

Multi-Source and Test-Time Domain Adaptation on Multivariate Signals using Spatio-Temporal Monge Alignment

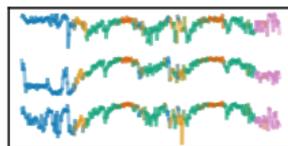
Théo Gnassounou, Antoine Collas, Rémi Flamary, Karim Lounici, Alexandre Gramfort

Huawei Seminar, 19-03-2025

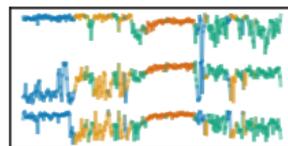


Sleep stage classification from EEG signals

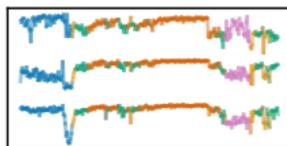
- **Multi-source** EEG signals from subjects/hospitals
- **Target** EEG signals from a new subject/hospital
- **No** access to the target labels
- **Shift** between the domains



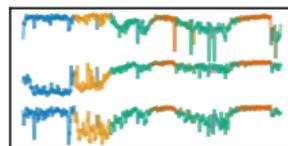
Domain 1
(X_1, y_1)



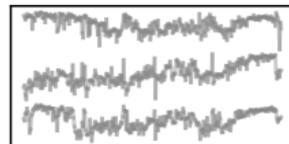
Domain 2
(X_2, y_2)



Domain 3
(X_3, y_3)



Domain 4
(X_4, y_4)

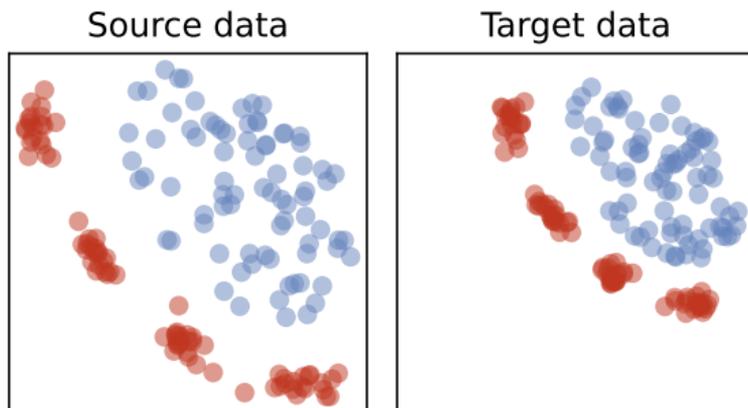


Domain 5
(X_5)

→ **Goal: Adapt** the source to the target to **classify** the target signals

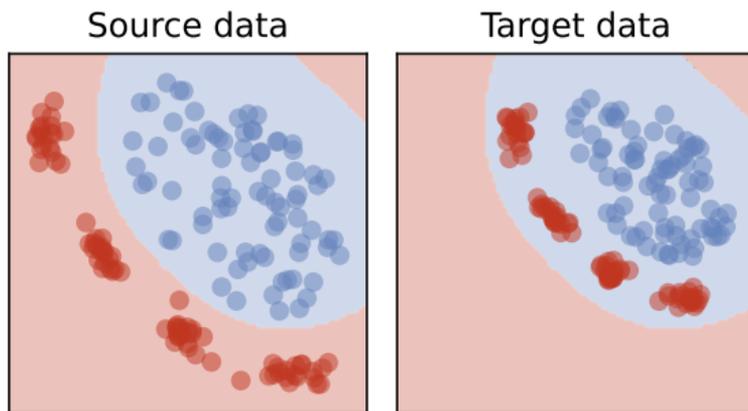
What is Domain Adaptation (DA)?

- Two type of domains: **Source** and **Target** .
- **Source** domains **with label** and **Target** domains **without label** .
- Assumption → **shift** between the distribution of the domain's data



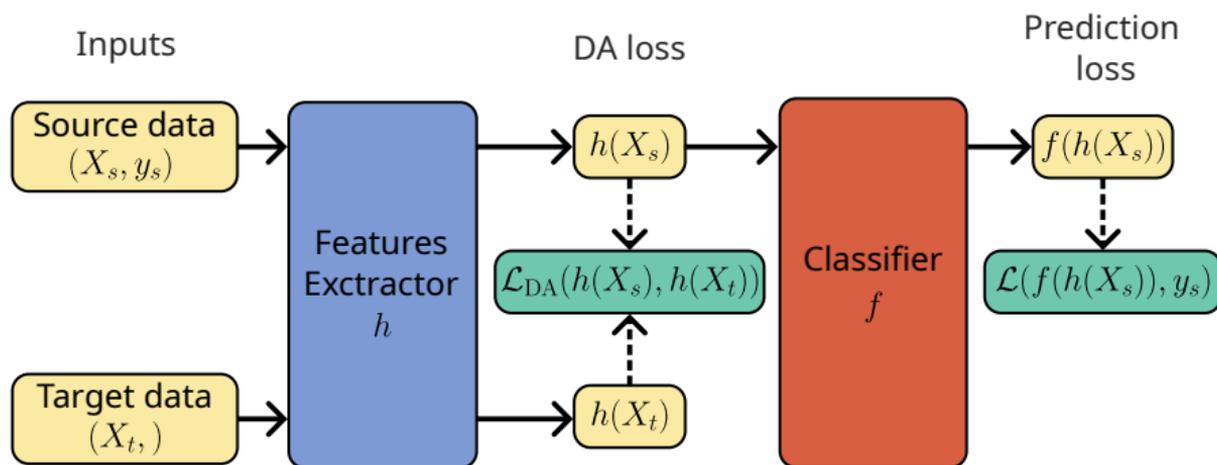
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→ **Problem: Drop in performance** when applying a model trained on the source to the target.

Traditional DA methods: Deep Learning



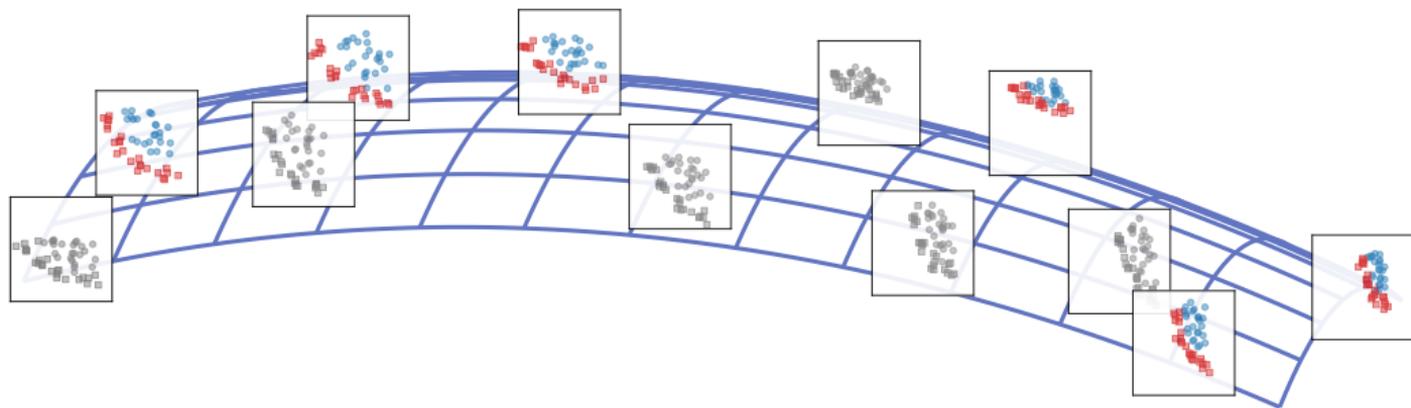
■ Reduce the **divergence** between the source and target features with:

- Correlation Alignment¹
- Domain Adversarial Neural Network²
- Joint Distribution Optimal Transport³
- ...

¹Sun et. al., 2016 ²Ganin et. al., 2016 ³Damodaran et. al., 2018

Multi-source multi-target Domain Adaptation

Domain manifold



→ Multiple **subjects** and **hospitals** with **different** EEG signals

Source-free Domain Adaptation (or Test-Time DA)

1. Train-time

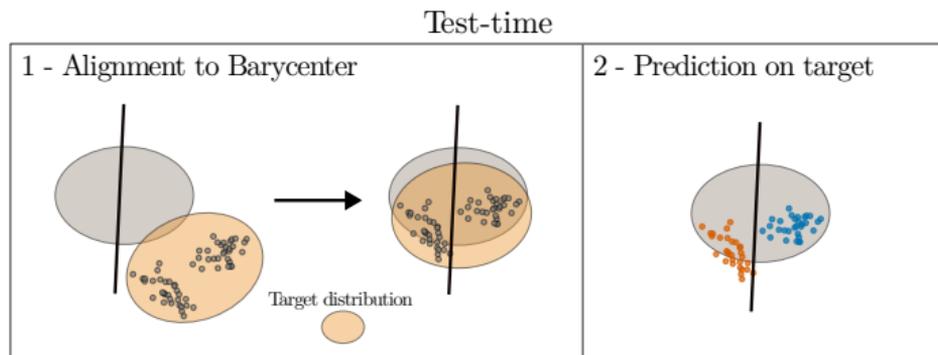
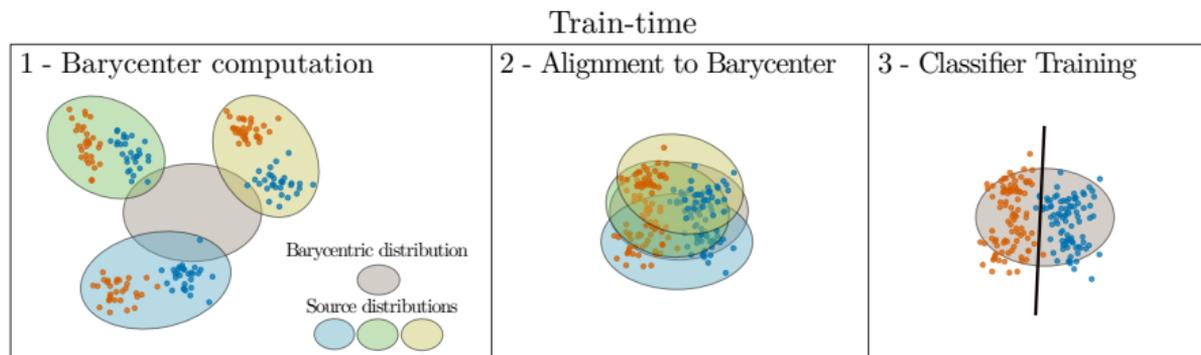
- Access to **Source** domains with labels
- **No** access to **Target** domains
- **Train** a model on the source domains with labels

2. Test-time

- **No** access to **Source** domains
- Access to **Target** domains **without** labels
- **Finetune** the model on the target domains without access to the target labels

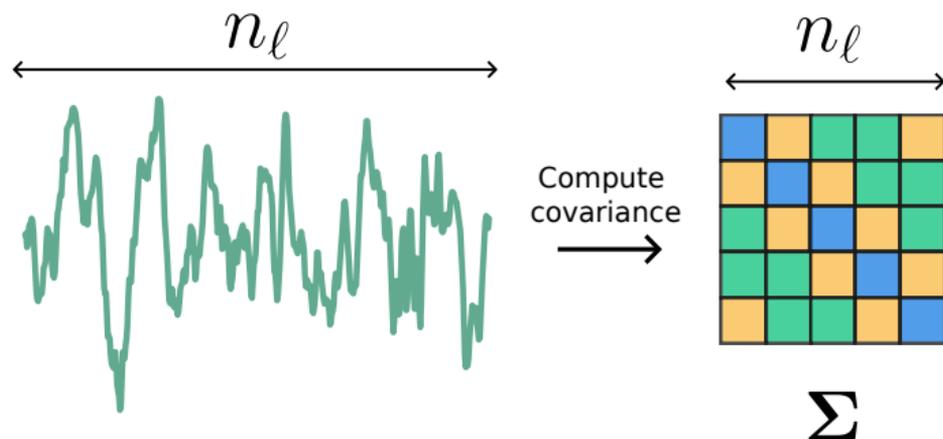
→ Practitioners **only** have access to the target data at test-time

Distribution alignment to barycenter to tackle domain shift



Assumptions on the signals

- Centered **Gaussian** distributions $\rightarrow \mathbf{X} \sim \mathcal{N}(\mathbf{0}, \Sigma)$ with $\Sigma \in \mathcal{S}_{n_\ell}^{++}$
- Σ is the "auto-covariance", computed with time-lagged. $\Sigma_{i,j} = \mathbf{X}_i \mathbf{X}_j$
- Stationarity+Periodicity** \rightarrow Covariance matrices are **Toeplitz circulant** matrices.

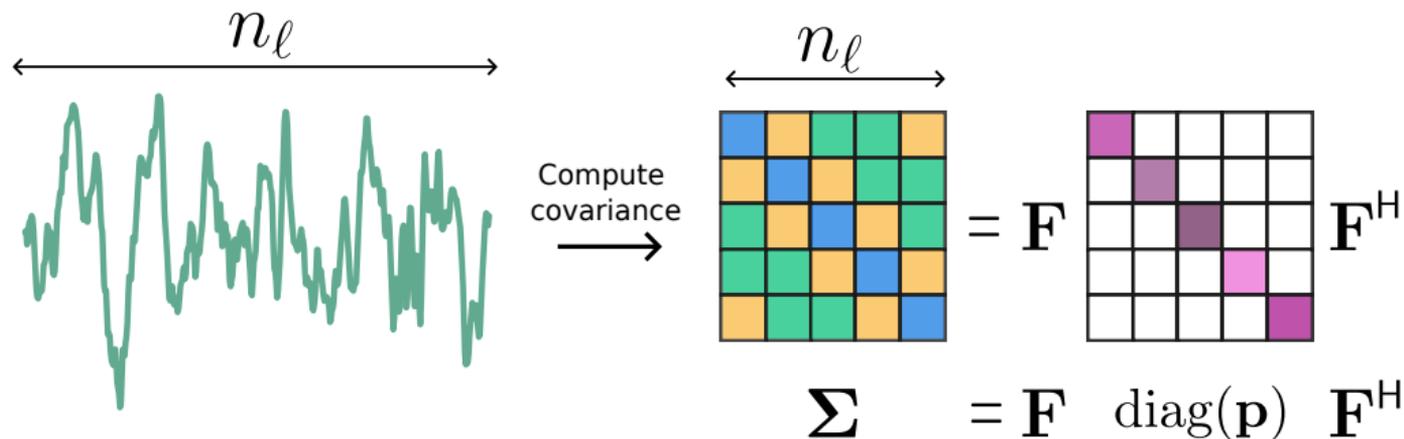


Assumptions on the signals

The Discrete Fourier Transform (DFT) can diagonalize the circulant matrix

$$\Sigma = \mathbf{F} \text{diag}(\mathbf{p}) \mathbf{F}^* ,$$

with \mathbf{F} and \mathbf{F}^* the Fourier transform operator and its inverse, and \mathbf{p} the Power Spectral Density (PSD) of the signal.



Monge mapping for Gaussian distributions

Let consider Gaussian distributions $\mu_d = \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_d)$ with $d \in \{s, t\}$. The OT cost, also called the **Bures-Wasserstein distance** when using a quadratic ground metric, is

$$\mathcal{W}_2^2(\mu_s, \mu_t) = \text{Tr} \left(\boldsymbol{\Sigma}_s + \boldsymbol{\Sigma}_t - 2 \left(\boldsymbol{\Sigma}_t^{\frac{1}{2}} \boldsymbol{\Sigma}_s \boldsymbol{\Sigma}_t^{\frac{1}{2}} \right)^{\frac{1}{2}} \right). \quad (1)$$

The OT mapping, also called **Monge mapping**, can be expressed as the following affine function :

$$m(\mathbf{x}) = \mathbf{A} \mathbf{x}, \quad \text{with} \quad \mathbf{A} = \boldsymbol{\Sigma}_s^{-\frac{1}{2}} \left(\boldsymbol{\Sigma}_s^{\frac{1}{2}} \boldsymbol{\Sigma}_t \boldsymbol{\Sigma}_s^{\frac{1}{2}} \right)^{\frac{1}{2}} \boldsymbol{\Sigma}_s^{-\frac{1}{2}} = \mathbf{A}^T. \quad (2)$$

Wasserstein barycenter between Gaussian distributions

Considering multiple Gaussian distributions μ_k . The barycenter $\bar{\mu}$ is expressed as

$$\bar{\mu} = \arg \min_{\mu} \frac{1}{K} \sum_{k=1}^K \mathcal{W}_2^2(\mu, \mu_k) . \quad (3)$$

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One uses the following optimality condition from¹:

$$\bar{\Sigma} = \frac{1}{K} \sum_{k=1}^K \left(\bar{\Sigma}^{\frac{1}{2}} \Sigma_k \bar{\Sigma}^{\frac{1}{2}} \right)^{\frac{1}{2}}, \quad (4)$$

Barycenter Covariance \uparrow $\bar{\Sigma}$ $\left(\bar{\Sigma}^{\frac{1}{2}} \Sigma_k \bar{\Sigma}^{\frac{1}{2}} \right)^{\frac{1}{2}}$ \uparrow Σ_k Domain k Covariance

¹Agueh et. al., 2011

Previously for Univariate Gaussian stationary signals

- **Stationary** Gaussian signals with **PSD** \mathbf{p}_s and \mathbf{p}_t
- **Monge mapping** between the two **univariate** signals
- After **diagonalization** of the covariance matrix, the mapping is expressed as a **convolution**¹:

$$m(\mathbf{x}) = \mathbf{h} * \mathbf{x}, \quad \text{with} \quad \mathbf{h} = \mathbf{F}^* \left(\mathbf{p}_t \odot^{\frac{1}{2}} \odot \mathbf{p}_s \odot^{-\frac{1}{2}} \right). \quad (5)$$

The diagram illustrates the components of the equation. A blue box labeled "Filter" points to the vector \mathbf{h} . A yellow box labeled "Target PSD" points to the term \mathbf{p}_t . A red box labeled "Source PSD" points to the term \mathbf{p}_s .

¹Flamary et. al., 2018

Wasserstein barycenter between Gaussian stationary signals

Lemma from¹

Consider K centered stationary Gaussian signals of PSD \mathbf{p}_k with $k \in [K]$, the Wasserstein barycenter of the K signals is a centered stationary Gaussian signal of PSD $\bar{\mathbf{p}}$ with:

$$\bar{\mathbf{p}} = \left(\frac{1}{K} \sum_{k=1}^K \mathbf{p}_k \odot^{\frac{1}{2}} \right) \odot^2. \quad (6)$$

Barycenter PSDDomain k PSD

Sketch of proof: the proof directly applies the optimality condition (7) of the barycenter. With factorized covariances, the matrix square root and the inverse can be simplified as element-wise square root and inverse.

¹Gnassounou et. al., 2023

New assumption on the signals

- **Multivariate** signals with cross covariance $\Sigma \in \mathcal{S}_{n_\ell n_c}^{++}$
- Reduction of parameters from $(n_\ell \times n_c)^2 \rightarrow n_\ell \times n_c^2$
- **P** is the cross-PSD matrix of the signal

$$\begin{pmatrix} \text{3x3 grid of } 3 \times 3 \text{ colored blocks} \end{pmatrix} \begin{matrix} \xrightarrow{n_c} \\ \xleftarrow{n_\ell} \end{matrix} = \mathbf{F} \begin{pmatrix} \text{3x3 grid of } 3 \times 3 \text{ colored blocks} \end{pmatrix} \mathbf{F}^H = \mathbf{F} \mathbf{U} \begin{pmatrix} \text{3x3 grid of } 3 \times 3 \text{ colored blocks} \end{pmatrix} \mathbf{U}^T \mathbf{F}^H$$

Σ
 \mathbf{P}

Monge mapping for Multivariate Gaussian stationary signals

- Let consider Gaussian distributions $\mu_d = \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_d)$ with $d \in \{s, t\}$ and $\boldsymbol{\Sigma}_d = \mathbf{F}\mathbf{U}\mathbf{Q}_d\mathbf{U}^T\mathbf{F}^H$

$$\begin{pmatrix} \text{diag}(\mathbf{p}_{1,1}) & \dots & \text{diag}(\mathbf{p}_{1,n_c}) \\ \dots & \dots & \dots \\ \text{diag}(\mathbf{p}_{n_c,1}) & \dots & \text{diag}(\mathbf{p}_{n_c,n_c}) \end{pmatrix} \triangleq \mathbf{U}\mathbf{P}_s^{-\frac{1}{2}} \left(\begin{matrix} \mathbf{P}_s^{\frac{1}{2}} & & \\ & \mathbf{P}_t & \\ & & \mathbf{P}_s^{\frac{1}{2}} \end{matrix} \right)^{\frac{1}{2}} \mathbf{P}_s^{-\frac{1}{2}}\mathbf{U}^T \in \mathcal{H}_{n_c f}^{++}$$

↑ Source Cross-PSD
↑ Target Cross-PSD

- Given a signal $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_{n_c}]^T \in \mathbb{R}^{n_c \times n_\ell}$ the Monge mapping is a sum of convolutions

$$m(\mathbf{X}) = \left[\sum_{j=1}^{n_c} \mathbf{h}_{1,j} * \mathbf{x}_j, \dots, \sum_{j=1}^{n_c} \mathbf{h}_{n_c,j} * \mathbf{x}_j \right]^T$$

where $\mathbf{h}_{i,j} = \frac{1}{\sqrt{f}} \mathbf{F}^H \mathbf{p}_{i,j} \in \mathbb{R}^f$.

↑ Filter between sensor i and j

Wasserstein barycenter for Multivariate Gaussian stationary signals

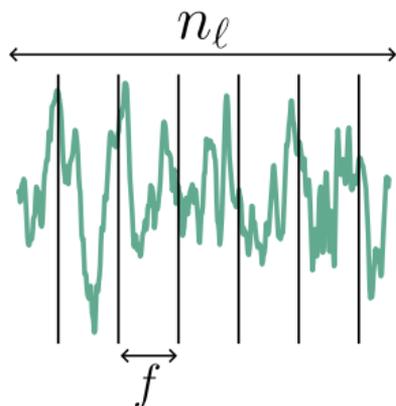
- No more closed form for the barycenter covariance $\bar{\Sigma}$.
- The barycenter PSD $\bar{\mathbf{P}}$ is expressed as

$$\bar{\mathbf{P}} = \frac{1}{K} \sum_{k=1}^K \left(\bar{\mathbf{P}}^{\frac{1}{2}} \mathbf{P} \bar{\mathbf{P}}^{\frac{1}{2}} \right)^{\frac{1}{2}}, \quad (7)$$

Barycenter cross-PSD Domain k cross-PSD

How to reduce the the number of parameters of the filter?

- $n_\ell \times n_c^2$ parameters for \mathbf{h} still highlight
- $n_\ell \rightarrow \mathbf{f}$
- Use **Welch** method to estimate the PSD
 - Cut the signal into segments
 - Compute the PSD of each segment
 - Average the PSD



Compute covariance
→

$$\begin{array}{c}
 \begin{array}{|c|c|c|}
 \hline
 \color{blue}{\square} & \color{orange}{\square} & \color{green}{\square} \\
 \hline
 \color{orange}{\square} & \color{blue}{\square} & \color{orange}{\square} \\
 \hline
 \color{green}{\square} & \color{orange}{\square} & \color{blue}{\square} \\
 \hline
 \end{array}
 & = \mathbf{F} &
 \begin{array}{|c|c|c|}
 \hline
 \color{purple}{\square} & \square & \square \\
 \hline
 \square & \color{purple}{\square} & \square \\
 \hline
 \square & \square & \color{pink}{\square} \\
 \hline
 \end{array}
 \mathbf{F}^H
 \end{array}$$

$$\Sigma = \mathbf{F} \text{diag}(\mathbf{p}) \mathbf{F}^H$$

$$\mathbf{P} = \begin{pmatrix}
 \begin{array}{|c|c|c|c|c|}
 \hline
 \color{blue}{\square} & \color{orange}{\square} & \color{green}{\square} & \color{red}{\square} & \color{purple}{\square} \\
 \hline
 \color{orange}{\square} & \color{blue}{\square} & \color{orange}{\square} & \color{green}{\square} & \color{red}{\square} \\
 \hline
 \color{green}{\square} & \color{orange}{\square} & \color{blue}{\square} & \color{orange}{\square} & \color{green}{\square} \\
 \hline
 \color{red}{\square} & \color{green}{\square} & \color{orange}{\square} & \color{blue}{\square} & \color{orange}{\square} \\
 \hline
 \color{purple}{\square} & \color{red}{\square} & \color{green}{\square} & \color{orange}{\square} & \color{blue}{\square} \\
 \hline
 \end{array}
 \end{pmatrix}$$

The matrix \mathbf{P} is a 5×5 grid. The top-left cell contains a 5×5 grid of colored squares. The cells on the main diagonal (top-left to bottom-right) contain a 5×5 grid of colored squares with a black 'X' over it. The other cells are empty. A double-headed arrow above the grid is labeled n_c , and a double-headed arrow below the grid is labeled $n_\ell \rightarrow f$.

Convolutional Monge Mapping Normalization (CMMN)

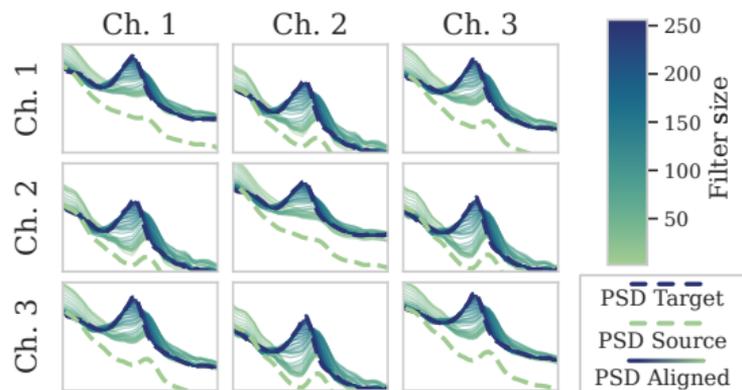
1. Train-time: Access to source domains

- Compute **cross-PSD** $\hat{\mathbf{P}}_k$ for each source domain.
- Compute **barycenter** $\hat{\mathbf{p}}$ with the PSD $\hat{\mathbf{P}}_k$.
- Compute the **convolutional filters** \mathbf{h}
- **Train a predictor** g on the normalized source data.

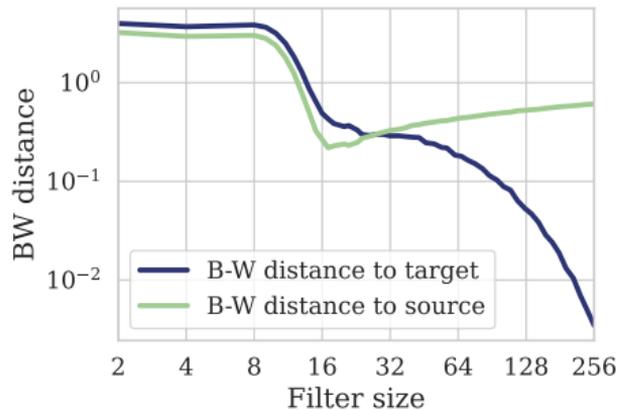
2. Test-time: Access to unseen target data

- Compute the **cross-PSD** $\hat{\mathbf{P}}_t$ for the target domain.
- Compute the **convolutional filter** \mathbf{h} between target domain and the barycenter $\bar{\mathbf{P}}$.
- Predict target labels with trained predictor g .

Illustration of the monge mapping for two signals

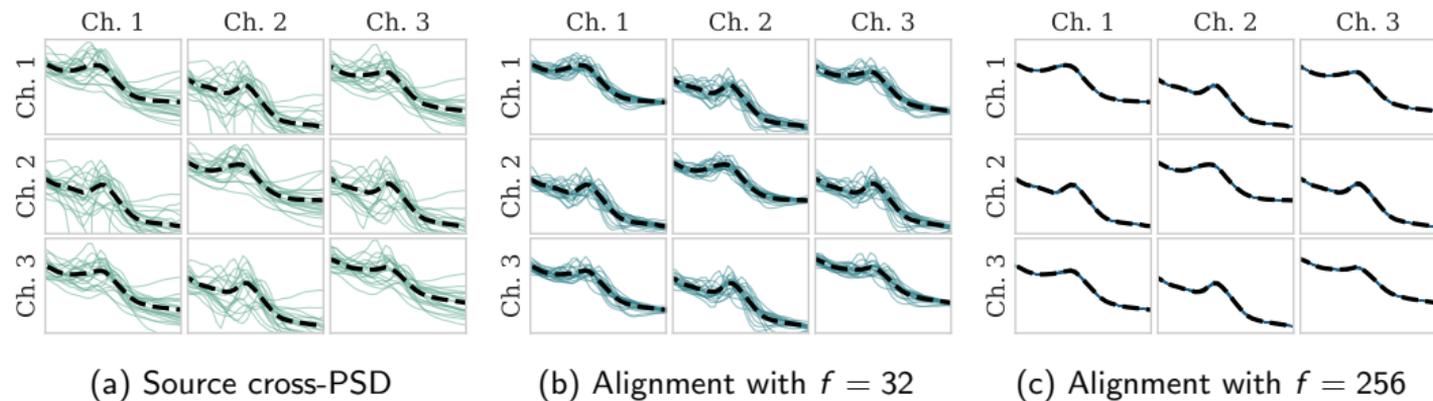


(a) Cross-PSD alignment



(b) Bures-Wasserstein distance

Cross-PSD alignment to barycenter for different filters size



Domain adaptation in biosignals

Possible variability in biosignals:

- Variability in the **patient population** : age, gender, height, diseased or healthy, different sleep stage proportion.

Domain adaptation in biosignals

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Domain adaptation in biosignals

Possible variability in biosignals:

- Variability in the **patient population** : age, gender, height, diseased or healthy, different sleep stage proportion.
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- Variability in **data interpretation by specialist** : different scoring criteria, subjectivity, tiredness.

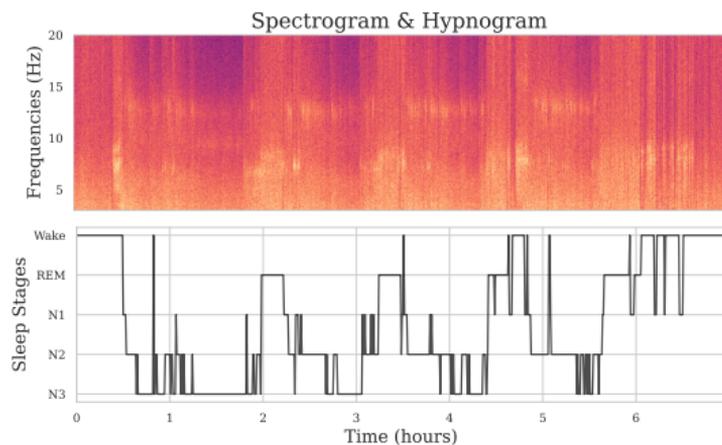
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→ **Domain Adaptation** problem.

Sleep Staging



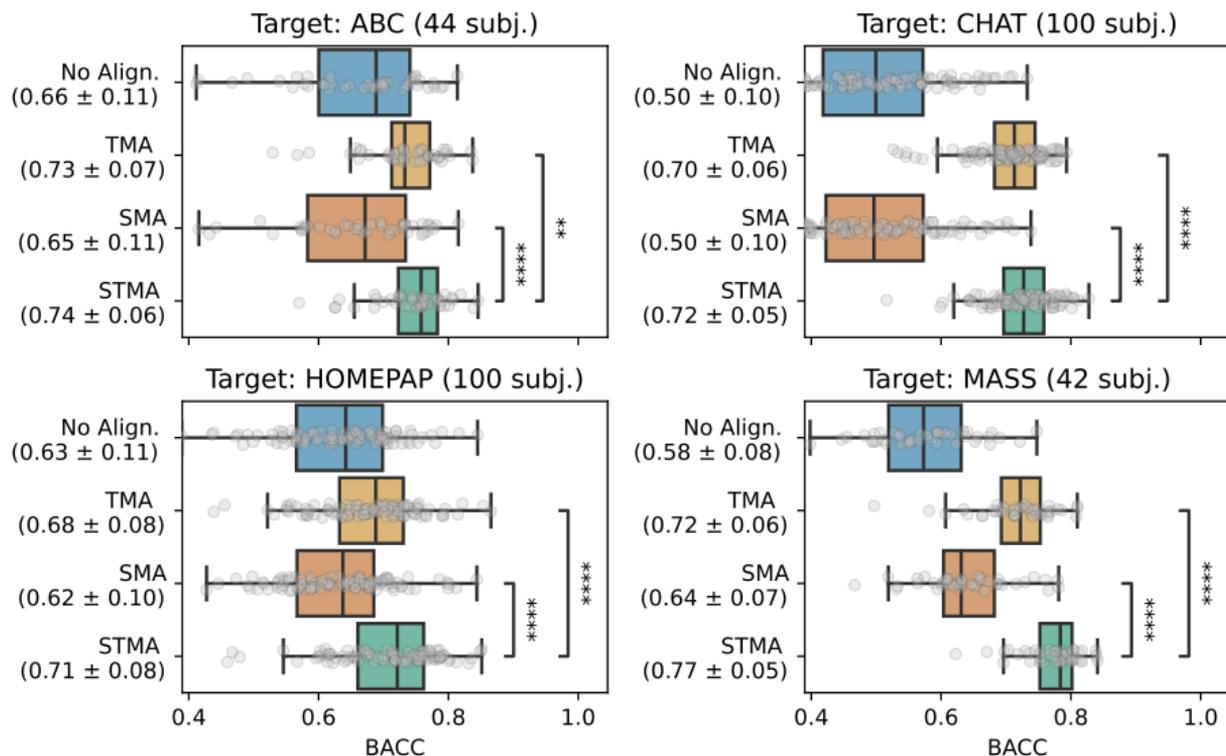
- **Classification** problem with **five** classes: Wake, N1, N2, N3, REM
- **Frequency** helps to classify sleep stage

Experimental setup

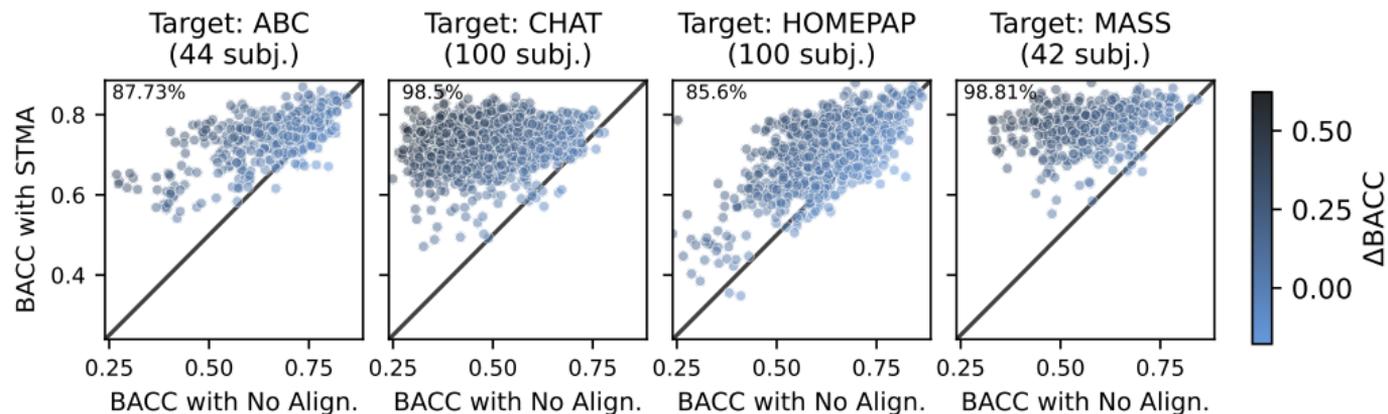
- **Four** different datasets: **ABC** , **CHAT** , **HOME PAP** and **MASS**
- Around **300** subjects in total
- One **domain** = One **subject**
- **Seven** EEG channels
- Use **CNN** architecture from¹

¹*Chambon et. al., 2018*

Results on Sleep data



Results on Sleep data



How to use DA?

Skada¹ is a **Python** library to **easily** use DA methods.

- **Homogeneous API** for all DA methods (Shallow and Deep learning).
- **Sklearn-like API** with estimator class (`.fit`, `.predict`, ...), pipeline, grid search ...
- **DA scorer** to validate hyper-parameters without using target label.



¹*Gnassounou et. al., 2024*

Data format in Skada

- $X \rightarrow$ 2D array of shape $(n_samples, n_features)$
- $y \rightarrow$ 1D array of shape $(n_samples,)$
- $sample_domain \rightarrow$ 1D array of shape $(n_samples,)$ giving the **domain** of each **sample**

```
1     from skada.datasets import make_shifted_datasets
2
3     X, y, sample_domain = make_shifted_datasets(
4         20, 20, shift='covariate_shift', random_state=42
5     )
```

- All shift are available in `make_shifted_datasets` function

Shallow DA in Skada

- Initialize the estimator
- Fit the model
- Don't forget to give the **sample domain**

```
1     from skada import LinOT
2
3     estimator = LinOT()
4     estimator.fit(X, y, sample_domain=sample_domain)
```

- ~ 20 shallow methods available in Skada

Pipeline DA in Skada

- Can be used with **Pipeline**

```
1     from skada import make_da_pipeline
2     from skada import LinOTAdapter, GaussianReweightAdapter
3     from sklearn.linear_model import LogisticRegression
4
5     pipeline = Pipeline(
6         LinOTAdapter(),
7         LogisticRegression()
8     )
9     pipeline.fit(X, y, sample_domain=sample_domain)
```

- Possibility to mixed DA adapters

```
1     pipeline = Pipeline(
2         LinOTAdapter(),
3         GaussianReweightAdapter(),
4         LogisticRegression()
5     )
```

DA scorer in Skada

- Possibility to use `cross_val_score` with **DA scorers**
- DA scorers are used to **validate** the **hyperparameters** without using the target labels

```
1     from skada.scorers import ImportanceWeightedScorer
2
3     scorer = ImportanceWeightedScorer()
4     score = cross_val_score(pipeline, X, y, sample_domain=sample_domain,
        ↪     scoring=scorer)
```

- 6 DA scorers available in Skada

Deep DA method in Skada

- Use **Skorch** → **Pytorch** wrapper for **Sklearn**
- Give an **architecture** and **hyperparameters**

```
1     from skada.deep import DeepCoral
2     from skada.deep.modules import ToyCNN
3
4     model = DeepCoral(
5         ToyCNN(),
6         batch_size=32,
7         max_epochs=5,
8         lr=1e-3,
9         reg=1,
10        layer_name="feature_extractor",
11    )
12    model.fit(X, y, sample_domain=sample_domain)
```

- ~ 10 Deep DA methods available in Skada

Conclusion

- Distribution shift is a **challenging** problem in **biosignals**
- Alignment of the **cross-PSD** is a **powerful** tool to tackle the problem
- Try **Skada** to easily use DA methods
- Don't hesitate to contribute to the library!

