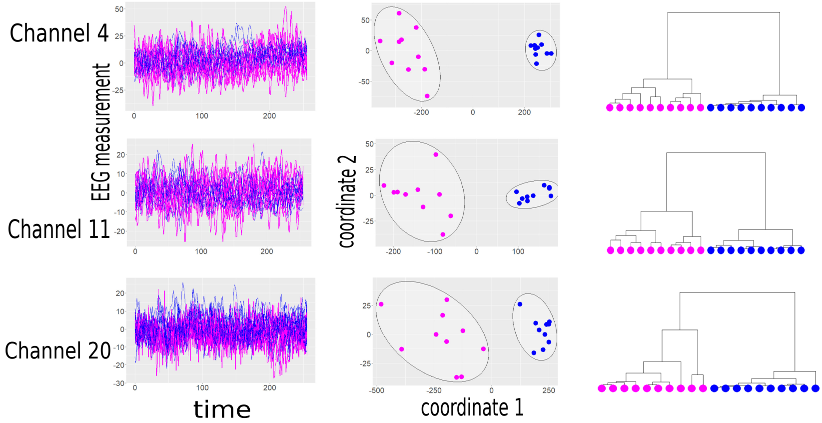
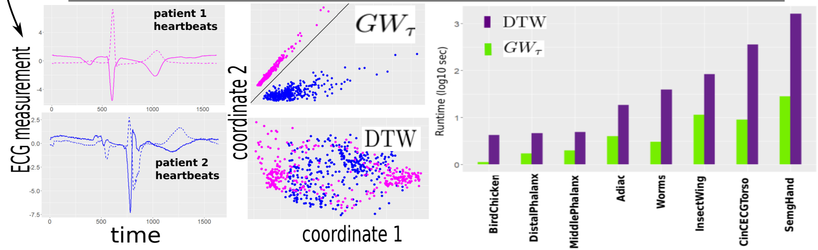
3. GW_τ is a metric on the space of (certain) equivalence classes of trajectories
4. Similar construction is defined for graphs in *Le, Ho, & Yamada 2022*
5. Can be computed in linear time (time series of the same length) or quadratic time (different lengths)

Performance of $GW_{\mathcal{T}}$ distance between time series: EEG dataset

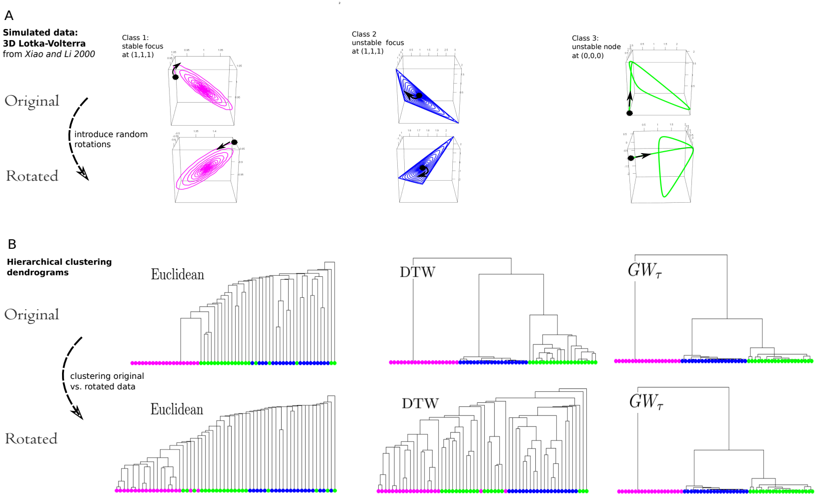


Performance of GW_τ distance between time series: 1-Nearest Neighbor classification of UCR Time Series Classification Archive data (*Dau et al. 2018*)

UCR dataset name	# classes	t.s. length	train size	test size	Euclidean error	GW_τ error	DTW error
CinCECGTorso	4	1639	40	1380	0.1029	0.1290*	0.3493
InsectWingbeatSound	11	265	220	1980	0.4384	0.5995*	0.6449
DistalPhalanxOutlineAgeGroup	3	80	400	139	0.3741	0.3237*	0.2302
Worms	5	900	181	77	0.5455	0.5325*	0.4156
Adiac	37	176	390	391	0.3887	0.3555**	0.3964
BirdChicken	2	512	20	20	0.4500	0.1500**	0.2500
MiddlePhalanxOutlineAgeGroup	3	80	400	154	0.4805	0.4740**	0.5000
SemgHandMovementCh2	6	1500	450	450	0.6311	0.3933**	0.4156

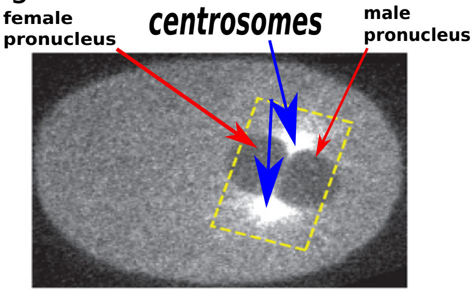


Performance of GW_τ distance between time series: 3D Lotka-Volterra dynamical system (*Xiao & Li 2000*) simulated data



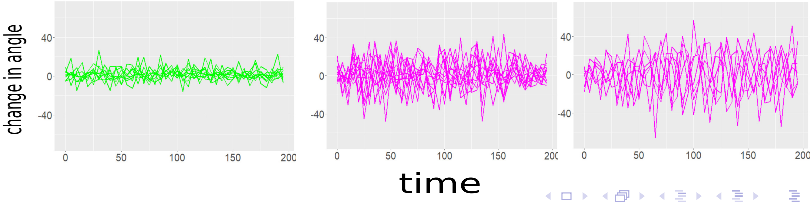
Performance of GW_τ distance between time series: data from Dawes lab (*Ignacio et al. 2022*)

C. elegans zygote

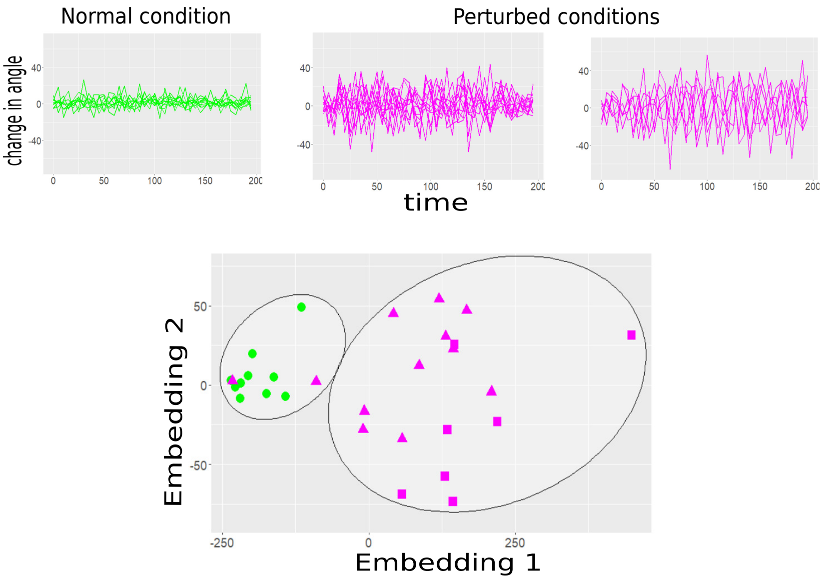


Normal condition

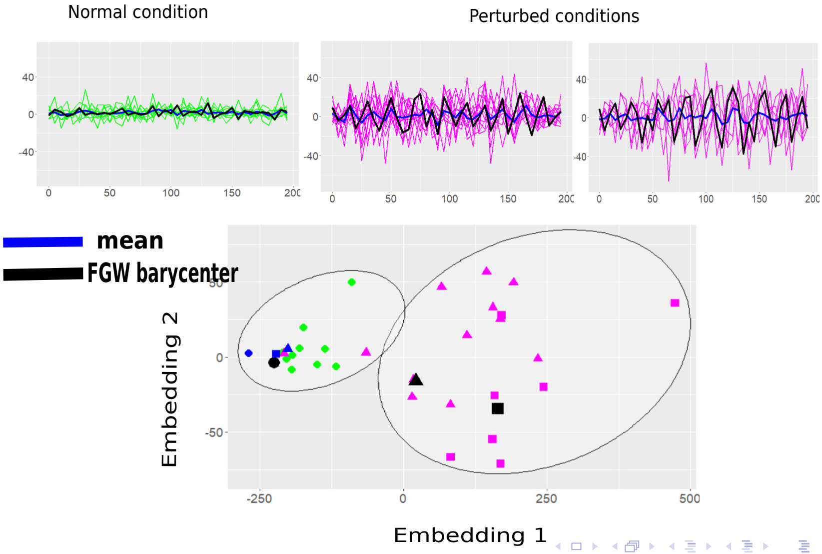
Perturbed conditions



Embedding result



Averaging result: on the use of Fused Gromov-Wasserstein barycenters of *Vayer et al. 2020*



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Nethan Ramachandran
Caroline Tatsuoka

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National Institutes of Health

Upcoming SMB 2023 presentations from Dawes Lab

Thursday at 6:00, Archie Griffin Ballroom:

Liam O'Brien *Changes in Approximate Symmetries of a Parametrized Turing Pattern*

Poster ID MFBM-10

Caroline Tatsuoka *Data Driven Modeling of Biological Systems with Deep Neural Networks*

Poster ID MFBM-17

End of Presentation

Thank you!

Questions?