Machine learning without human supervision on neuroscience data

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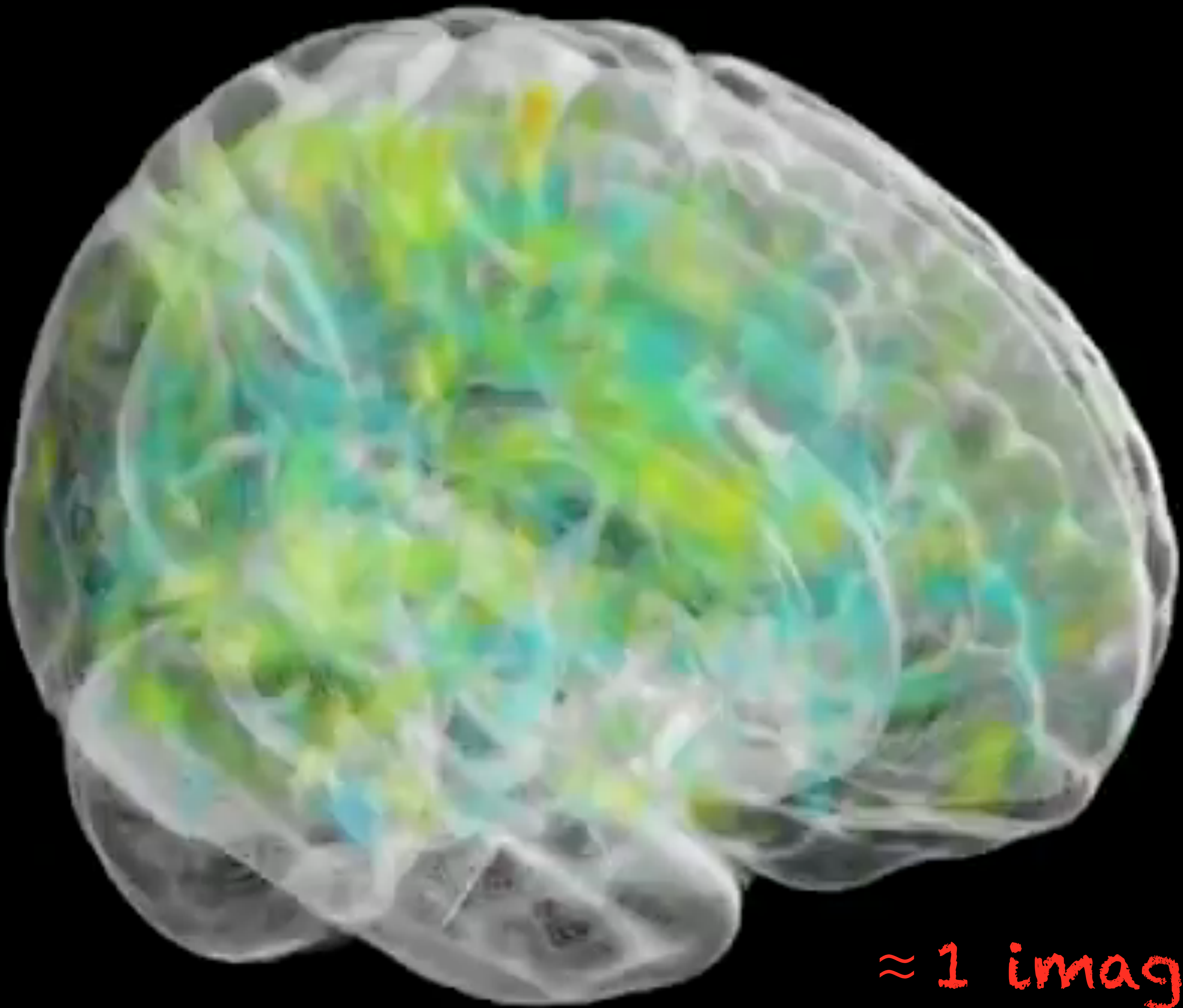
Nantes - June 2022

Functional MRI



≈ 1 image / 2s

http://www.youtube.com/watch?v=uhCF-zlk0jY

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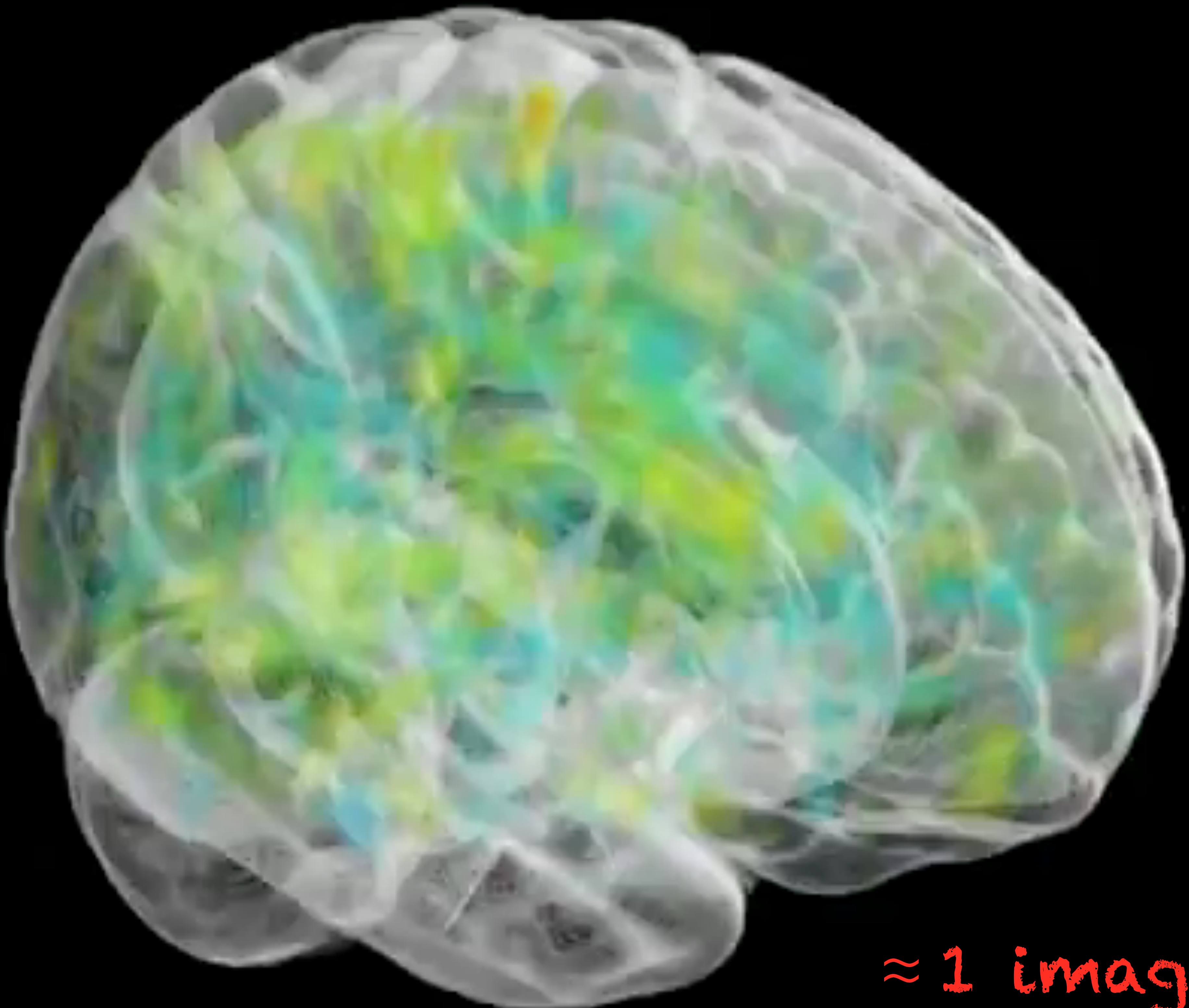

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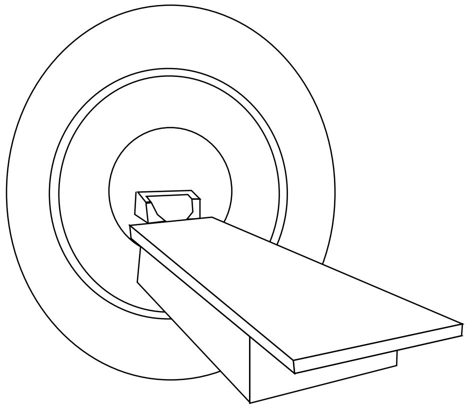
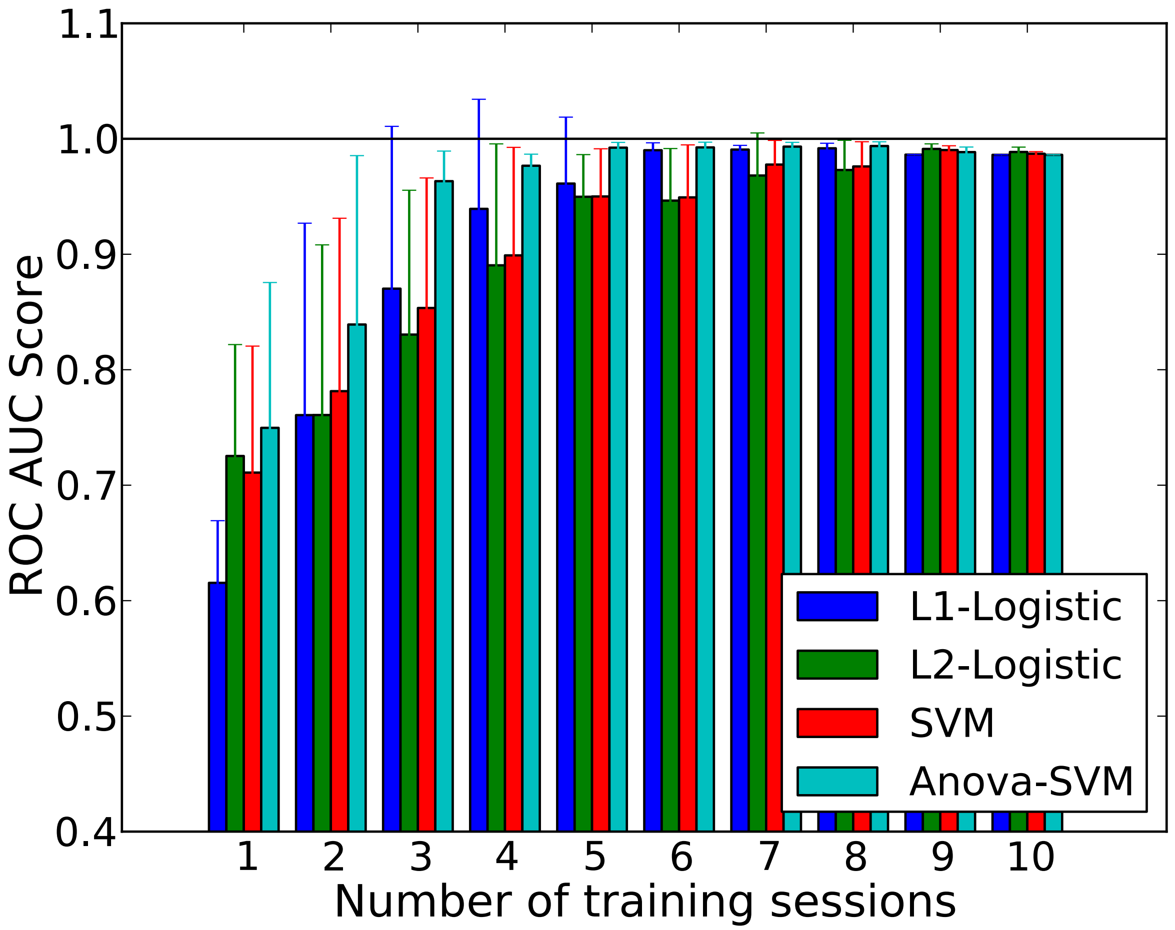
Supervised Learning on fMRI: Face vs. House



Binary classification results



[Gramfort et al. 2011]

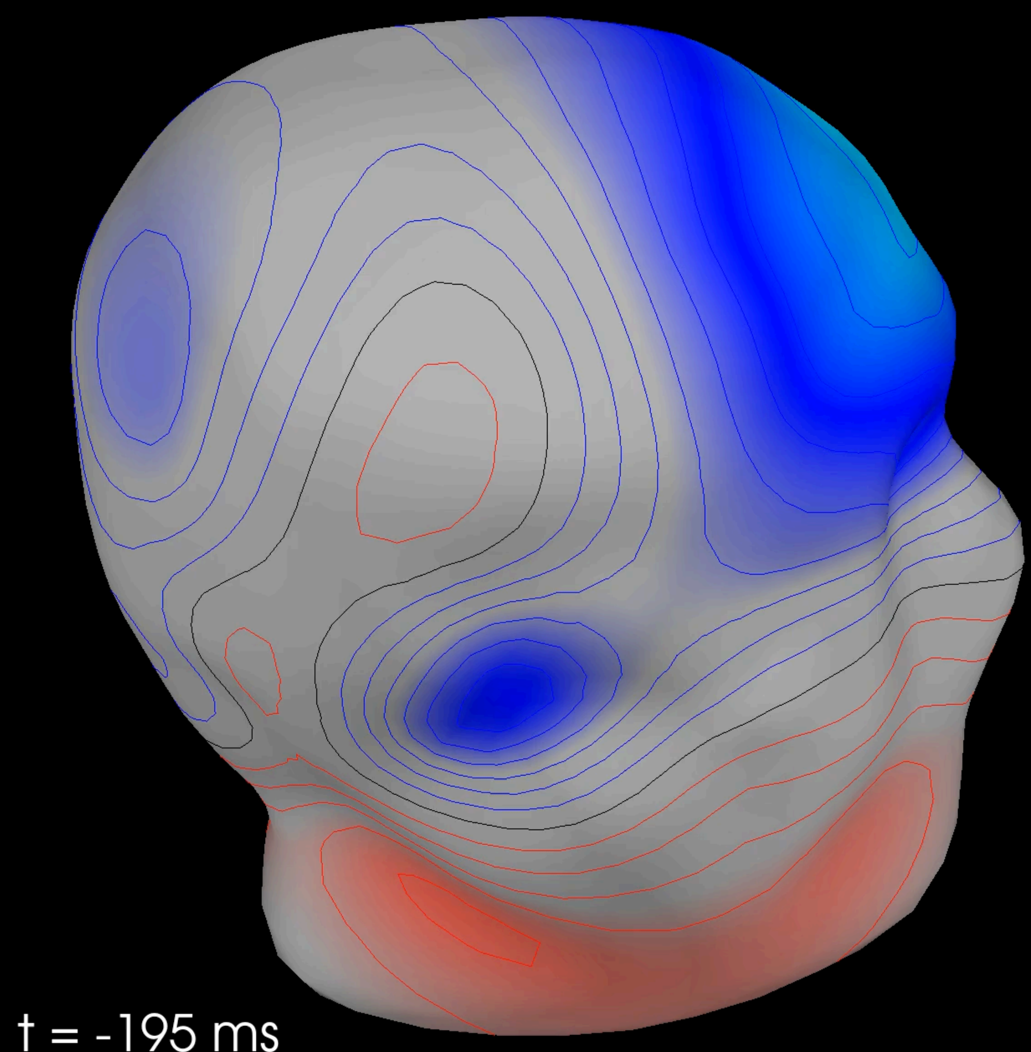
- The more data the better
- Almost no noise

It's often much harder:

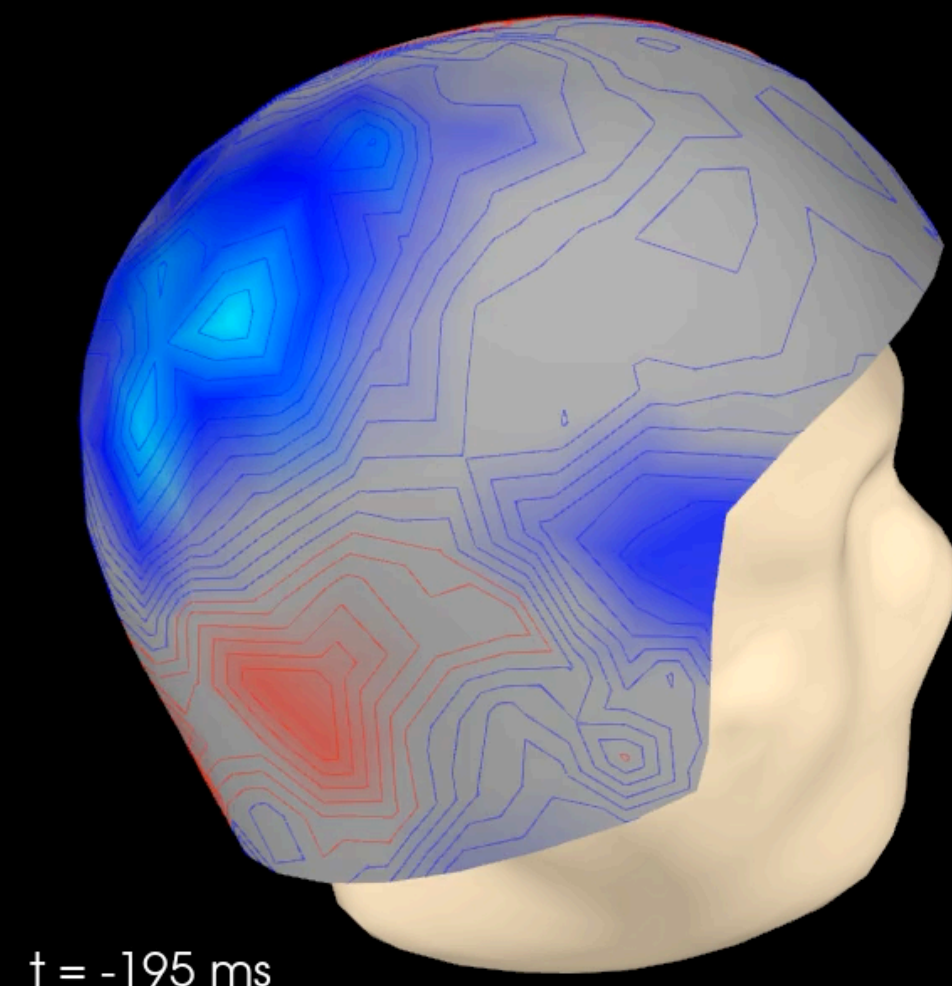
- Smaller effect sizes
- Intersubject variability
- Device variability etc.

[Pedregosa, Varoquaux, Gramfort et al. JMLR 2011]

Electroencephalography (EEG)
Electric Potential [V]



Magnetoencephalography (MEG)
Magnetic field [T]



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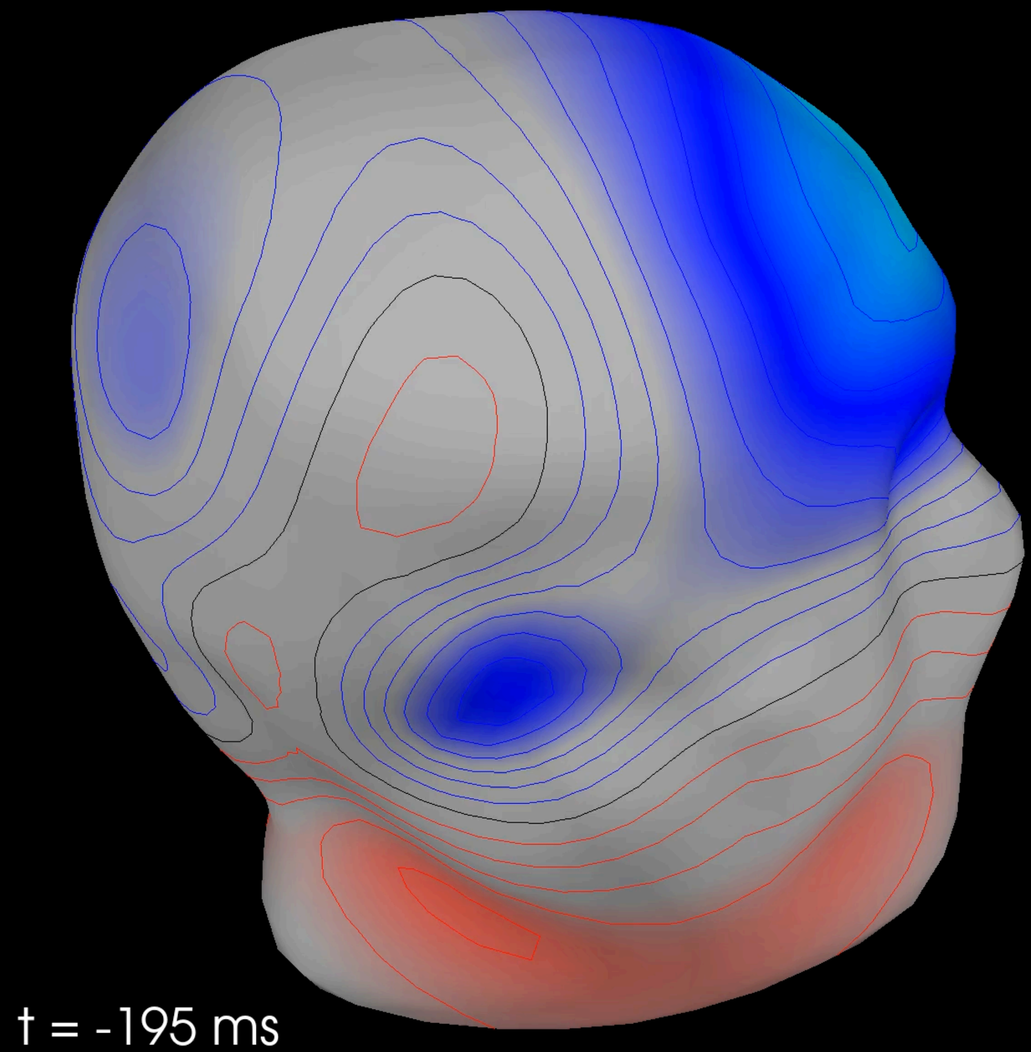

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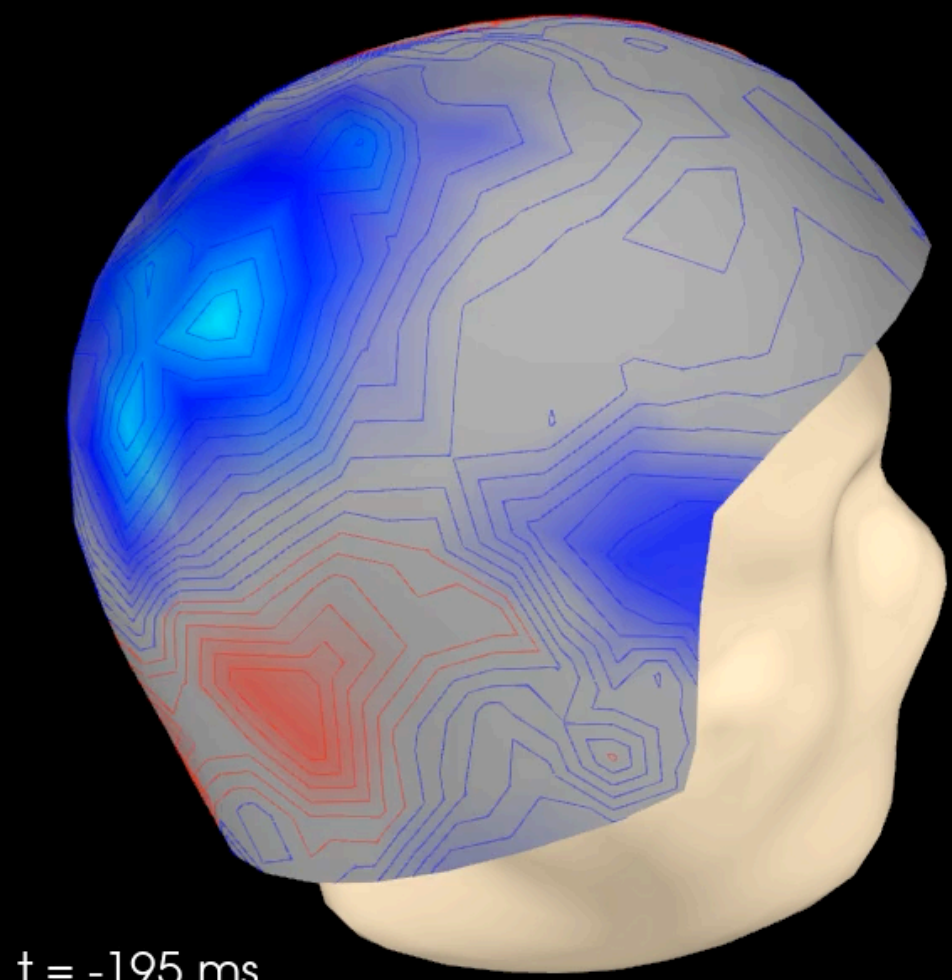

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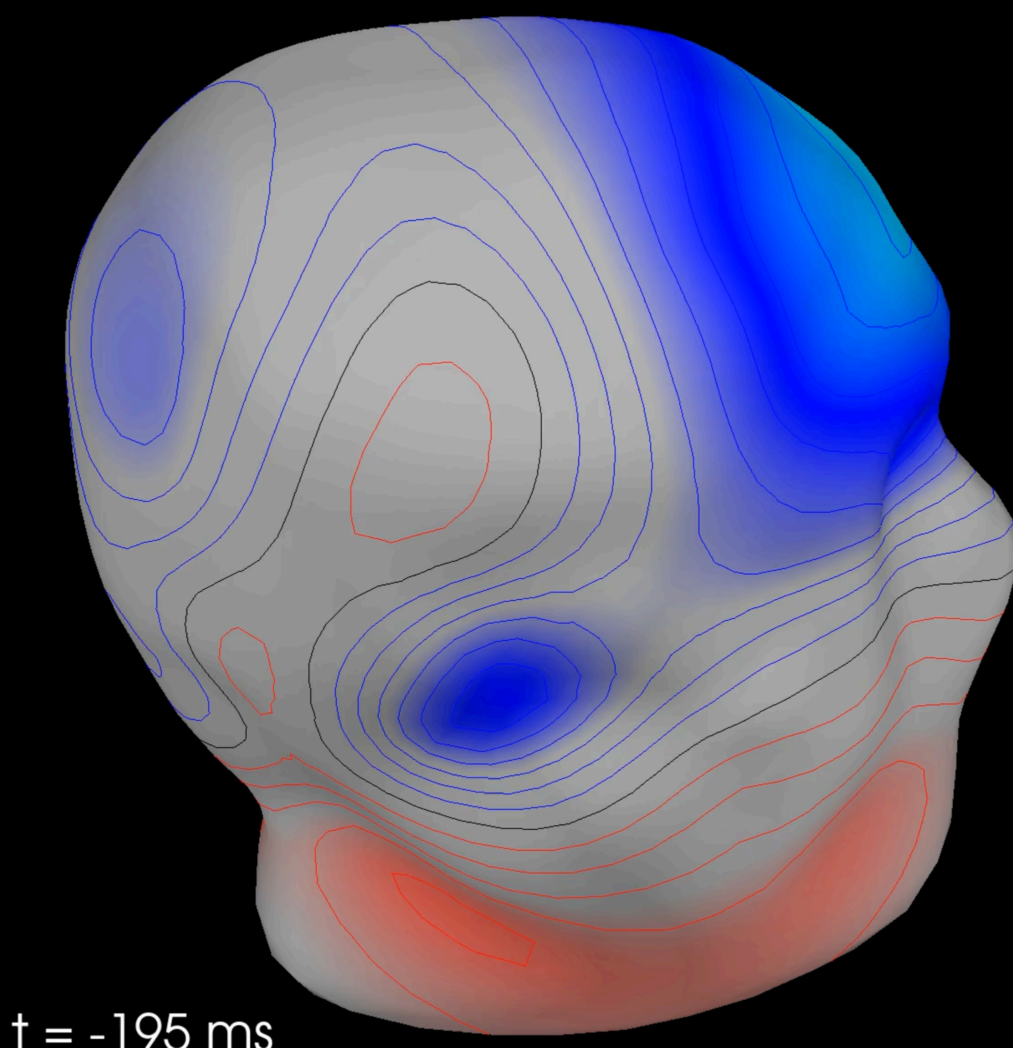

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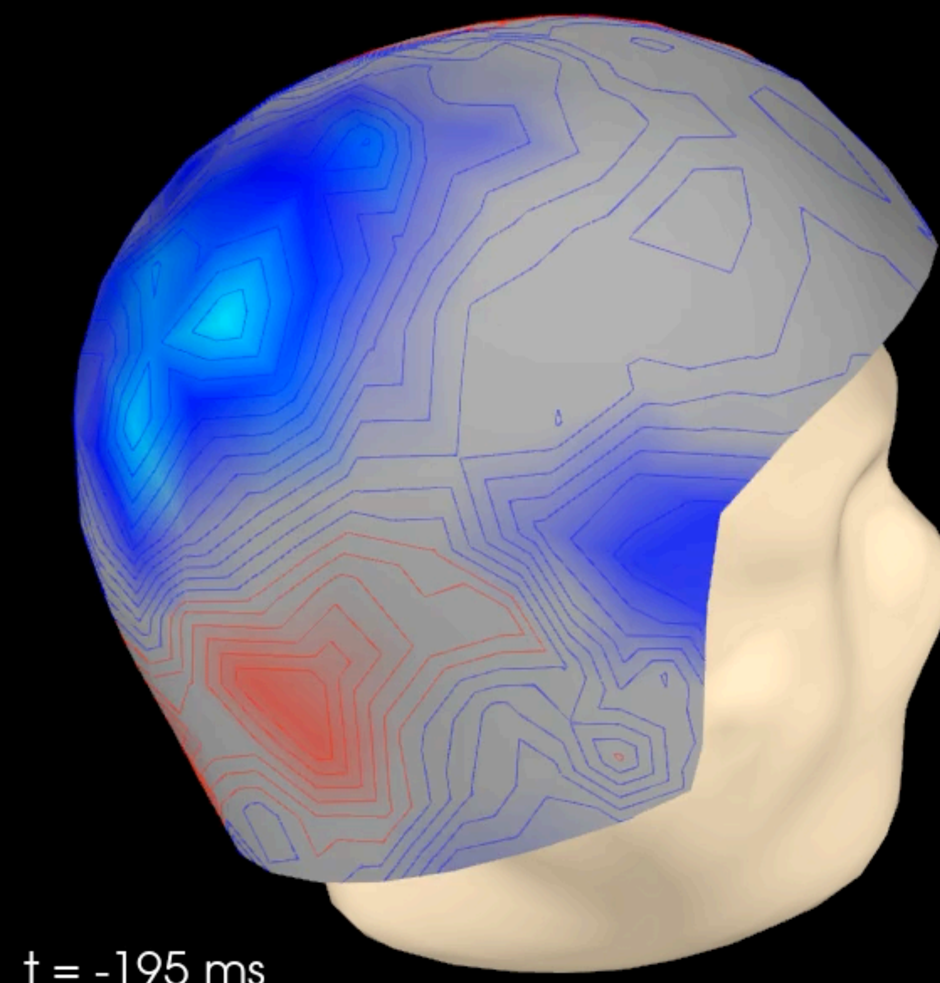
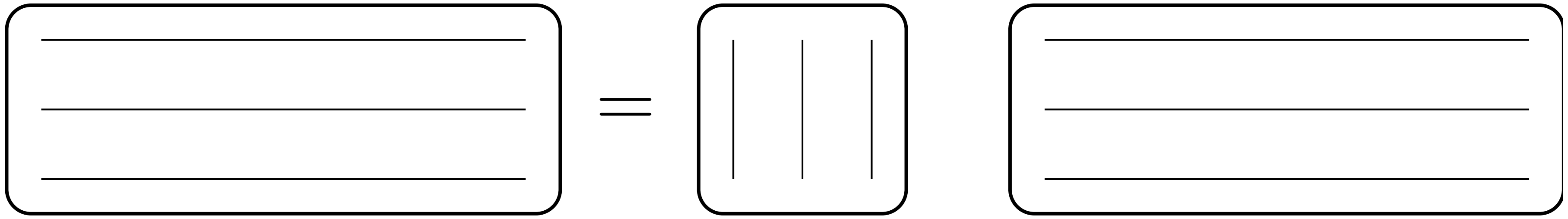


Outline: From unsupervised to self-supervised

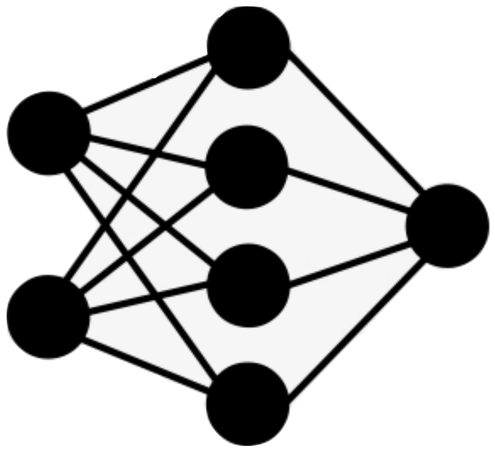
Unsupervised learning: From ICA to multiview ICA

P. Ablin, J-F Cardoso, A. Gramfort (2017), Faster independent component analysis by preconditioning with Hessian approximations, IEEE Trans. Sig. Proc.

H. Richard, L. Gresele, A. Hyvärinen, B. Thirion, A. Gramfort, P. Ablin (2020), Modeling Shared Responses in Neuroimaging Studies through MultiView ICA, Proc. NeurIPS



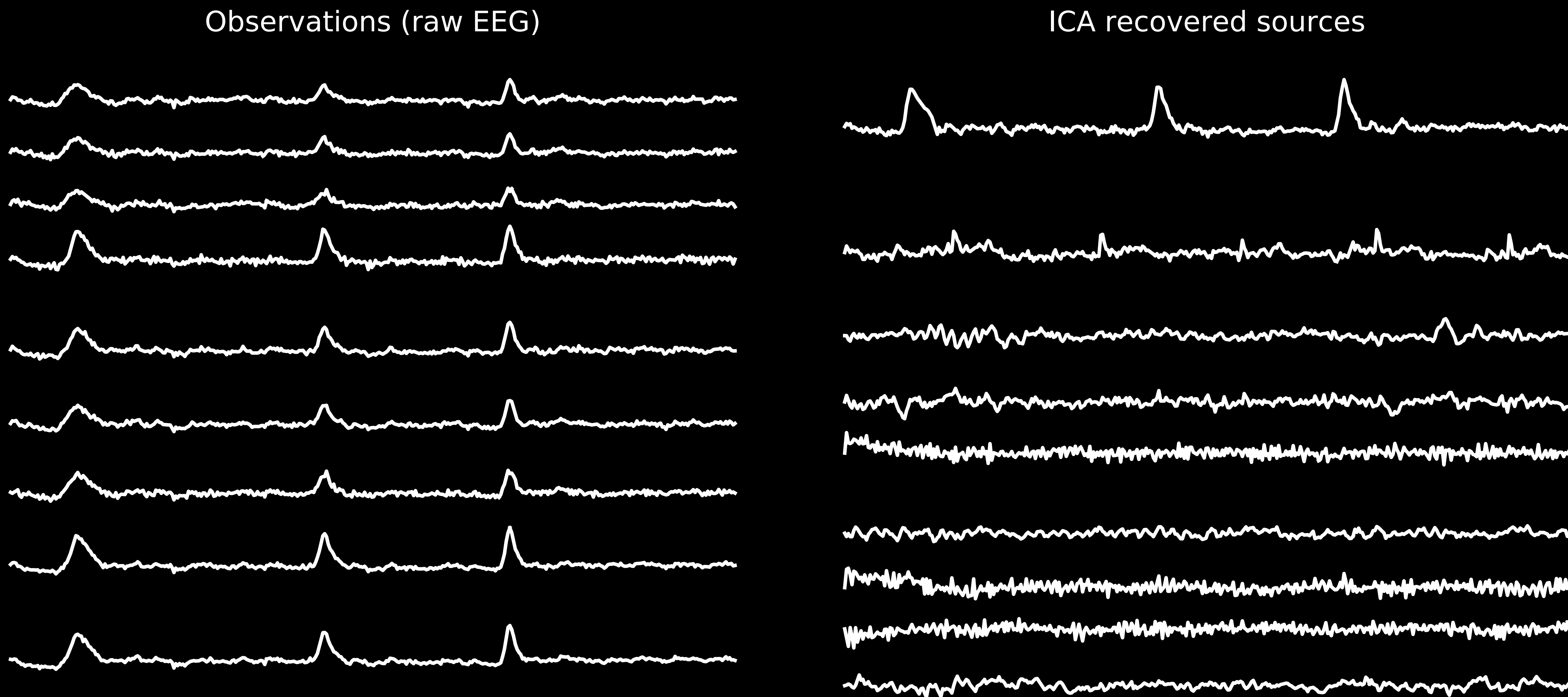
Self-supervised learning on EEG data



Banville, H., Chehab, O., Hyvärinen, A., Engemann, D. and Gramfort, A. (2020), Uncovering the structure of clinical EEG signals with self-supervised learning, Journal of Neural Engineering

1

From Independent Component Analysis (ICA) to multivew ICA

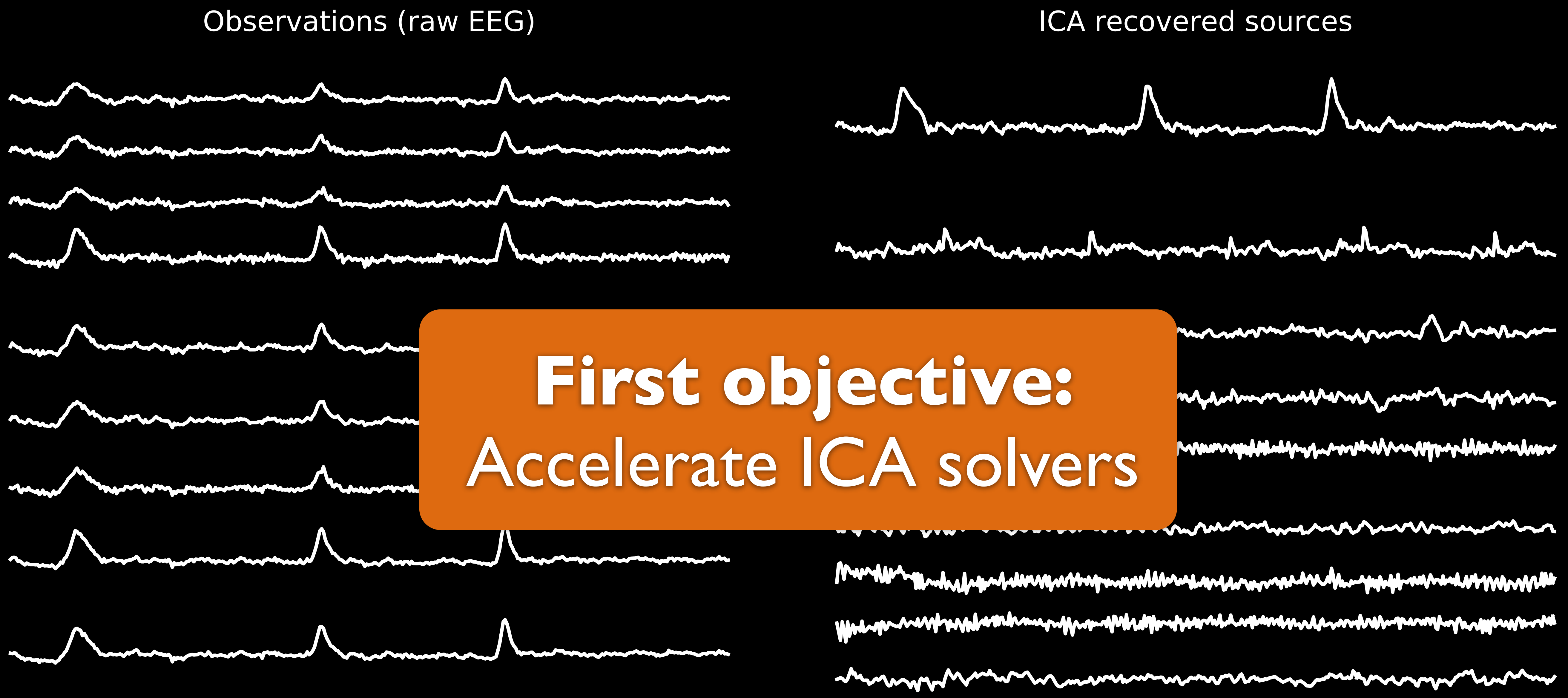


[Faster independent component analysis by preconditioning with Hessian approximations, P. Ablin, J.-F. Cardoso & A. Gramfort 2017 IEEE Trans. Signal Processing]

Code: https://pierreablin.github.io/picard

1

From Independent Component Analysis (ICA) to multiview ICA



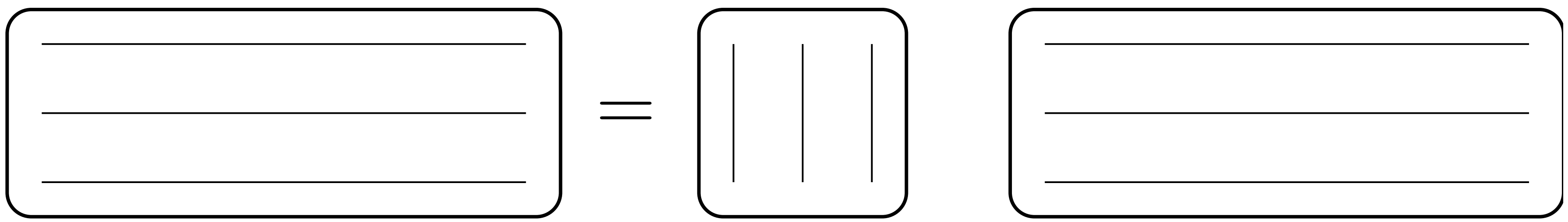
First objective:
Accelerate ICA solvers

[Faster independent component analysis by preconditioning with Hessian approximations, P. Ablin, J.-F. Cardoso & A. Gramfort 2017 IEEE Trans. Signal Processing]

Code: https://pierreablin.github.io/picard

Linear ICA model: $\mathbf{X} = \mathbf{AS}$

- **Assumption:** Observed signals are a linear mix of independent identically distributed signals.



$\mathbf{X} \in \mathbb{R}^{N \times T}$ $\quad$ $\mathbf{A} \in \mathbb{R}^{N \times N}$ $\quad$ $\mathbf{S} \in \mathbb{R}^{N \times T}$

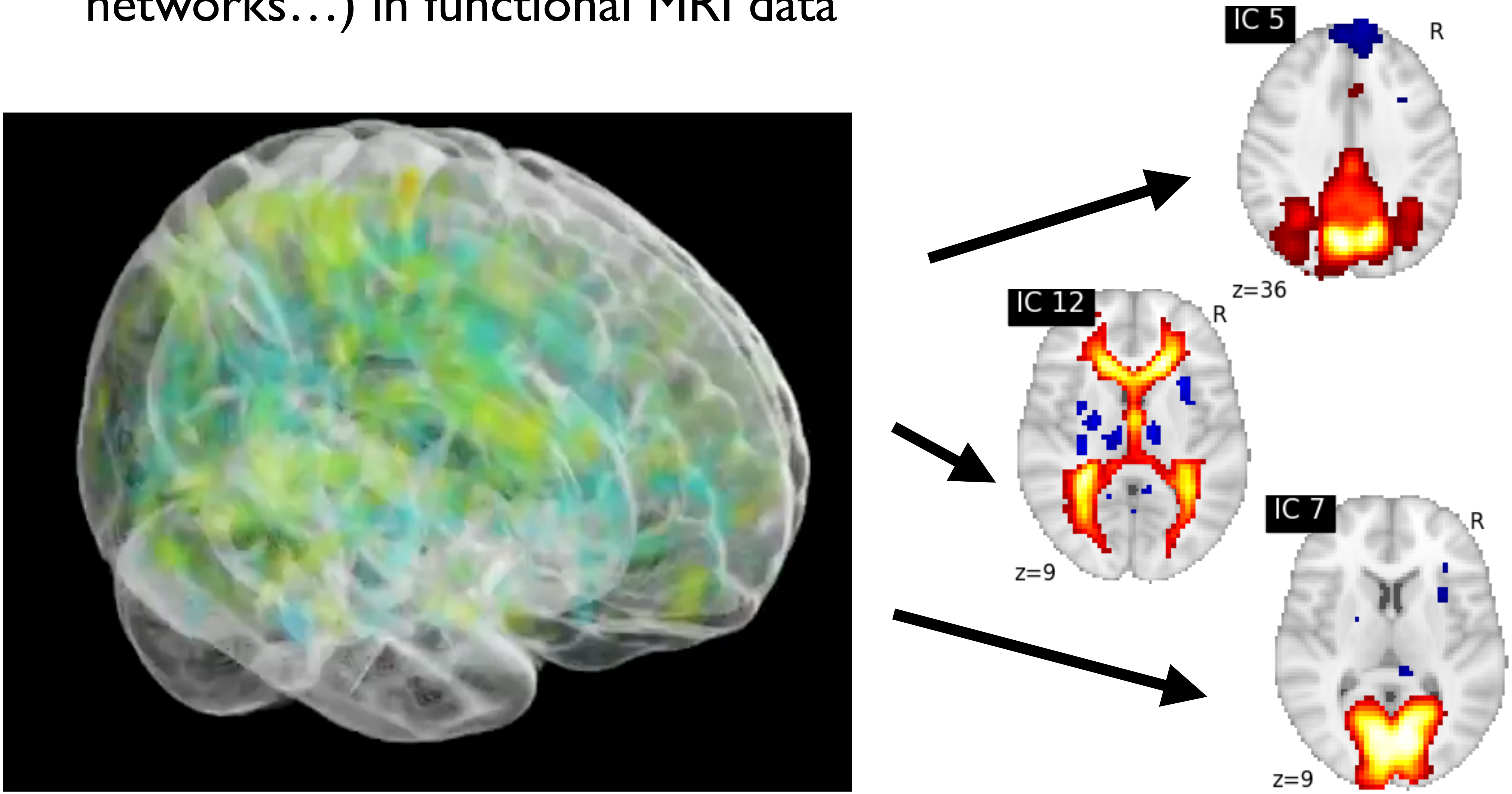
- N: Number of signals
- T: Number of samples
- $\mathbf{X}$: Observed signals
- $\mathbf{S}$: Independent **sources** signals
- $\mathbf{A}$: **Mixing matrix**

Both $\mathbf{A}$ and $\mathbf{S}$ are unknown

[Jutten & Herault 91, Bell & Sejnowski 1995, Hyvärinen 1997]

Why should you care?

- Used in neuroimaging to find "brain networks" (not neural networks…) in functional MRI data



Source: http://nilearn.github.io/auto_examples/03_connectivity/plot_canica_resting_state.html

Why should you care?

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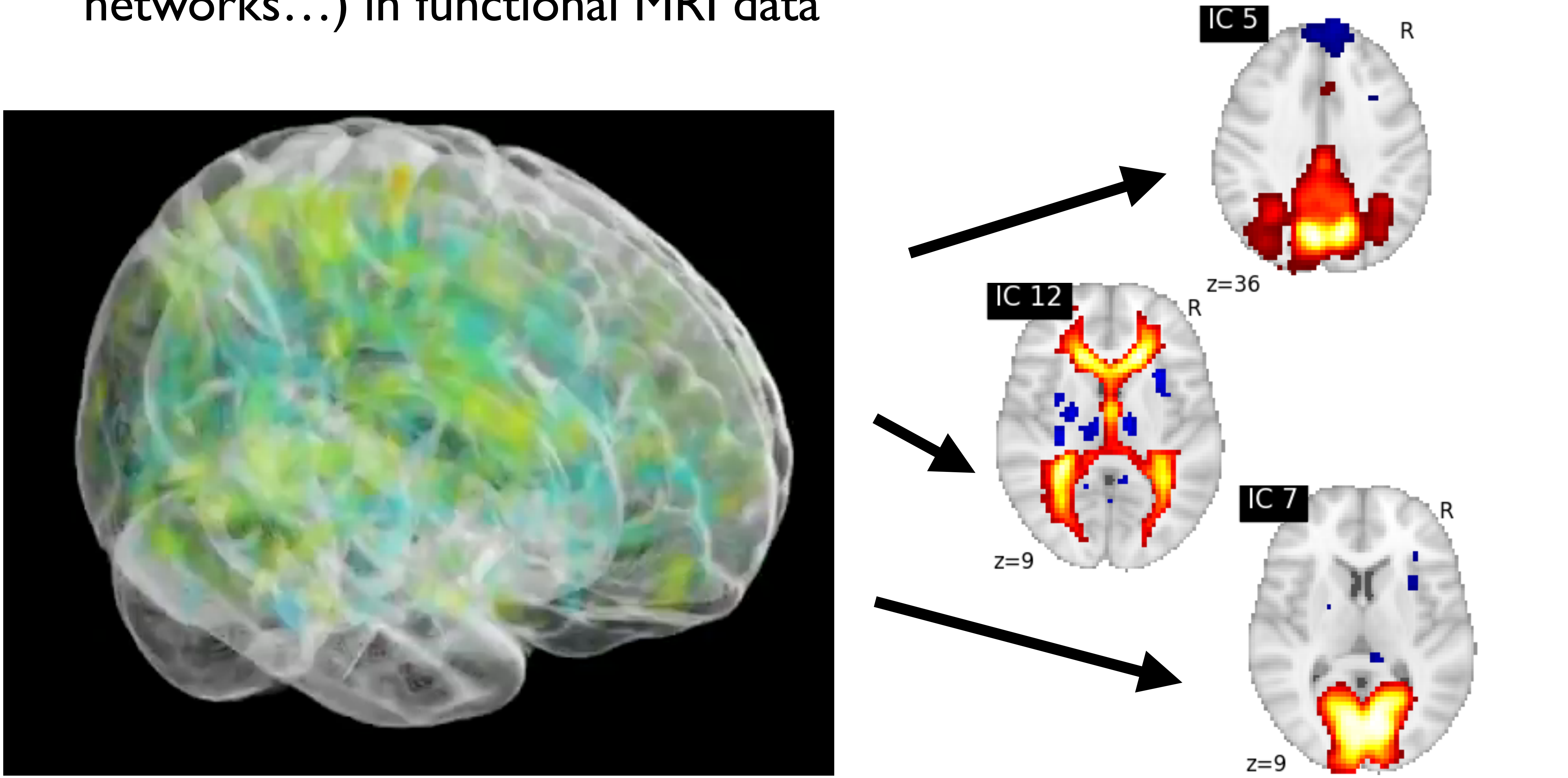
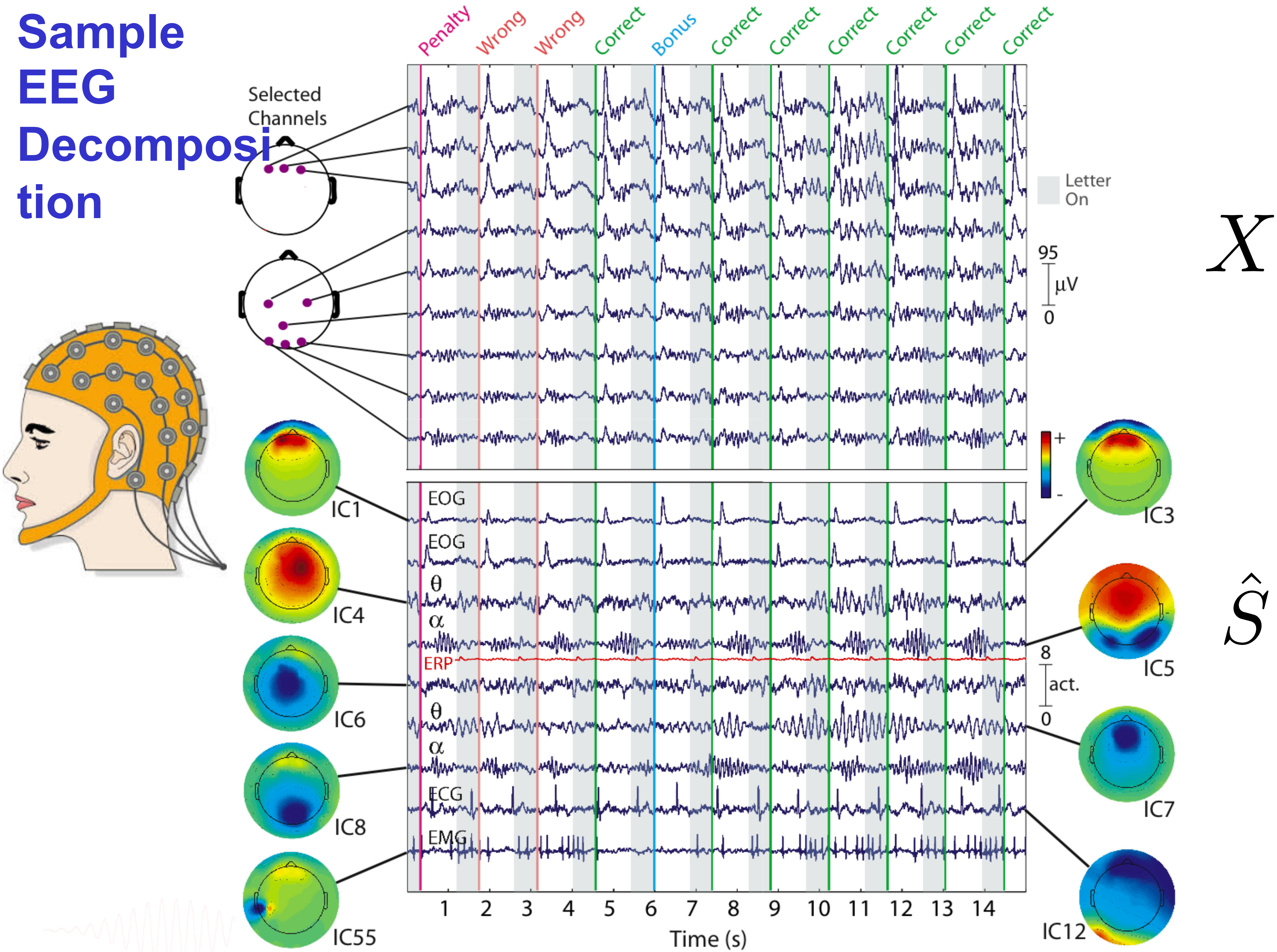


Source: http://nilearn.github.io/auto_examples/03_connectivity/plot_canica_resting_state.html

Sample EEG Decomposition



Source: EEGLAB software documentation

Principles of (non-Gaussian) ICA

$$\mathbf{X} = \mathbf{A}\mathbf{S}$$

Objective: Find $\mathbf{W}$ s.t. $\mathbf{W}\mathbf{X}$ has maximally <u>independent</u> rows.

Model: Let $\mathbf{Y} = \mathbf{W}\mathbf{X}$ denote the unmixed data

$$p(\mathbf{Y}(t)) = p_1(\mathbf{Y}_1(t))\ldots p_N(\mathbf{Y}_N(t))$$

Principles of (non-Gaussian) ICA

$$\mathbf{X} = \mathbf{AS}$$

Objective: Find $\mathbf{W}$ s.t. $\mathbf{WX}$ has maximally <u>independent</u> rows.

Model: Let $\mathbf{Y} = \mathbf{WX}$ denote the unmixed data

$$p(\mathbf{Y}(t)) = p_1(\mathbf{Y}_1(t))\ldots p_N(\mathbf{Y}_N(t))$$

Likelihood: With $\mathbf{Y} = g(\mathbf{X}) = \mathbf{WX}$

$$p(\mathbf{X}) = p(g(\mathbf{X}))\,|\det J_{g(\mathbf{X})}| = p(\mathbf{Y})\,|\det \mathbf{W}\,|$$

cf. RealNVP [Dinh et al. 2016]

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leads to:

cf. RealNVP [Dinh et al. 2016]

$$\boxed{\mathscr{L}(\mathbf{W}) = \log|\det \mathbf{W}| + \mathbb{E}_t\left(\sum_{i=1}^{N} \log p_i(\mathbf{Y}_i(t))\right)}$$

[Pham & Garat 1997]

Optimization problem

$$\boxed{\min_{\mathbf{W}\in\mathbb{R}^{N\times N}} -\log|\det \mathbf{W}| - \frac{1}{T}\sum_{t=1}^{T}\left(\sum_{i=1}^{N}\log p_i(\mathbf{Y}_i(t))\right)}$$

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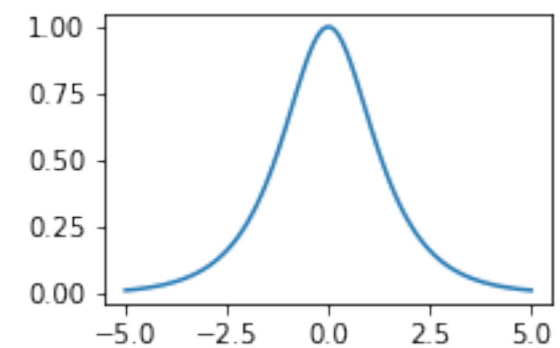
- Infomax model *[Bell & Sejnowski 1995]*

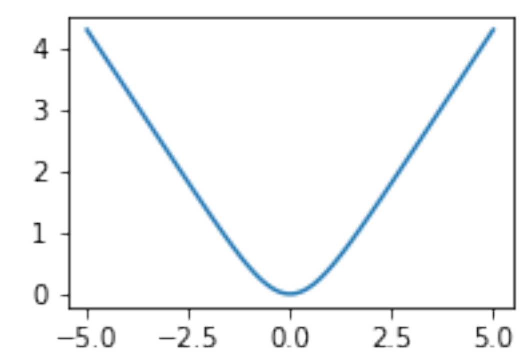
Density

$$p_i(\,\cdot\,) \propto \frac{1}{\cosh(\,\cdot\,)}$$



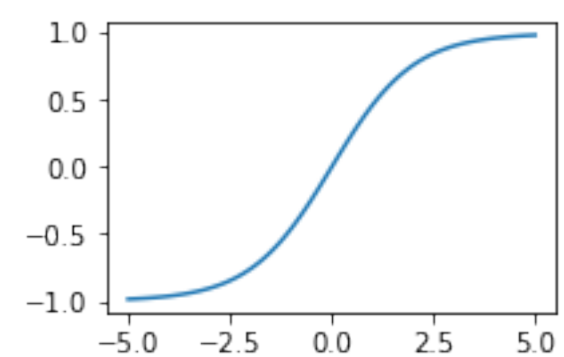
Heavy-tail
"sparse"

$$-\log(p_i(\,\cdot\,)) = \log(\cosh(\,\cdot\,)) + c$$



Score function:

$$\psi_i(\,\cdot\,) = -\log(p_i(\,\cdot\,))' = \tanh(\,\cdot\,/2)$$



Geometry of the problem

- non-convex (multiple minima)
- Optimization on the invertible matrices manifold
- Use of a **relative** framework

Absolute

$$\mathbf{W}_{n+1} = \mathbf{W}_n + \delta\mathbf{W}$$

Relative

$$\mathbf{W}_{n+1} = (I_N + \delta\mathbf{W})\mathbf{W}_n$$

Relative gradient / Hessian

Relative matrix form Taylor expansion:

$$\mathcal{L}((I+\mathcal{E})W) = \mathcal{L}(W) + \langle G|\mathcal{E}\rangle + \frac{1}{2}\langle \mathcal{E}|H|\mathcal{E}\rangle + \mathcal{O}(||\mathcal{E}||^3)$$

- Gradient is a $N \times N$ matrix:

$$G_{ij} = E[\psi_i(y_i)y_j] - \delta_{ij}$$

simple expressions

- Hessian is a $N \times N \times N \times N$ Fourth order tensor.

$$H_{ijkl} = \delta_{il}\delta_{jk} + \delta_{ik}E[\psi_i'(y_i)y_j y_l]$$

(relative) Newton method

$$H_{ijkl} = \delta_{il}\delta_{jk} + \delta_{ik} E[\psi_i'(y_i) y_j y_l]$$

One iteration: $\boxed{W_{n+1} = (I - H^{-1}G)W_n}$

Problem:

Large linear system / regularization needed

Newton method is possible but not practical

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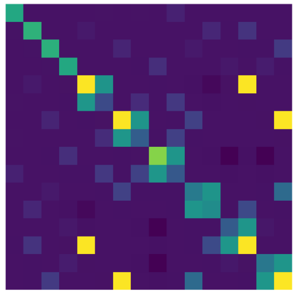
but if model holds:

$$\delta_{ik}E[\psi_i'(y_i)y_jy_l] \quad = \quad \delta_{ik}\delta_{jl}E[\psi_i'(y_i)]E[y_j^2]$$



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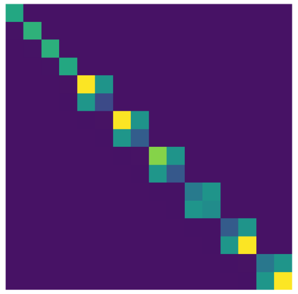
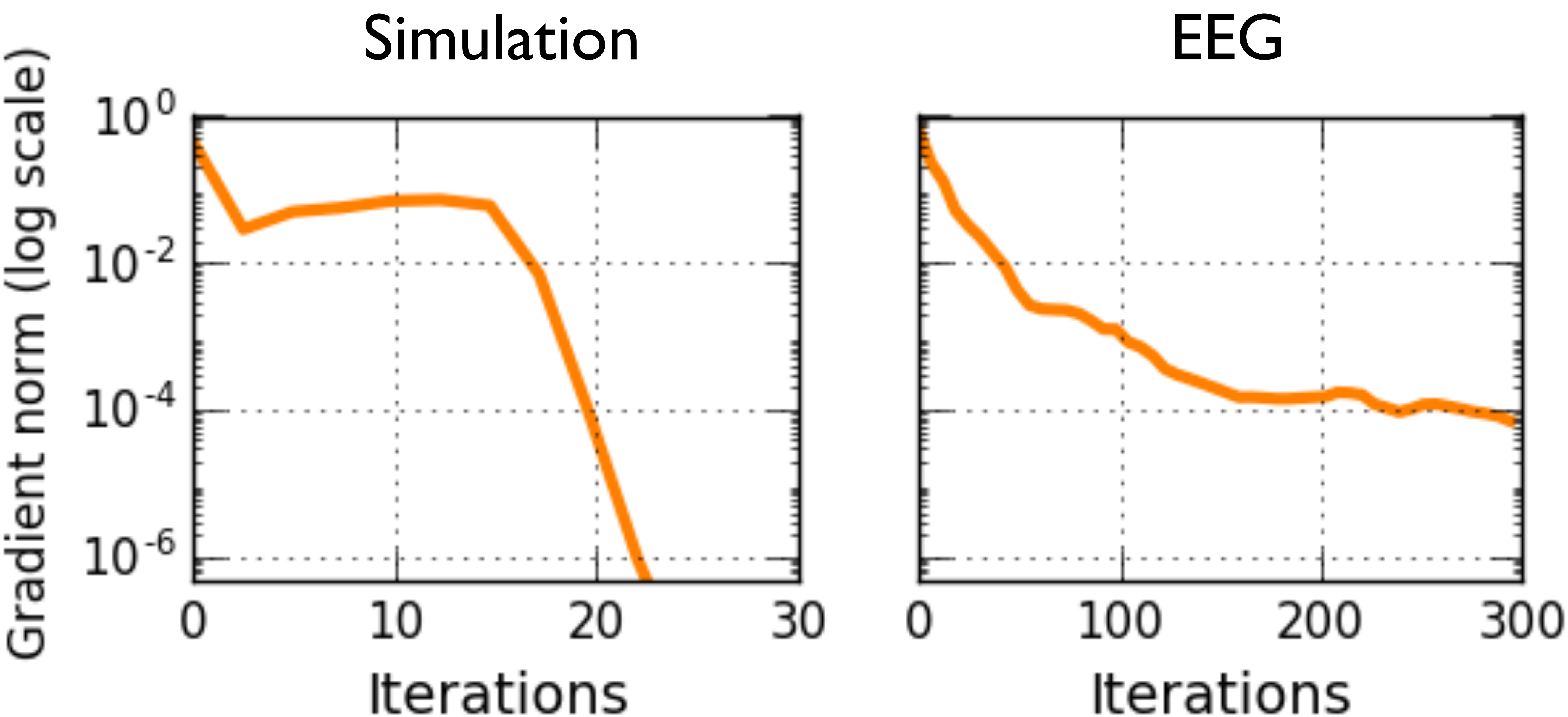


But…



It does not work with real data !

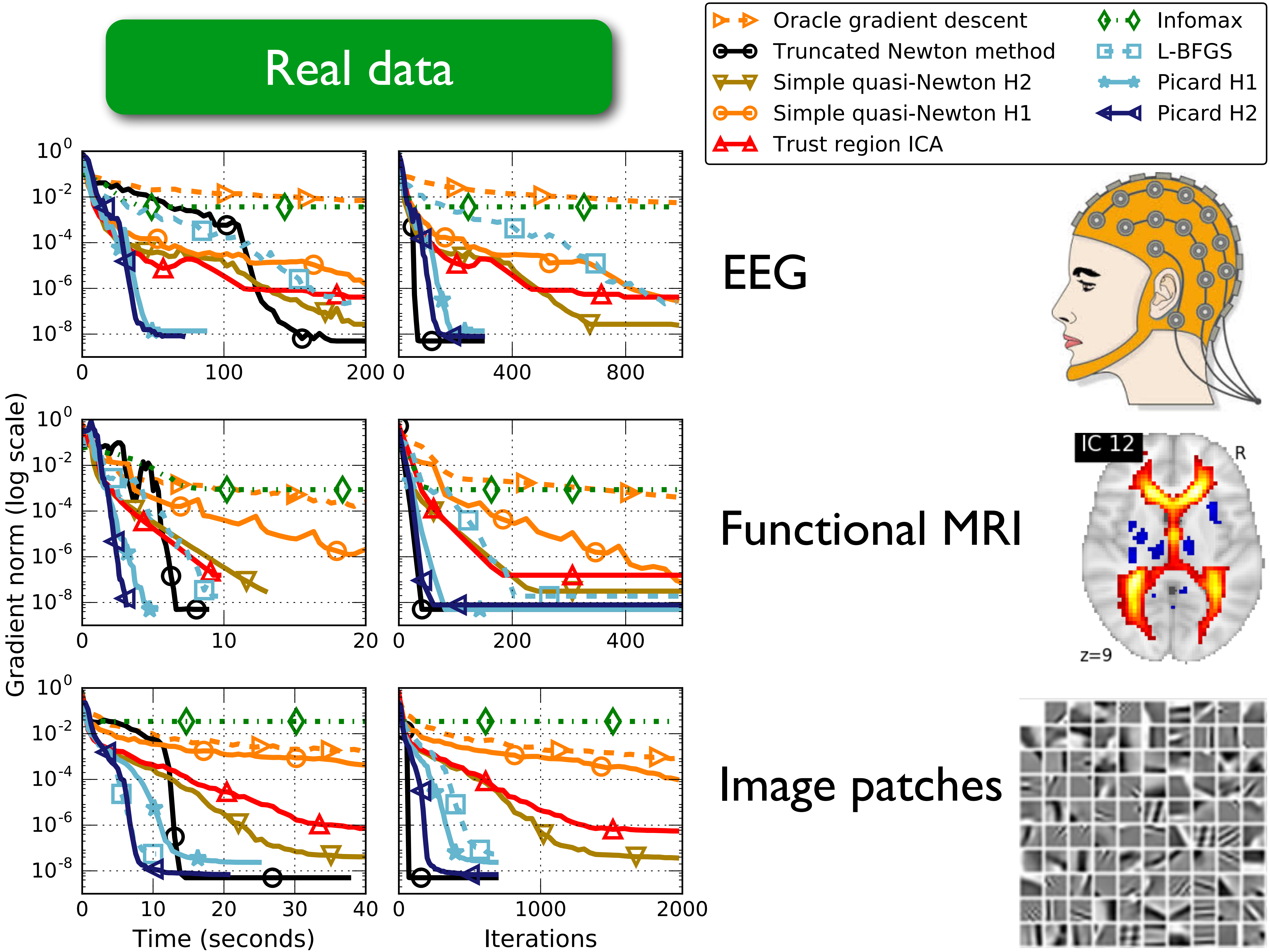
L-BFGS algorithm with Hessian approx.

Idea:

- Combine L-BFGS with Hessian approx.
- Replace diagonal initial guess by Hessian approx.
- The rest is the same (although written with relative gradients)…

[Liu, D. C., & Nocedal, J. « On the limited memory BFGS method for large scale optimization. » *Mathematical programming, 1989*]

[P. Ablin, J.-F. Cardoso, A. Gramfort, Faster ICA by preconditioning with Hessian approximations, IEEE TSP 2017]

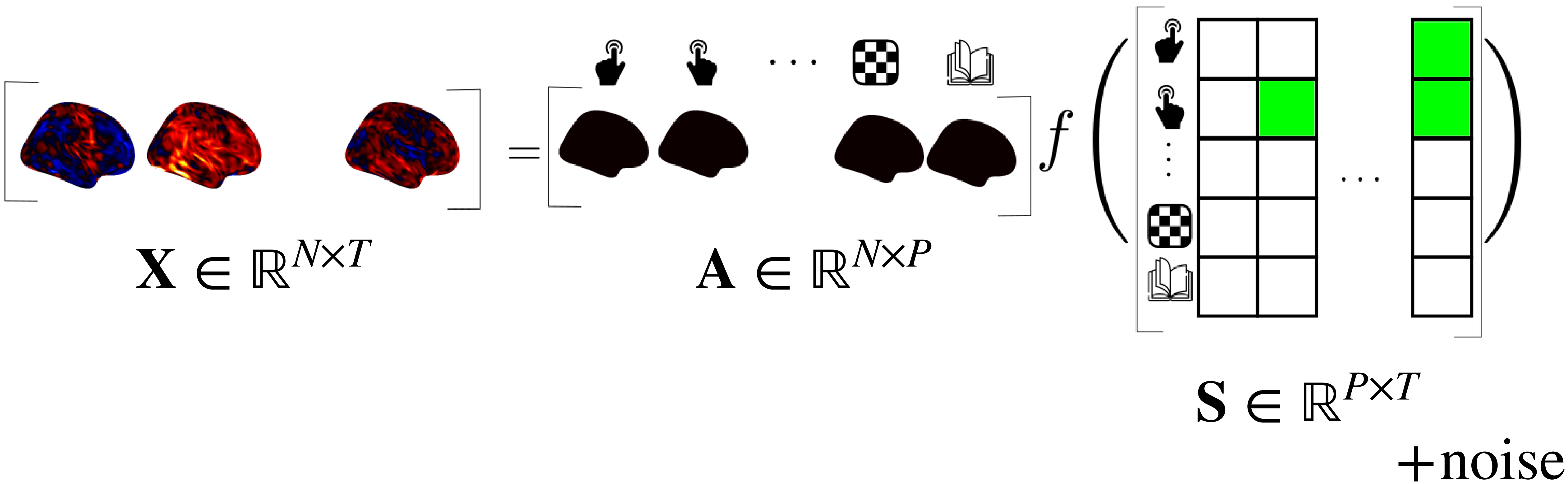

Real data
Oracle gradient descent
Truncated Newton method
Simple quasi-Newton H2
Simple quasi-Newton H1
Trust region ICA
Infomax
L-BFGS
Picard H1
Picard H2
EEG
Functional MRI
IC 12
R
z=9
Image patches
Gradient norm (log scale)
Time (seconds)
Iterations

What if you have multiple sets $\mathbf{X}$, e.g. from a population?
Multiview ICA

[Modeling Shared Responses in Neuroimaging Studies through MultiView ICA
Richard, H., Gresele, L., Hyvärinen, A., Thirion, B., Gramfort, A., Ablin, P. (2020). Proc. NeurIPS]
[Shared Independent Component Analysis for Multi-Subject Neuroimaging
Richard, H., Ablin, P., Thirion, B., Gramfort, A., Hyvärinen, A. (2021). Proc. NeurIPS]

Towards naturalistic stimuli

Controlled stimuli



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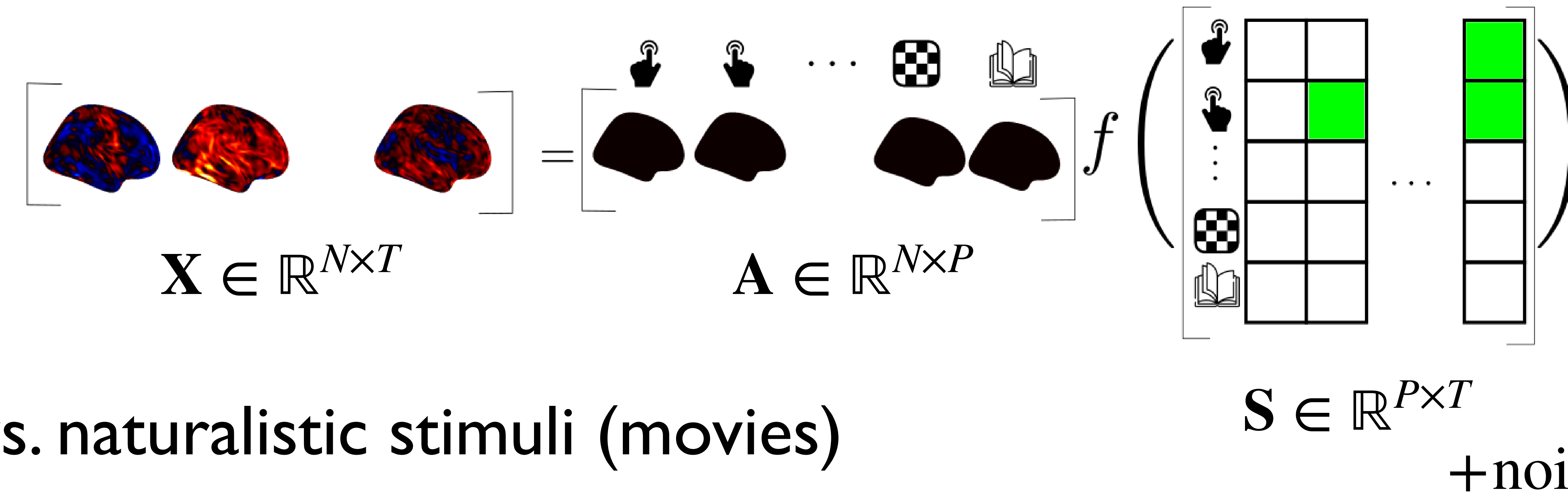
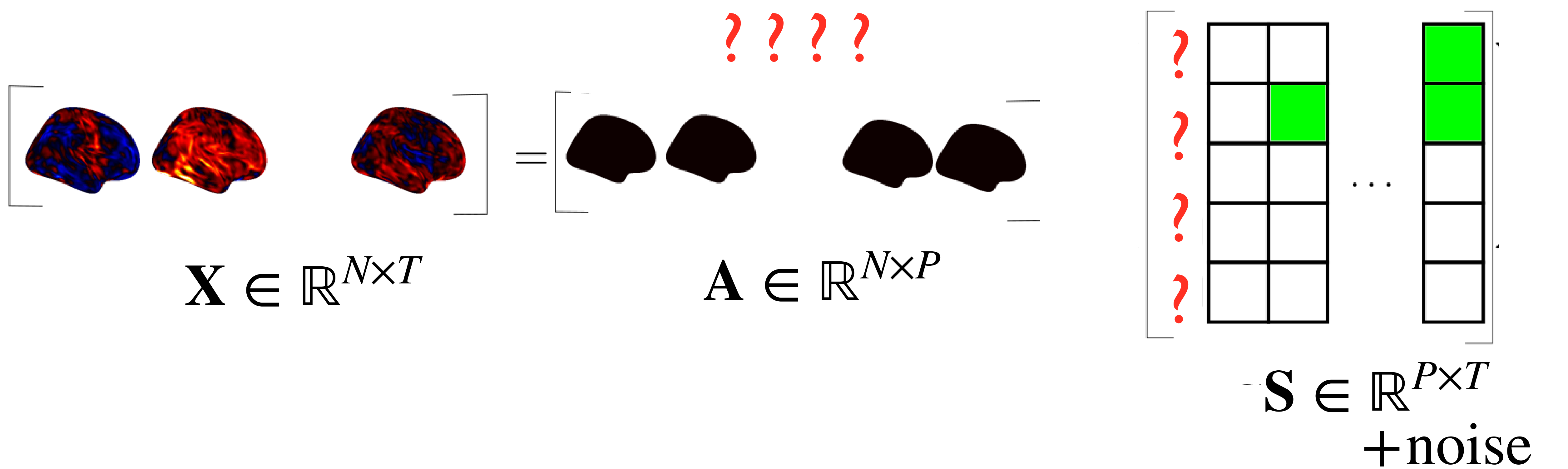


vs. naturalistic stimuli (movies)



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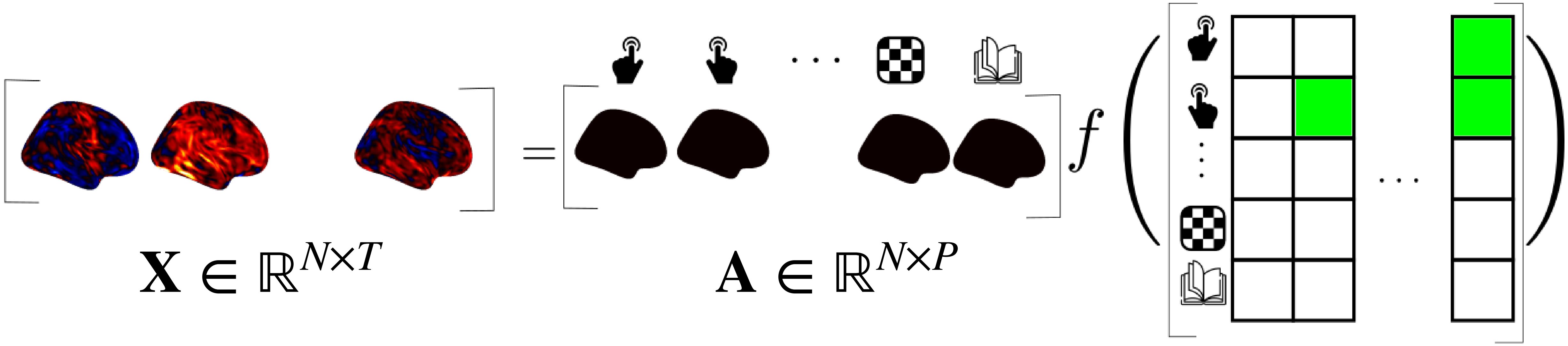
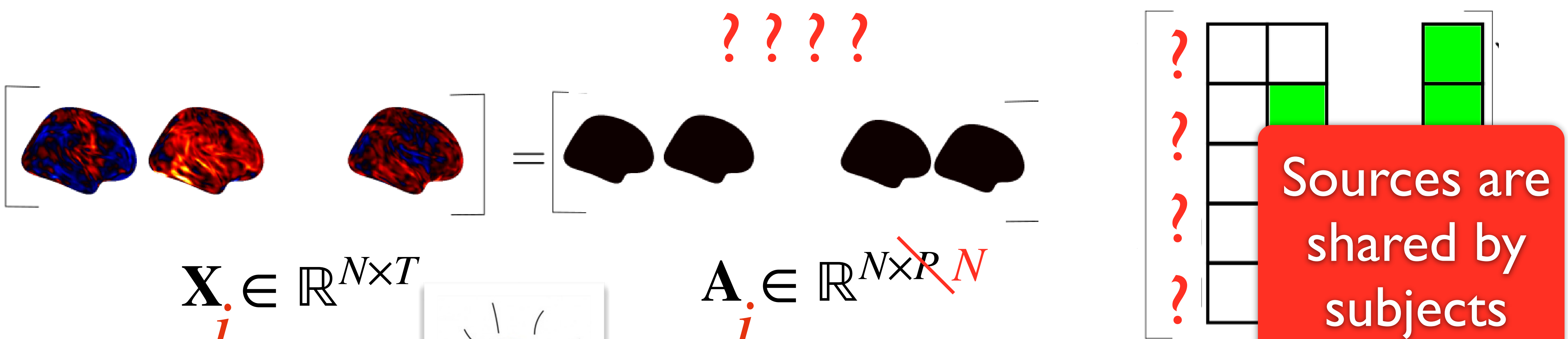


$$\mathbf{X} \in \mathbb{R}^{N\times T} = \mathbf{A} \in \mathbb{R}^{N\times P} \; f\left(\mathbf{S} \in \mathbb{R}^{P\times T}\right)$$

+noise

vs. naturalistic stimuli (movies)



$\mathbf{X}_i \in \mathbb{R}^{N\times T}$

$\mathbf{A}_i \in \mathbb{R}^{N\times \cancel{P}\, N}$

$i = 1,\dots,M$

subjects/views

Sources are shared by subjects

$\mathbf{S} \in \mathbb{R}^{P\times T}$

+noise

Multiview ICA

Model: $\mathbf{X}^i = \mathbf{A}^i(\mathbf{S} + \mathbf{N}^i),\ i = 1,\ldots,M$ $\mathbf{X}^i$ *Data for subject i*

Assumptions:

density as in Infomax (1/cosh)

Source independence: $p(\mathbf{S}(t)) = q(\mathbf{S}_1(t))\ldots q(\mathbf{S}_N(t))$

Gaussian noise: $\mathbf{N}^i_j(t) \sim \mathcal{N}(0,\sigma^2)$ *independent across components and independent from sources*

[Richard et al. NeurIPS 2020]

Multiview ICA

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Gaussian noise: $\mathbf{N}^i_j(t) \sim \mathcal{N}(0,\sigma^2)$ *independent across components and independent from sources*

$$\boxed{\mathscr{L}(\mathbf{W}^i) = -\sum_{i=1}^{M} \underbrace{\log|\det \mathbf{W}^i| + f(\tilde{\mathbf{S}})}_{\text{“ICA term”}} + \frac{1}{2\sigma^2}\sum_{i=1}^{M} \underbrace{\|\mathbf{W}^i\mathbf{X}^i - \tilde{\mathbf{S}}\|^2}_{\text{“Error term”}}}$$

$\mathbf{W}^i$ *Unmixing matrix for subject i*

$$\tilde{\mathbf{S}} = \frac{1}{M}\sum_{i=1}^{M}\mathbf{W}^i\mathbf{X}^i \qquad f(\mathbf{S}) = \sum_{j=1}^{N} f(\mathbf{S}_j)$$

$$f(\mathbf{S}_j) = \int \exp\left(-\frac{1}{2\sigma^2}Mz^2\right) q(\mathbf{S}_j - z)dz$$

Smoothed density

[Richard et al. NeurIPS 2020]

Optimization (same recipe)

Objective: Minimize the negative log-likelihood $\mathscr{L}$ using a block-coordinate Newton descent

$$\mathbf{W}^i = (\mathbf{I} + \rho \mathbf{D}^i)\mathbf{W}^i$$

Multiplicative updates

$$\mathbf{D}^i = -(\tilde{\mathbf{H}}^i)^{-1}\mathbf{G}^i$$

Relative "Newton descent" direction

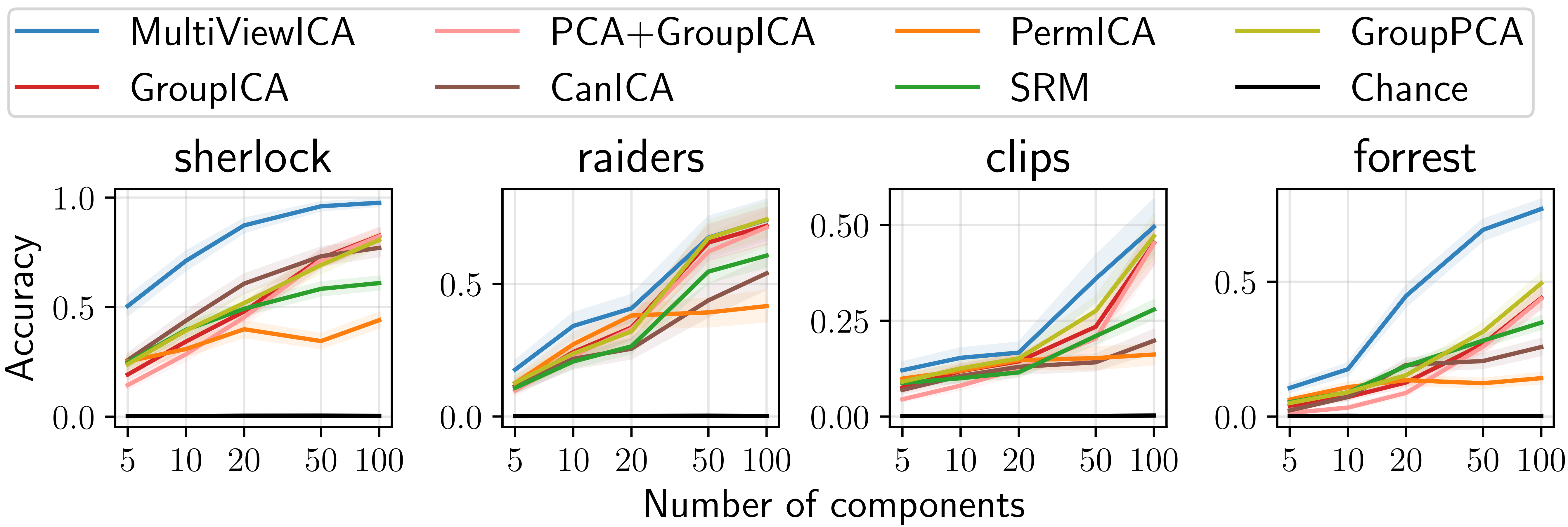
$$\tilde{\mathbf{H}}^i$$

Sparse Hessian ($N \times N \times N \times N$)
Approximation with N^2 non-zeros

[Ablin et al. IEEE TSP 2017, Richard et al. NeurIPS 2020]

fMRI time segment matching

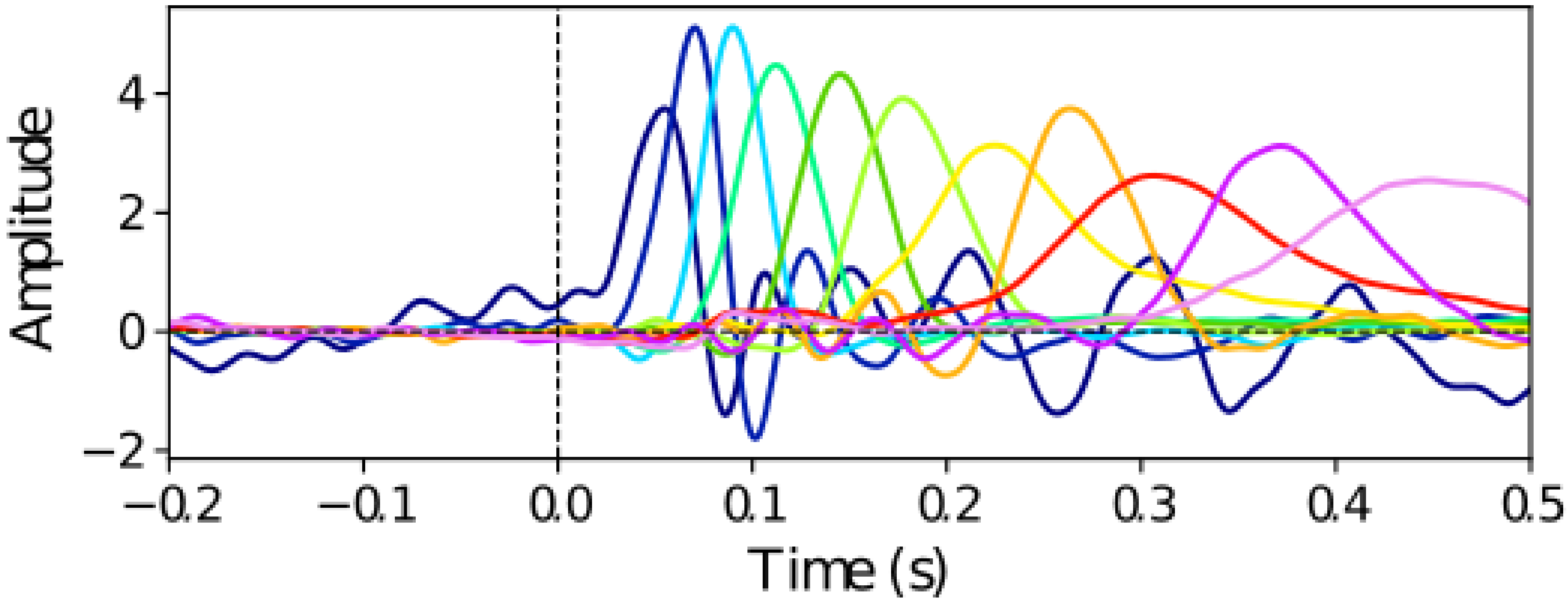
We select a target time-segment (9 consecutive timeframes) in the shared responses and try to localize the corresponding time-segment in the sources of the left-out subject using a maximum-correlation classifier

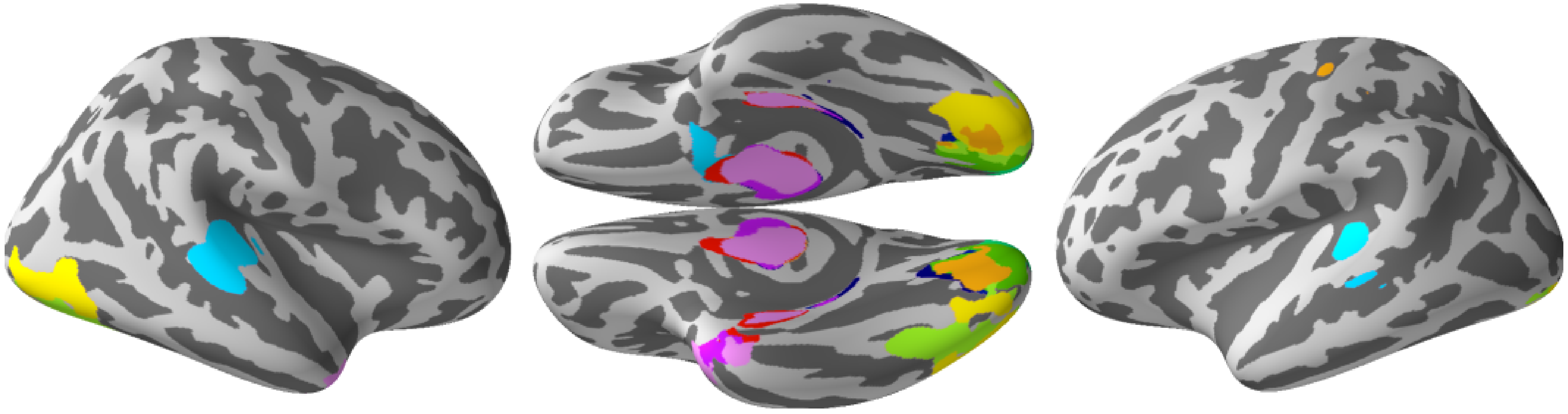


[Richard et al. NeurIPS 2020] 22

Experiment on MEG data

MEG data from Cam-CAN dataset
with 200 subjects attending to audiovisual stimuli

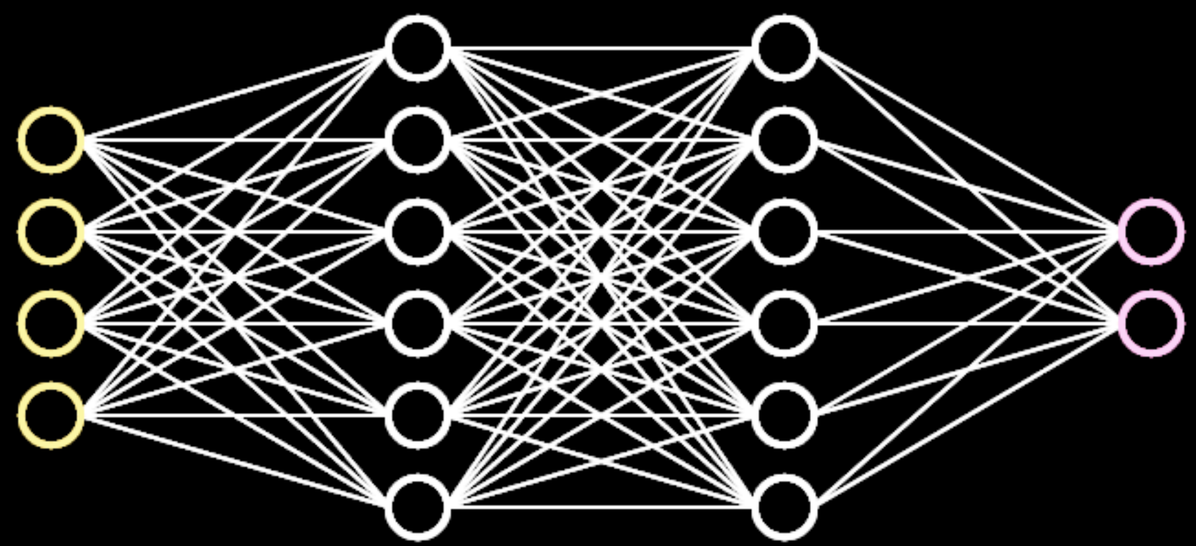




[Richard et al. NeurIPS 2020]

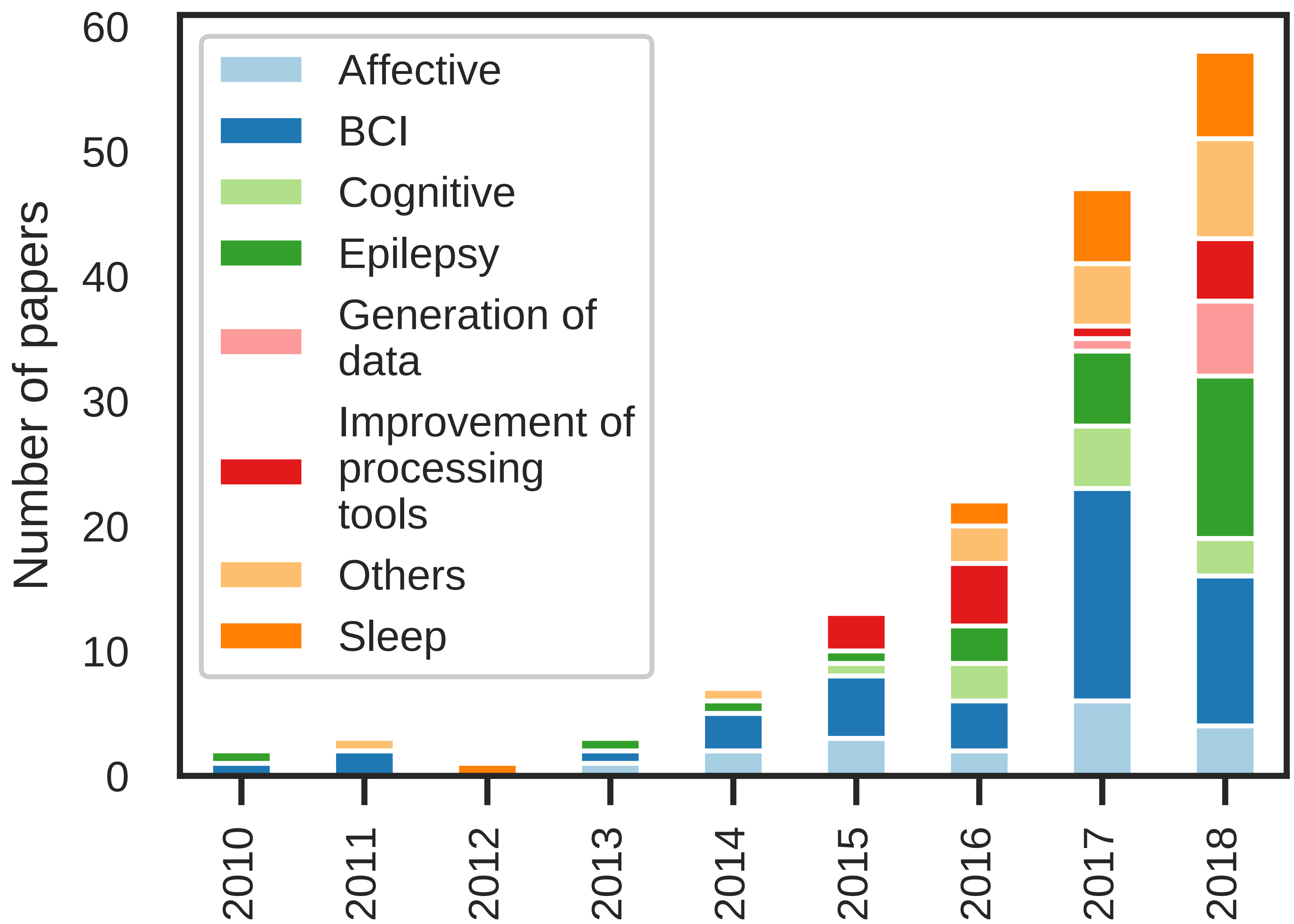
2

Self-supervised learning on EEG



Uncovering the structure of clinical EEG signals with self-supervised learning
Banville, H., Chehab, O., Hyvärinen, A., Engemann, D. and Gramfort, A. (2020)
Journal of Neural Engineering & ArXiv abs/2007.16104
Self-supervised representation learning from electroencephalography signals
Banville, H., Albuquerque, I., Moffat, G., Engemann, D. and Gramfort, A. (2019)
Proc. Machine Learning for Signal Processing (MLSP) .

Deep Learning papers on EEG



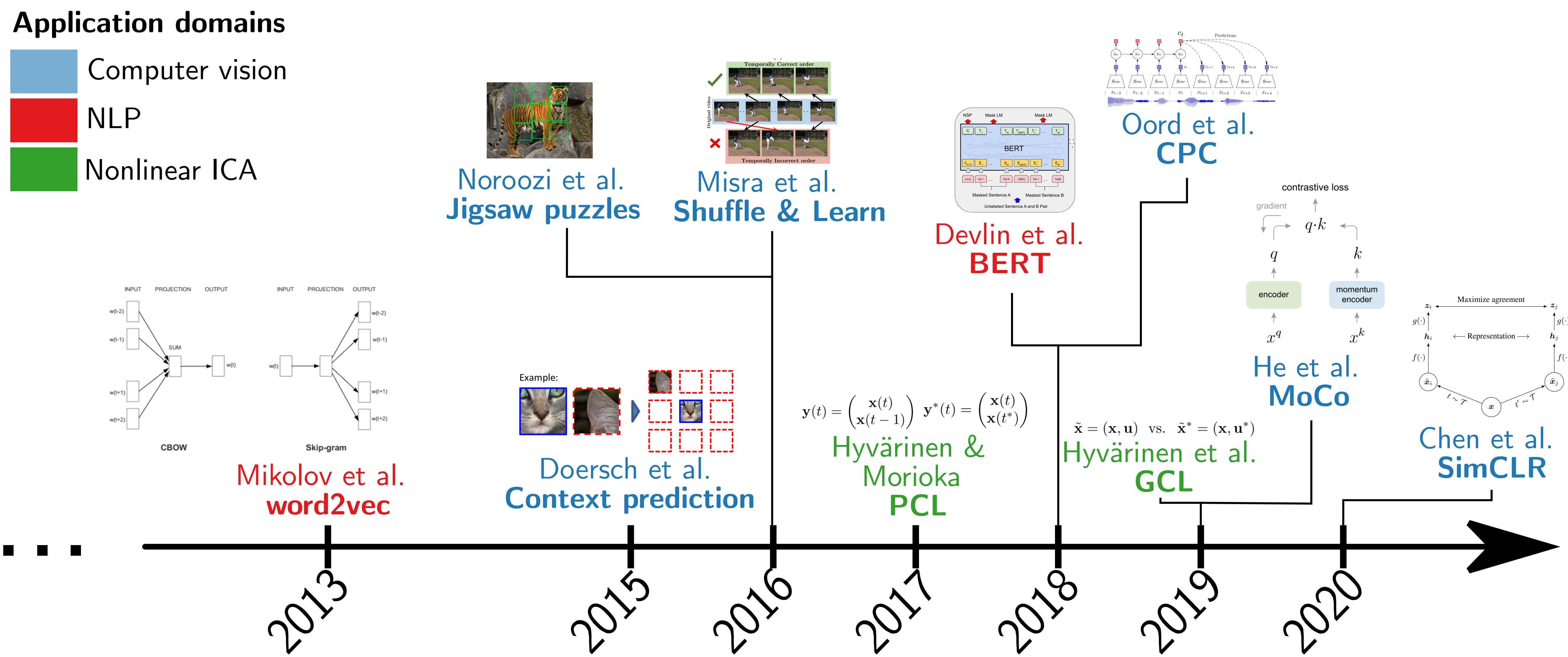
[Deep learning-based electroencephalography analysis: a systematic review
Roy, Y., Banville, H., Albuquerque, I., Gramfort, A., Falk, T. and Faubert, J. (2019)
Journal of Neural Engineering 16: (051001).]

Self-supervision

[Noroozi & Favaro 2016] use a deep neural network to solve the Jigsaw puzzle

Use the **structure** of the data to pretrain a **feature extractor** with a supervised *pretext task* – then use the features on a *downstream task*.

(Partial) History of SSL beyond EEG



Remarks: Heavily based on contrastive learning and possibly data augmentation techniques

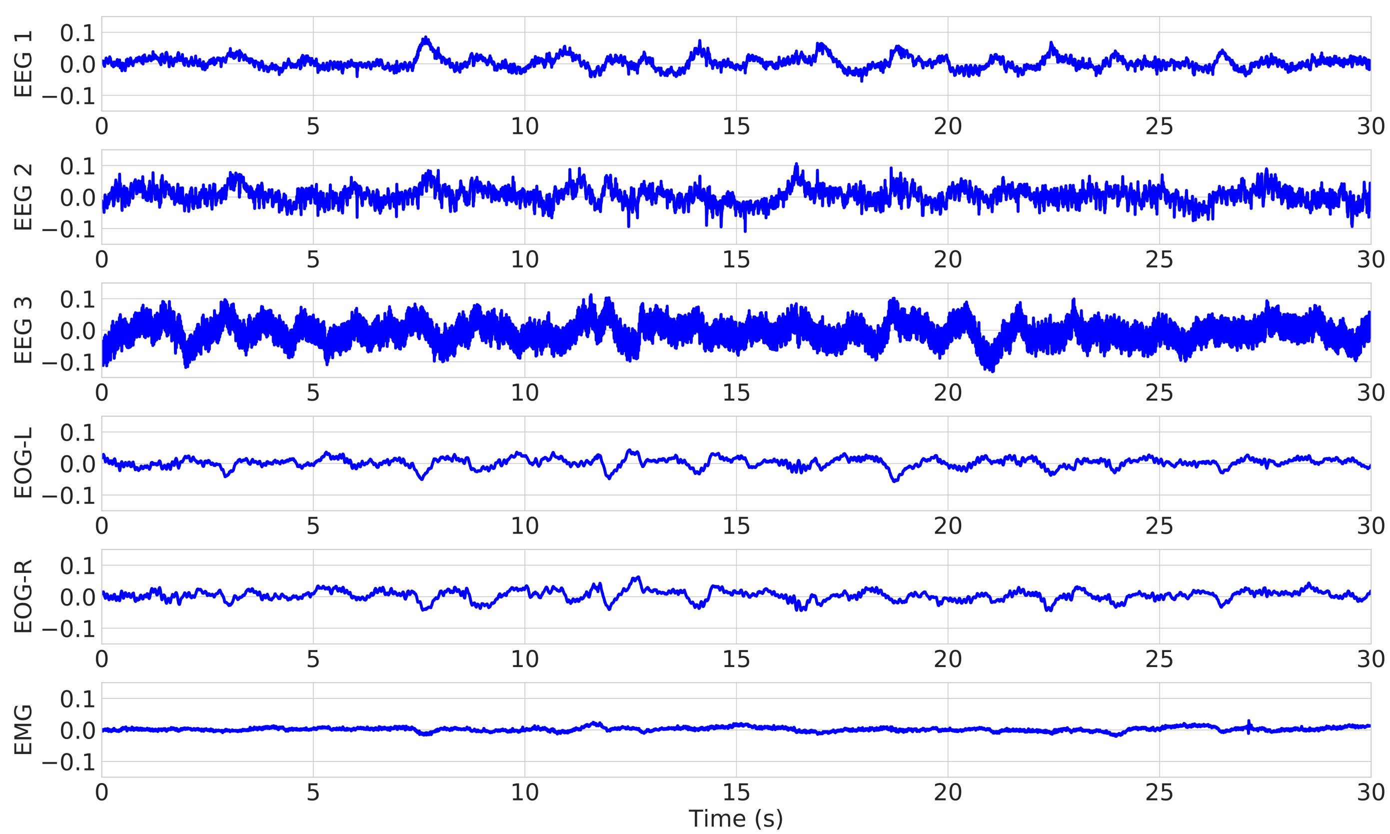
Polysomnography (PSG)

- Clinical exam
- Electrophysiological signals

Electro-encephalography (EEG)

Electro-oculography (EOG)

Electro-myography (EMG)



Polysomnography (PSG)

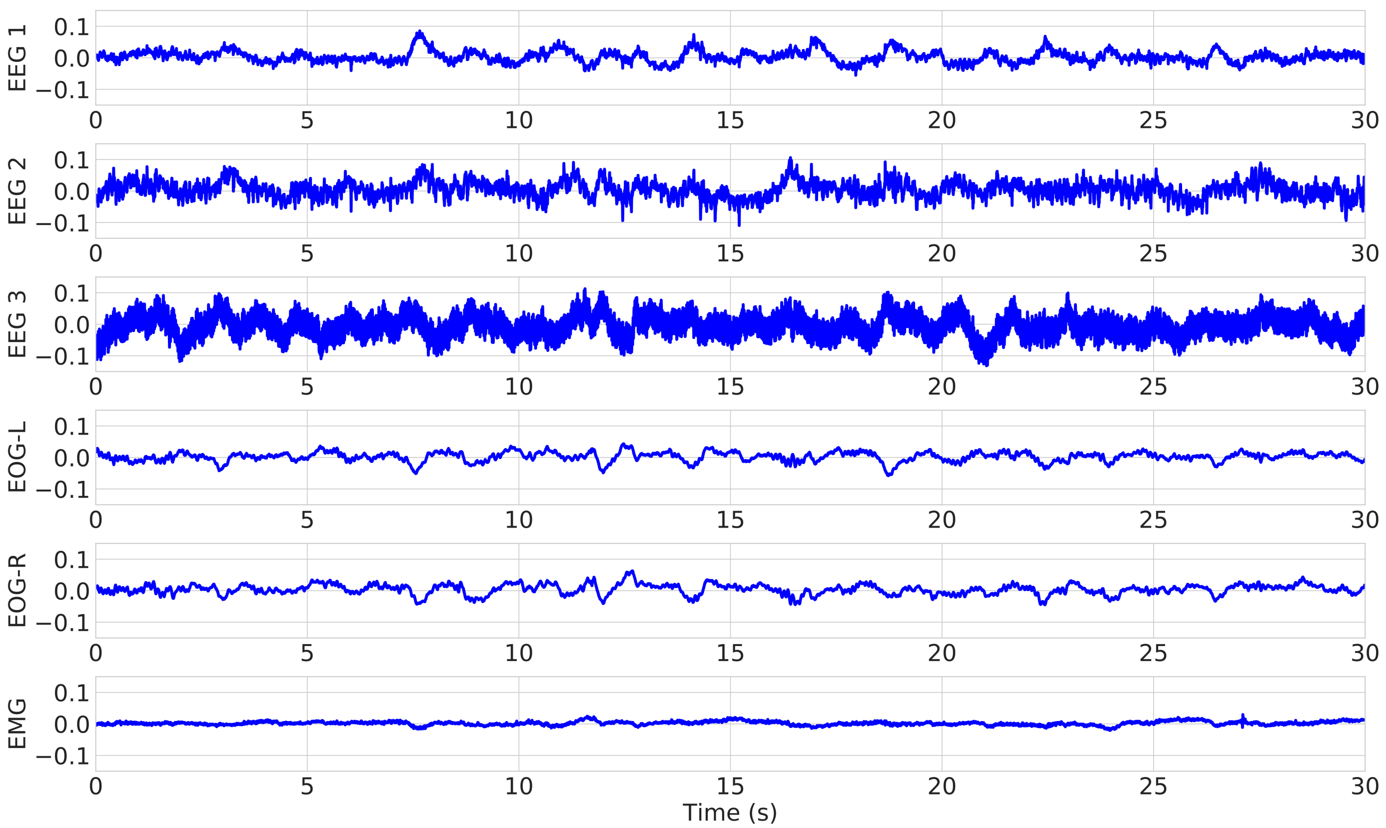
- Clinical exam
- Electrophysiological signals

Routinely annotated by sleep experts

Electro-encephalography (EEG)

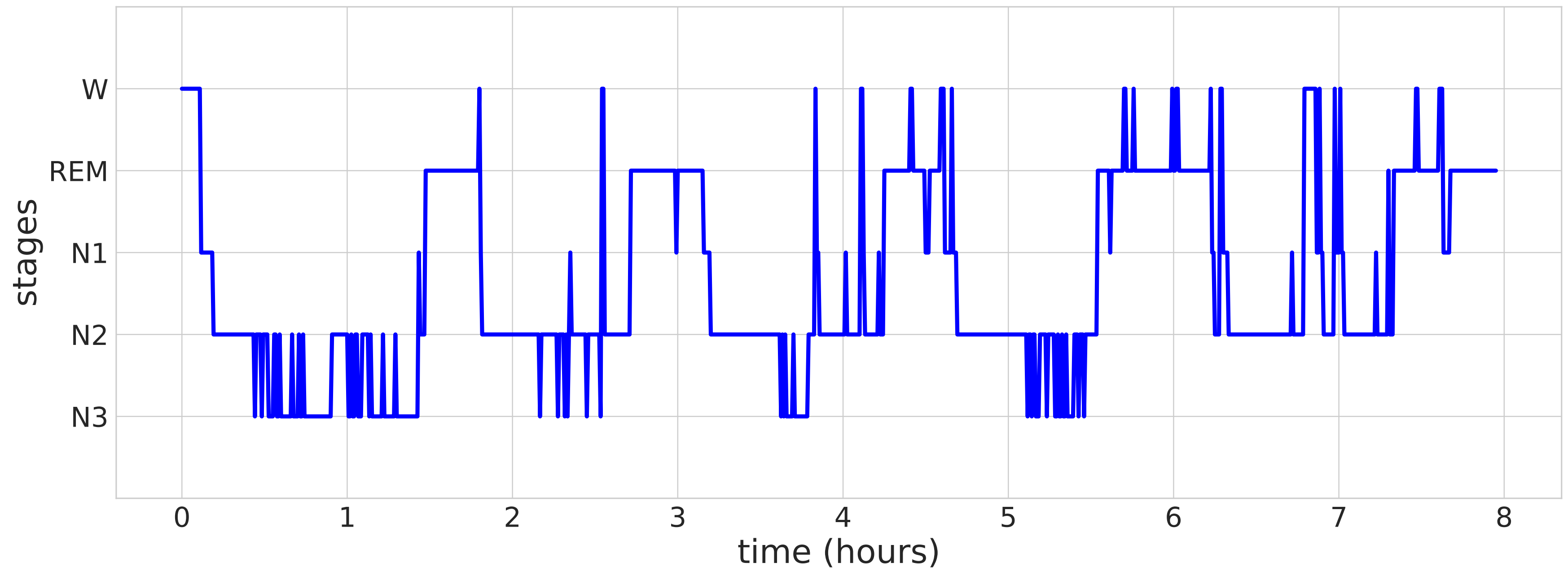
Electro-oculography (EOG)

Electro-myography (EMG)



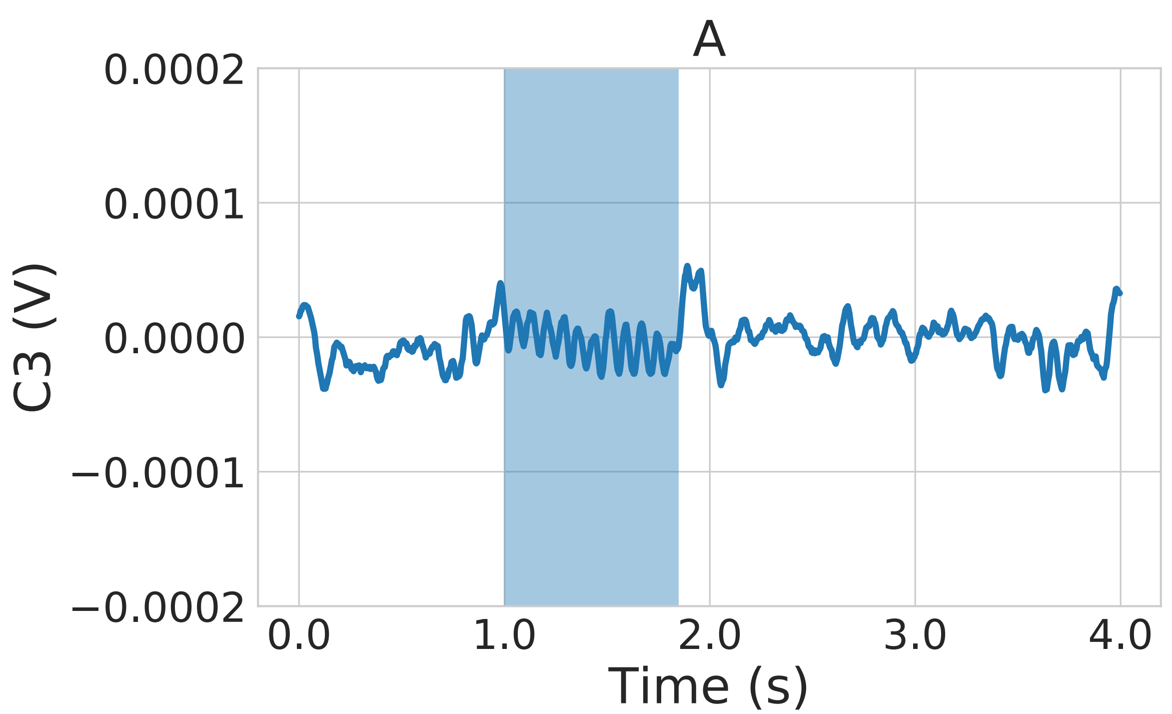
2 types of annotations

Hypnogram of sleep stages



[S. Chambon et al. (2018), IEEE Trans. Neural Systems and Rehabilitation Engineering]

Micro-events: Spindles, K-complex etc.

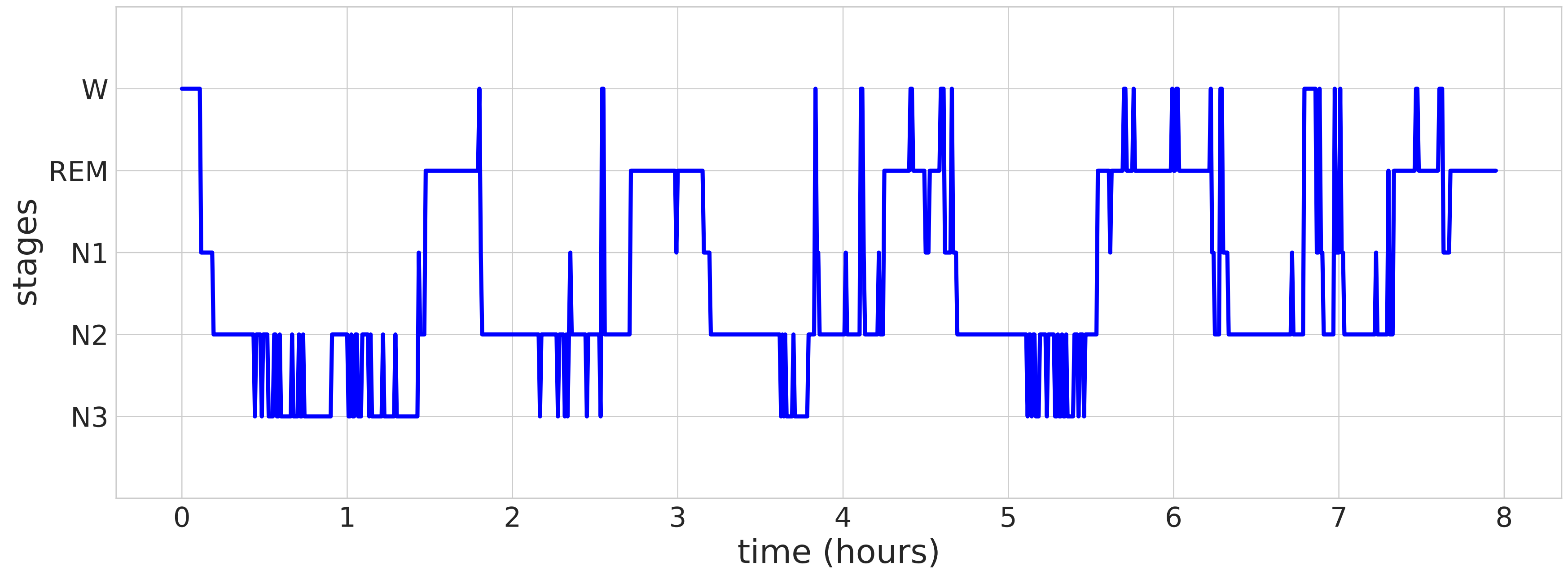


[S. Chambon et al. (2018), J. of Neuroscience Methods]

2 types of annotations

Hypnogram of sleep stages

Classification problem



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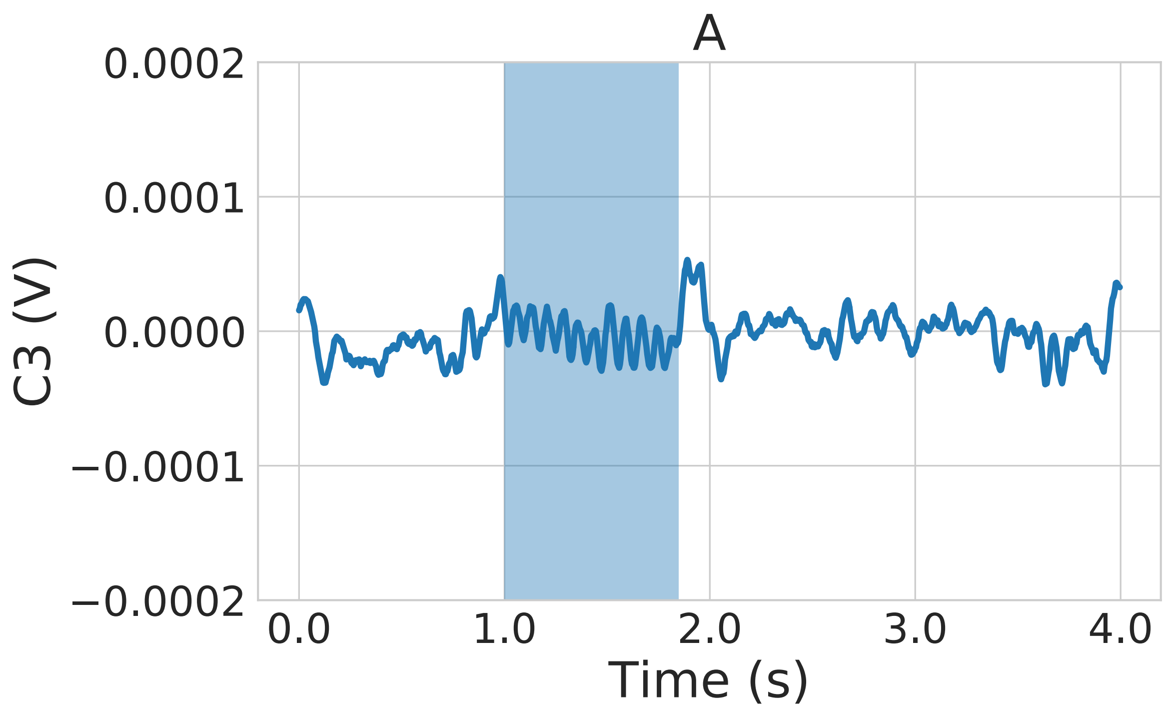

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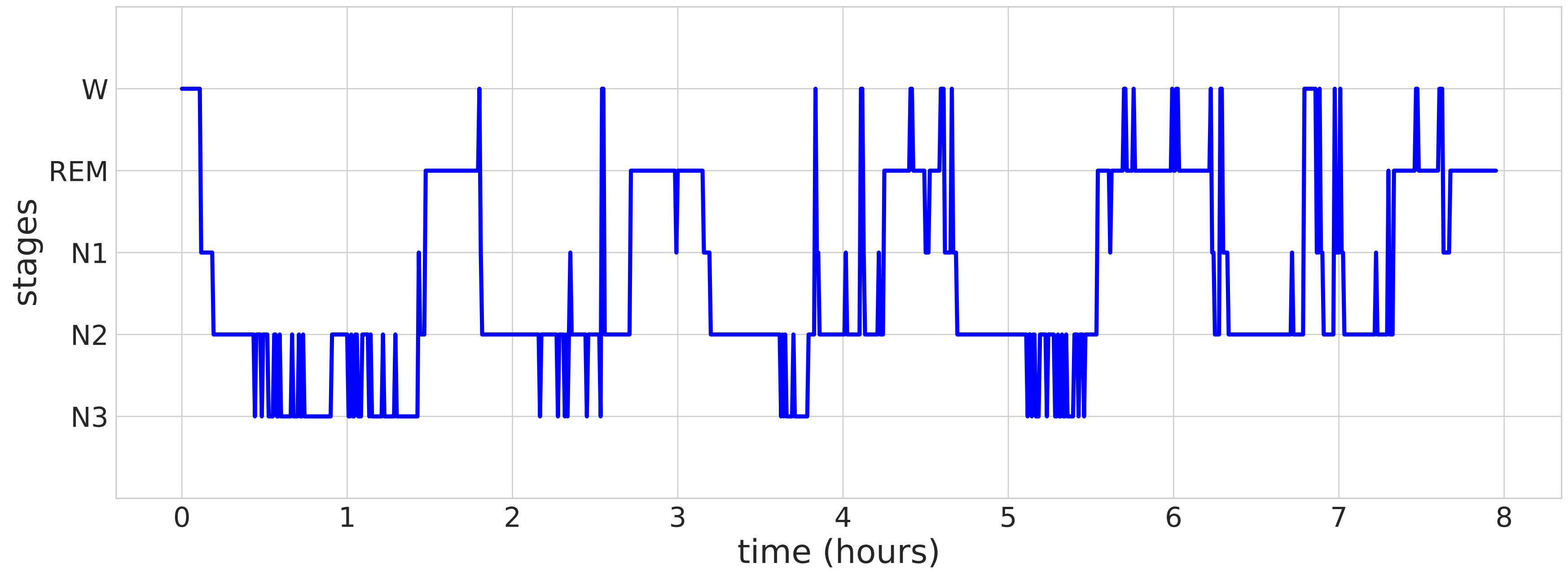

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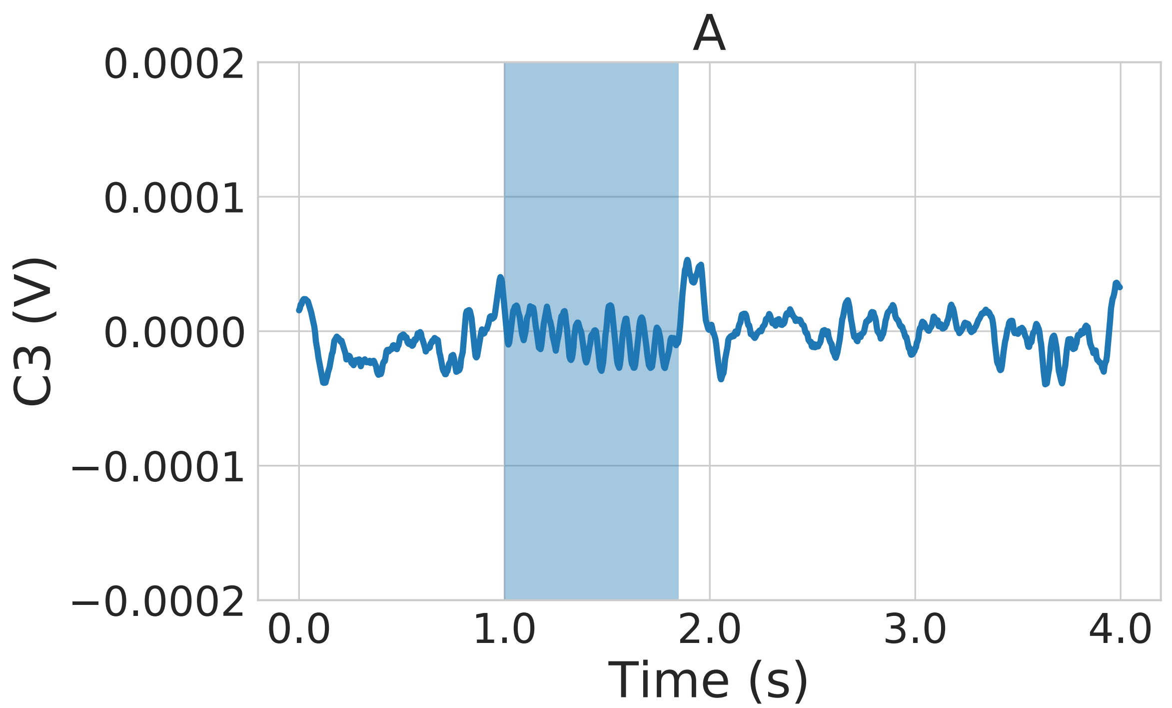
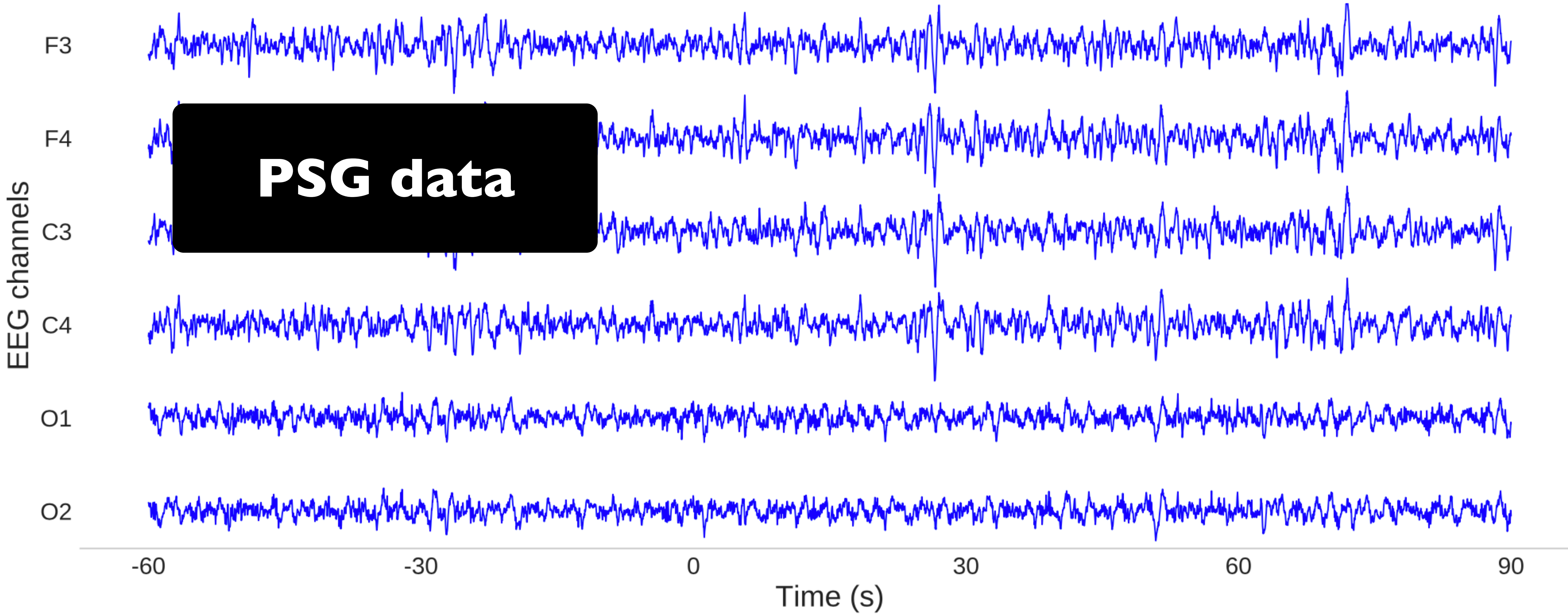
Micro-events: Spindles, K-complex etc.

Joint detection and classification problem

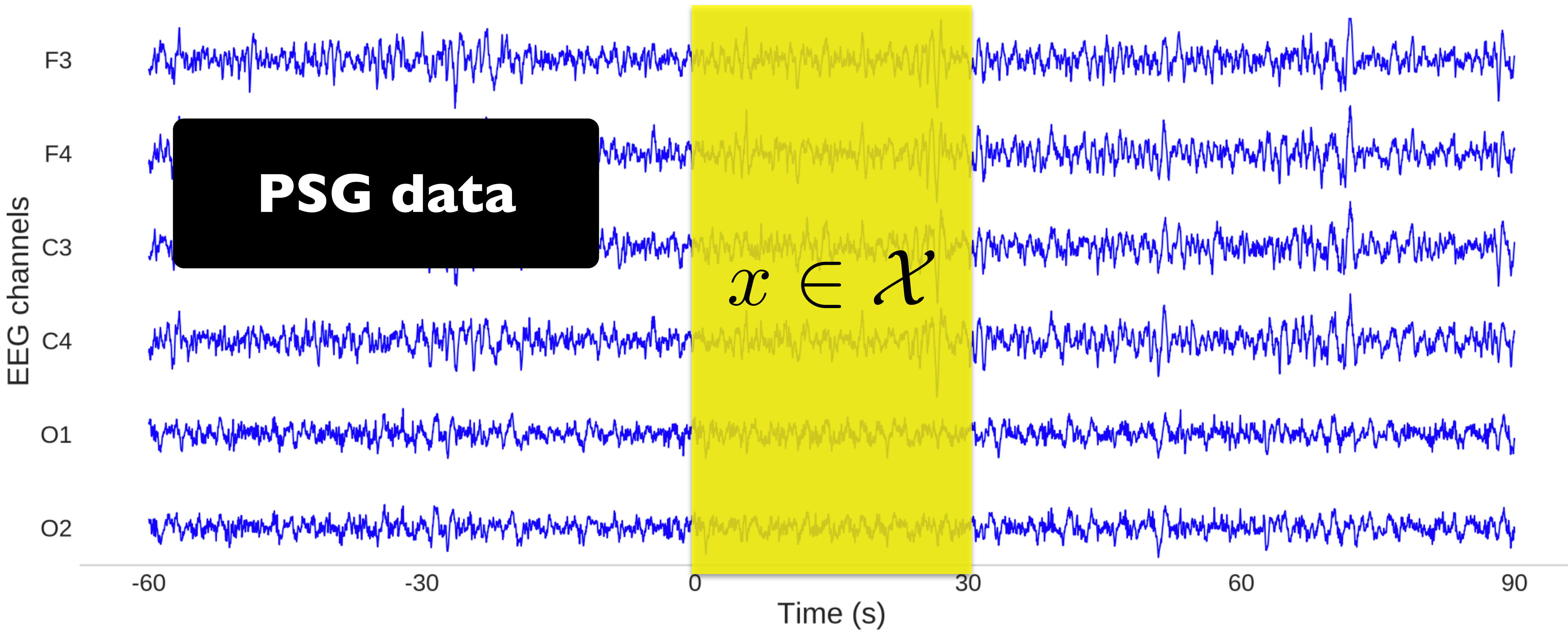


[S. Chambon et al. (2018), J. of Neuroscience Methods]

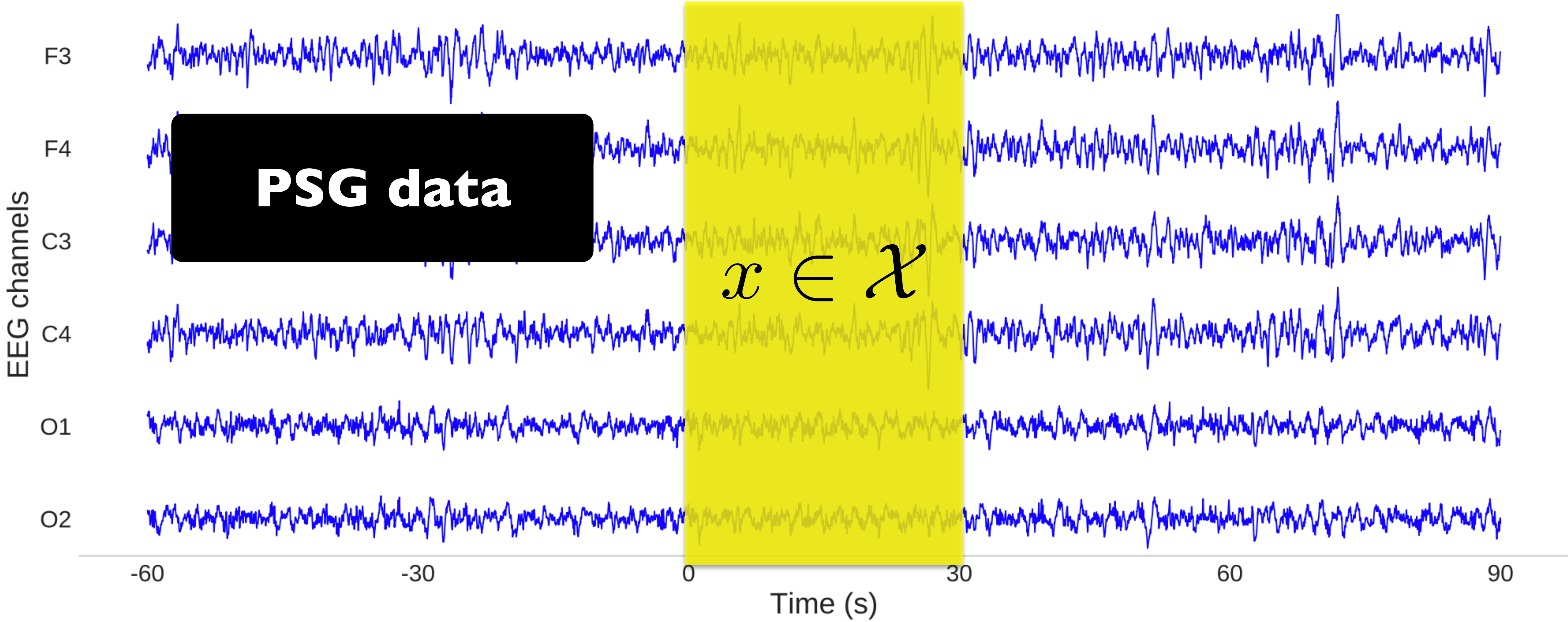
Sleep scoring: Downstream Task



Sleep scoring: Downstream Task



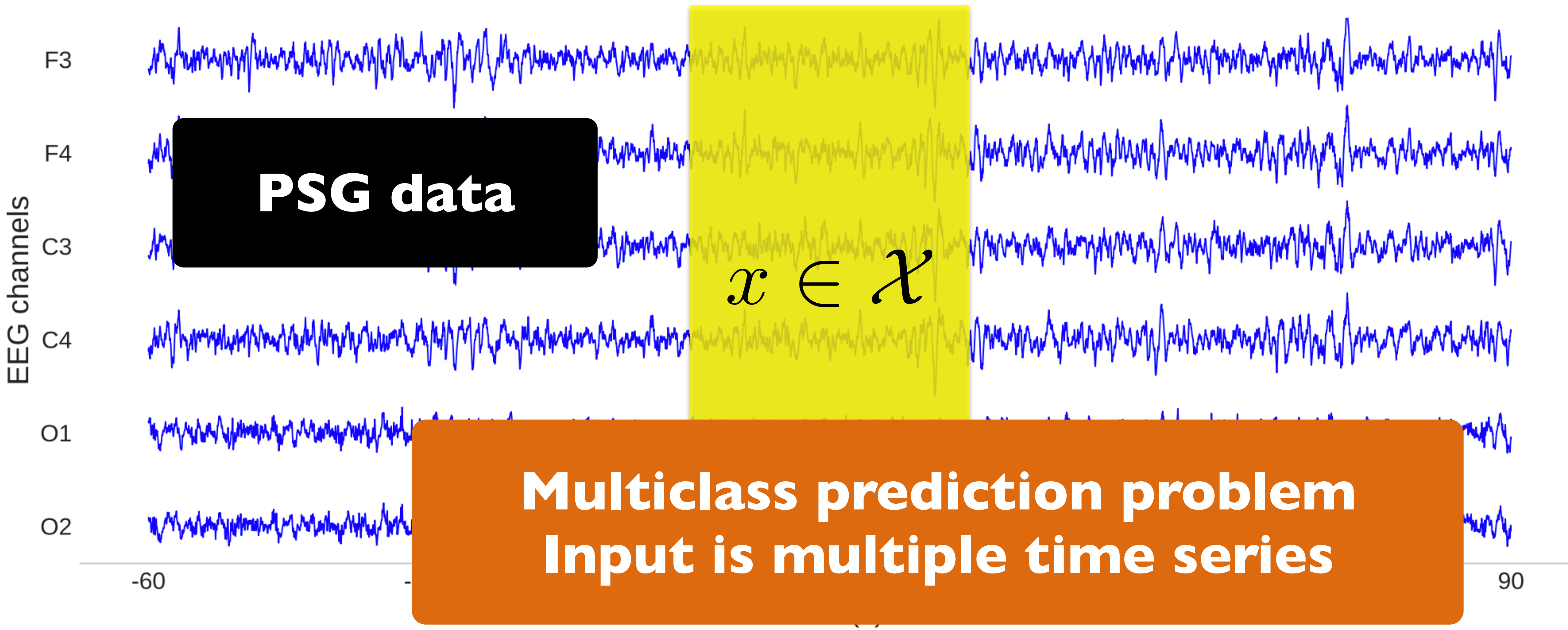
Sleep scoring: Downstream Task



Learn: $\hat{f} : \mathcal{X} \rightarrow \mathcal{Y}$

$$\mathcal{Y} = \{\text{Awake, REM, Stage 1, Stage 2, etc.}\}$$

Sleep scoring: Downstream Task



Multiclass prediction problem
Input is multiple time series

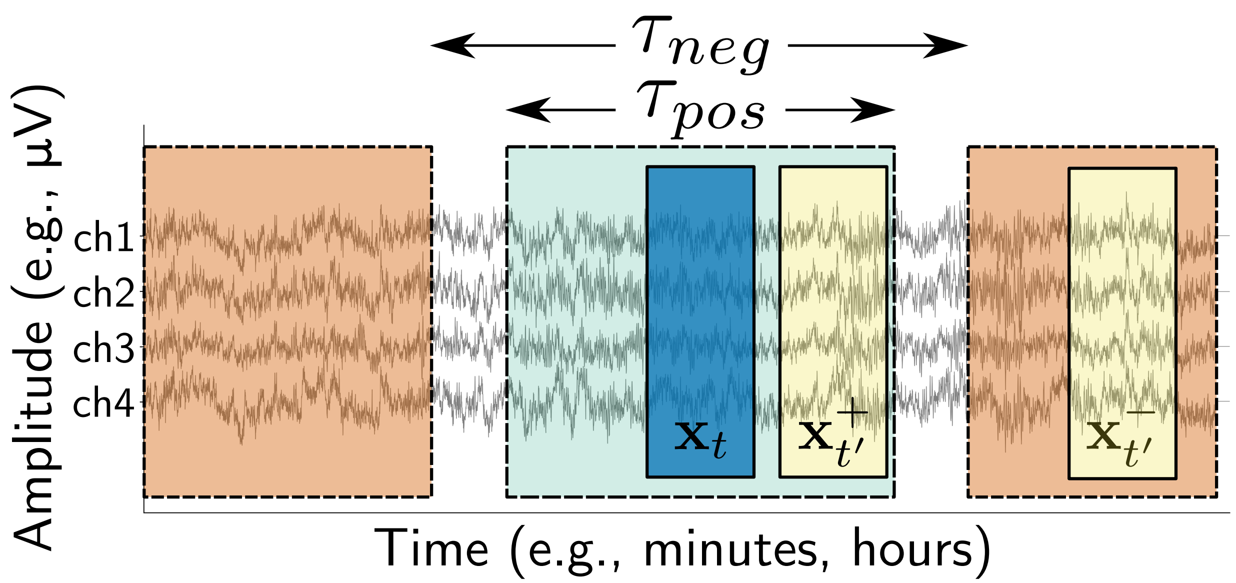
Learn: $\hat{f} : \mathcal{X} \rightarrow \mathcal{Y}$

$$\mathcal{Y} = \{\text{Awake, REM, Stage 1, Stage 2, etc.}\}$$

Pretext Task

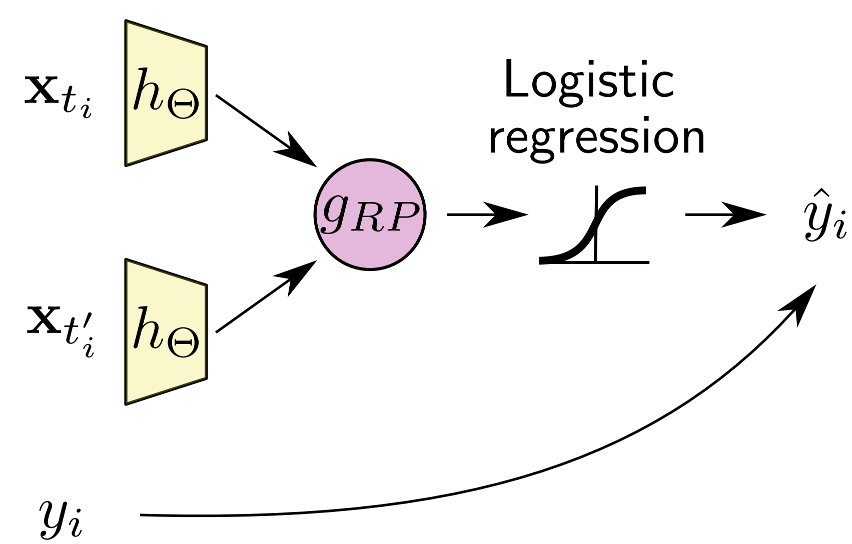
Relative positioning (RP)

1 Sampling



$$y_i = \begin{cases} 1, & \text{if } |t_i - t_i'| \leq \tau_{pos} \\ \text{-}1, & \text{if } |t_i - t_i'| > \tau_{neg} \end{cases}$$

2 Training



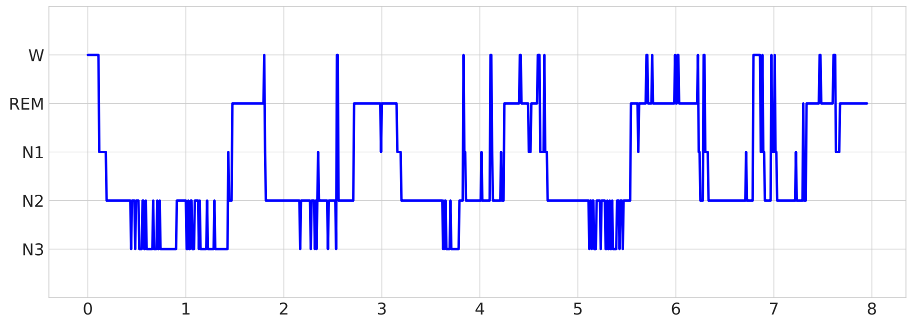
Predict if 2 windows of data are close in time

Related to PCL [Hyvärinen et al. 2017]

Downstream tasks on clinical EEG

Sleep staging:

Predict sleep stage from EEG (5-class: W, N1, N2, N3, R)



Hypnogram

- **Dataset:** Physionet Challenge 2018 (PC18) [Ghassemi et al. 2018]

Downstream tasks on clinical EEG

Sleep staging:

Predict sleep stage from EEG
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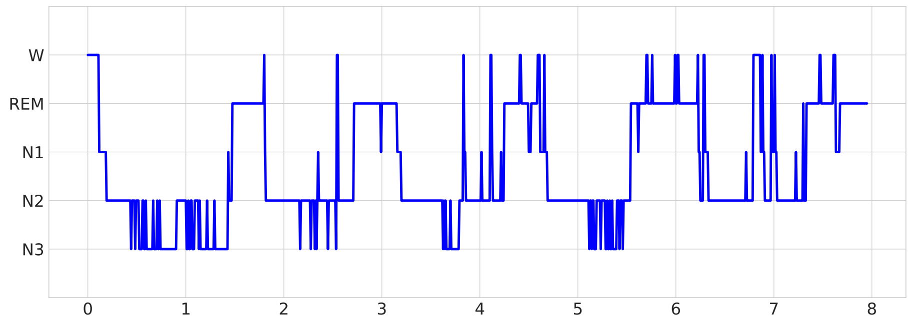


Hypnogram

- **Dataset:** Physionet Challenge 2018 (PC18) [Ghassemi et al. 2018]

Pathology detection:

Is someone's EEG pathological?
(2-class: normal, abnormal)

- **Dataset:** TUH Abnormal EEG (TUHab) [López 2017]

Datasets

Two public datasets with hundreds of recordings:

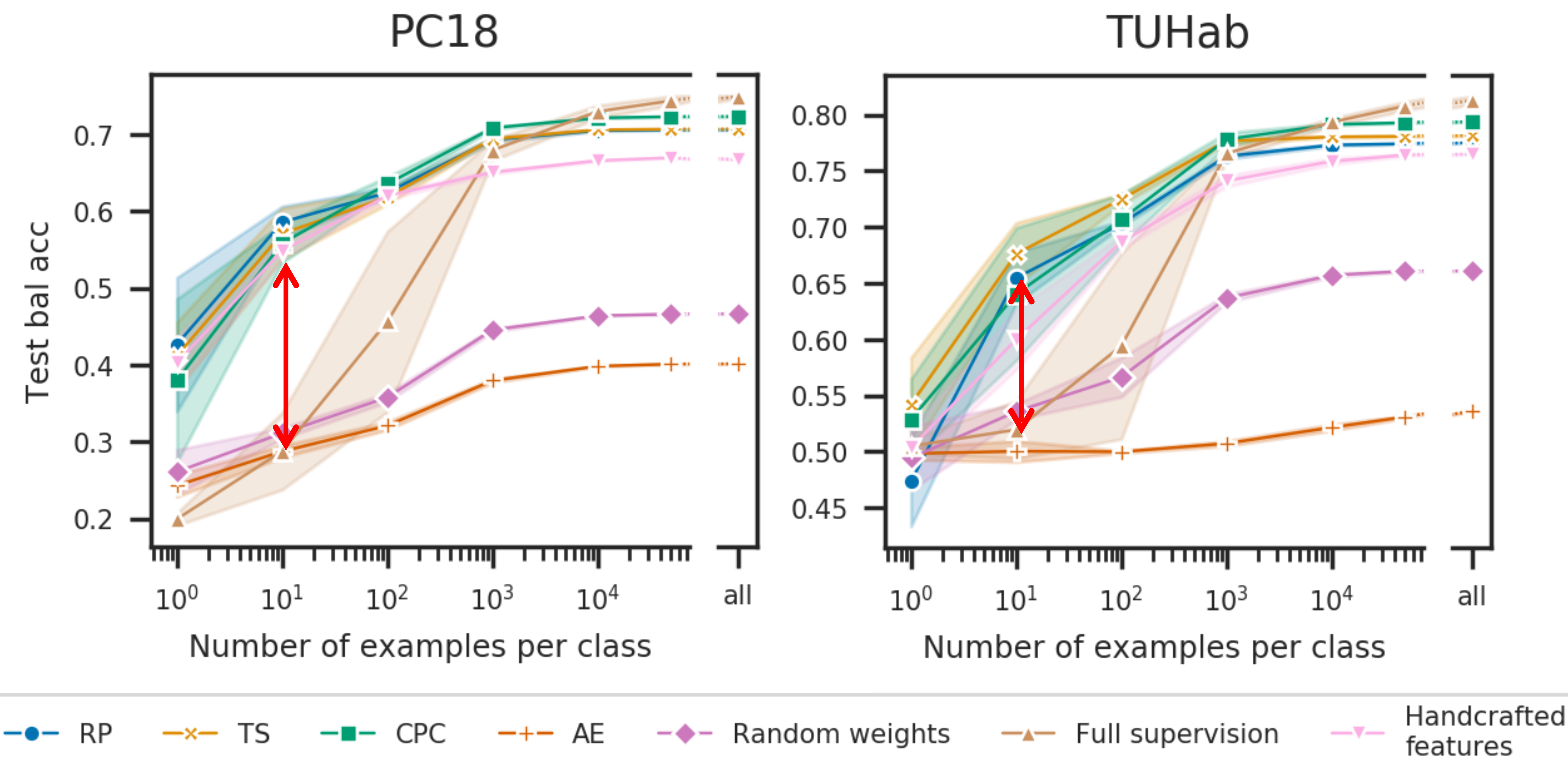
- **Sleep staging**: Physionet Challenge 2018 (PC18) [Ghassemi et al. 2018]
- **Pathology detection**: TUH Abnormal EEG (TUHab) [López 2017]

	PC18 (train)
	# windows
W	158,020
N1	136,858
N2	377,426
N3	102,492
R	116,872
Total	891,668
# unique subjects	994
# recordings	$\boxed{994}$
Sampling frequency	200 Hz
# EEG channels	6
Reference	M1 or M2

	TUHab (train)	TUHab (eval)
	# recordings	# recordings
Normal	1371	150
Abnormal	1346	126
Total	2717	276
# unique subjects	2329	
# recordings	$\boxed{2993}$	
Sampling frequency	250, 256, 512 Hz	
# EEG channels	27 to 36	
Reference	Common average	

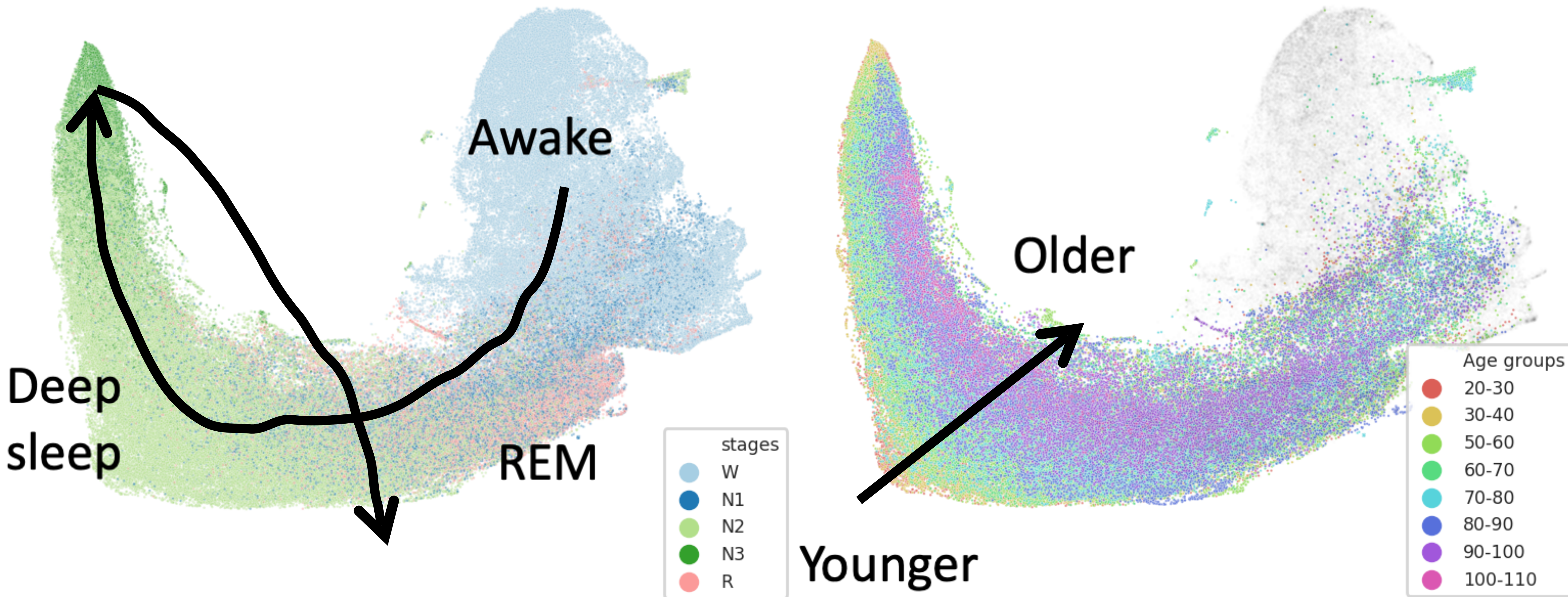
Results: Prediction accuracy

Using a CNN (2 conv/relu/mp) layers described in [Chambon et al. 2017]



SSL is **better than full supervision** when limited data is available, and **competitive** when all data is available.

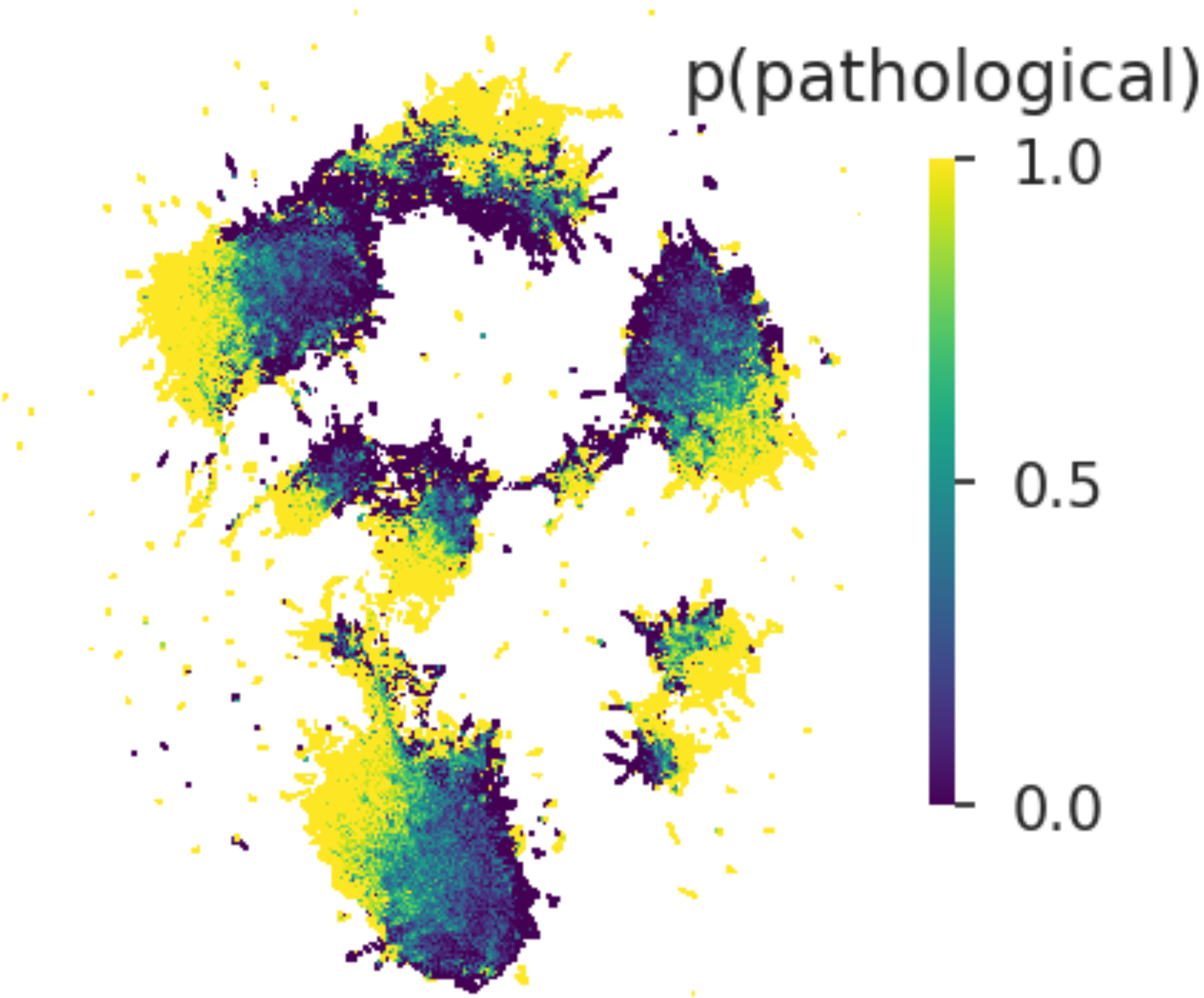
Results on sleep EEG

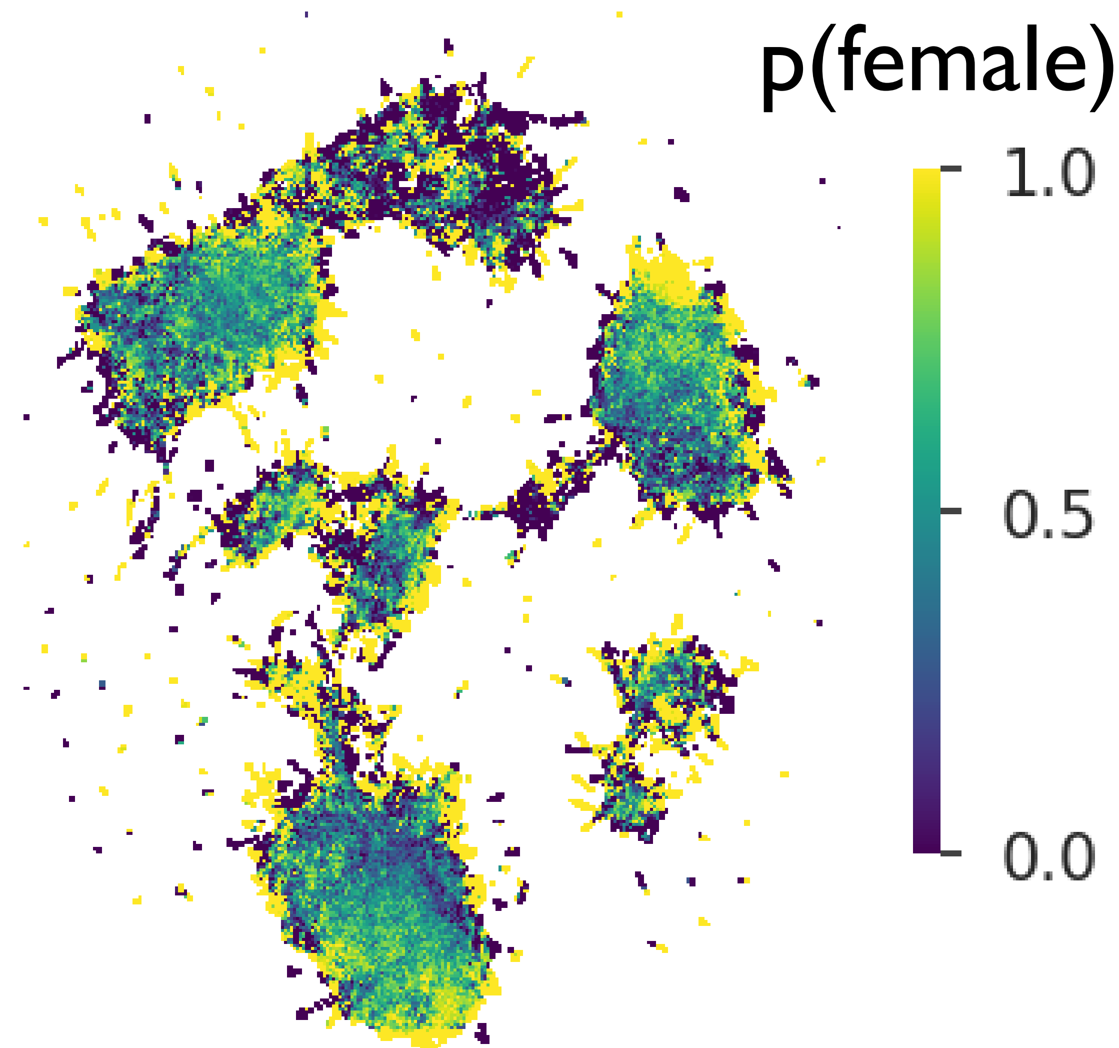


SSL can **uncover structure** without human supervision

[Banville et al. MLSP 2019]

Results on TUH data





SSL can **uncover clinically-relevant structure**
without human supervision


"All models are wrong but some come with good open source implementation and good documentation so use those."

Home Installation Documentation Examples

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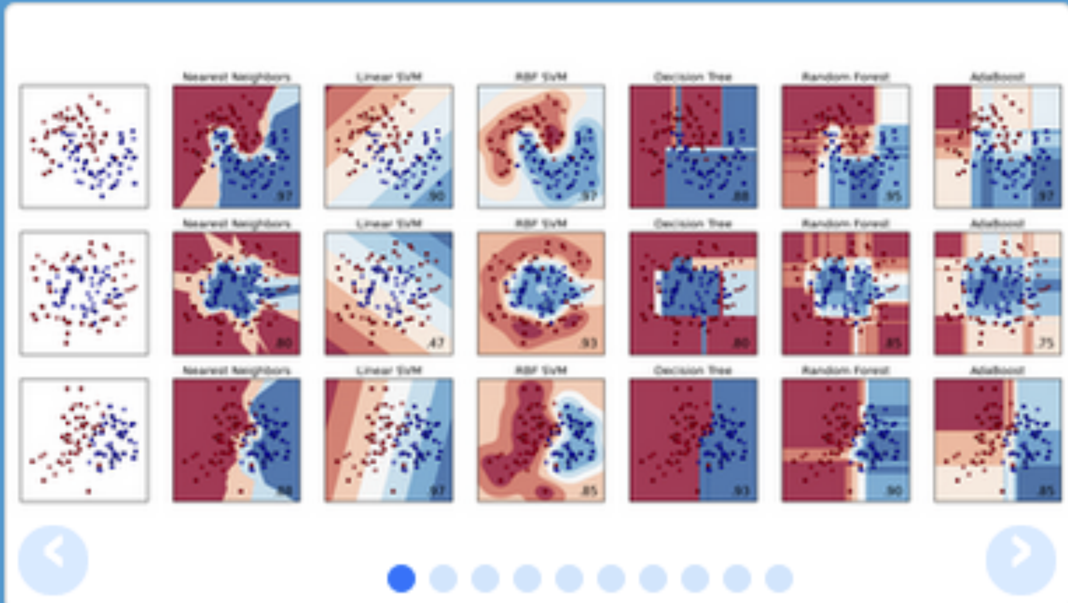


scikit-learn

Machine Learning in Python

- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

Classification

Identifying to which category an object belongs to.

Applications: Spam detection, Image recognition.
Algorithms: *SVM*, *nearest neighbors*, *random forest*, ... — *Examples*

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, Stock prices.
Algorithms: *SVR*, *ridge regression*, *Lasso*, ... — *Examples*

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: *k-Means*, *spectral clustering*, *mean-shift*, ... — *Examples*

Dimensionality reduction

Reducing the number of random variables to consider.

Applications: Visualization, Increased efficiency
Algorithms: *PCA*, *feature selection*, *non-*

Model selection

Comparing, validating and choosing parameters and models.

Goal: Improved accuracy via parameter tuning
Modules: *grid search*, *cross validation*

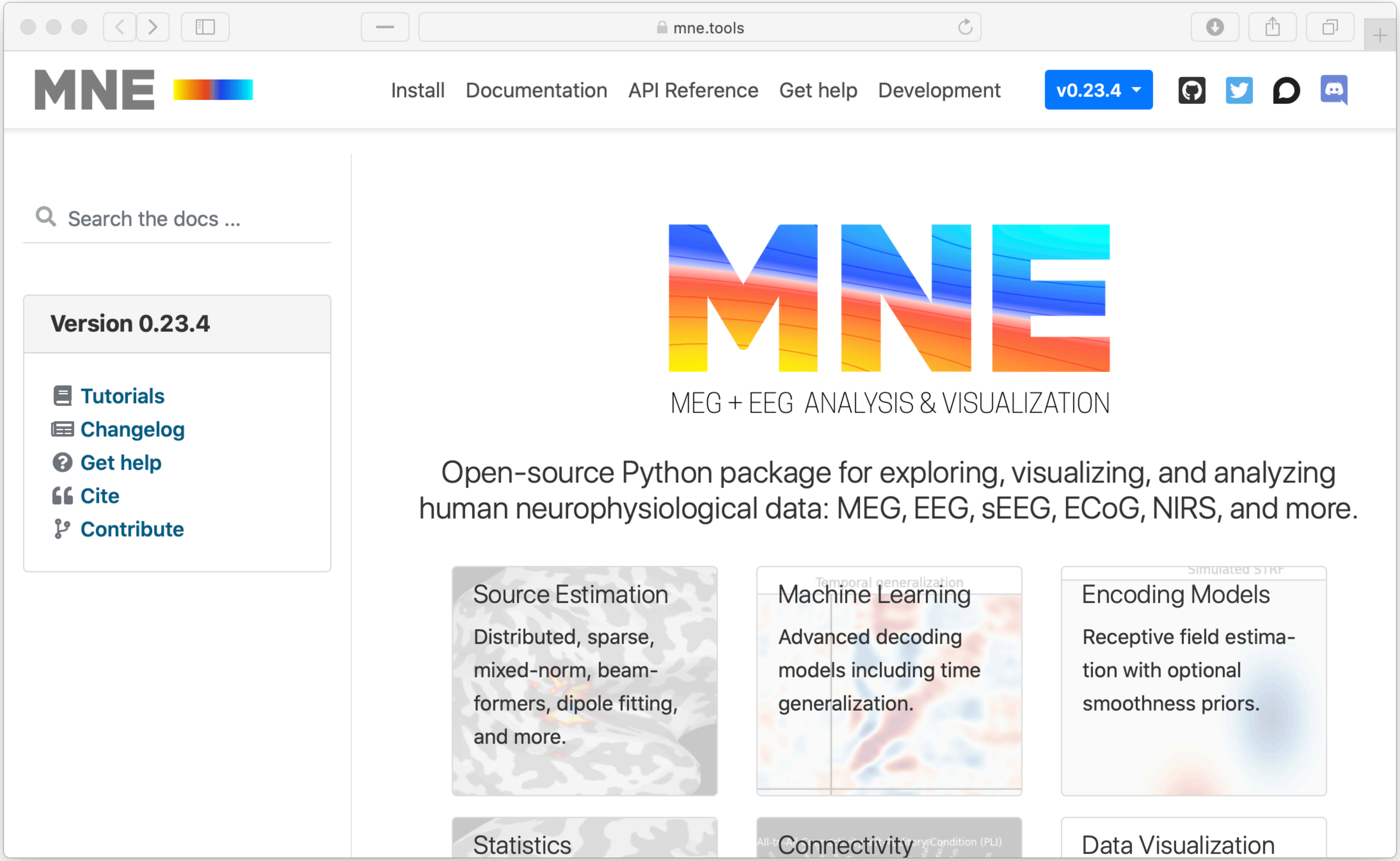
Preprocessing

Feature extraction and normalization.

Application: Transforming input data such as text for use with machine learning algorithms.
Modules: *preprocessing*, *feature extraction*.

http://scikit-learn.org

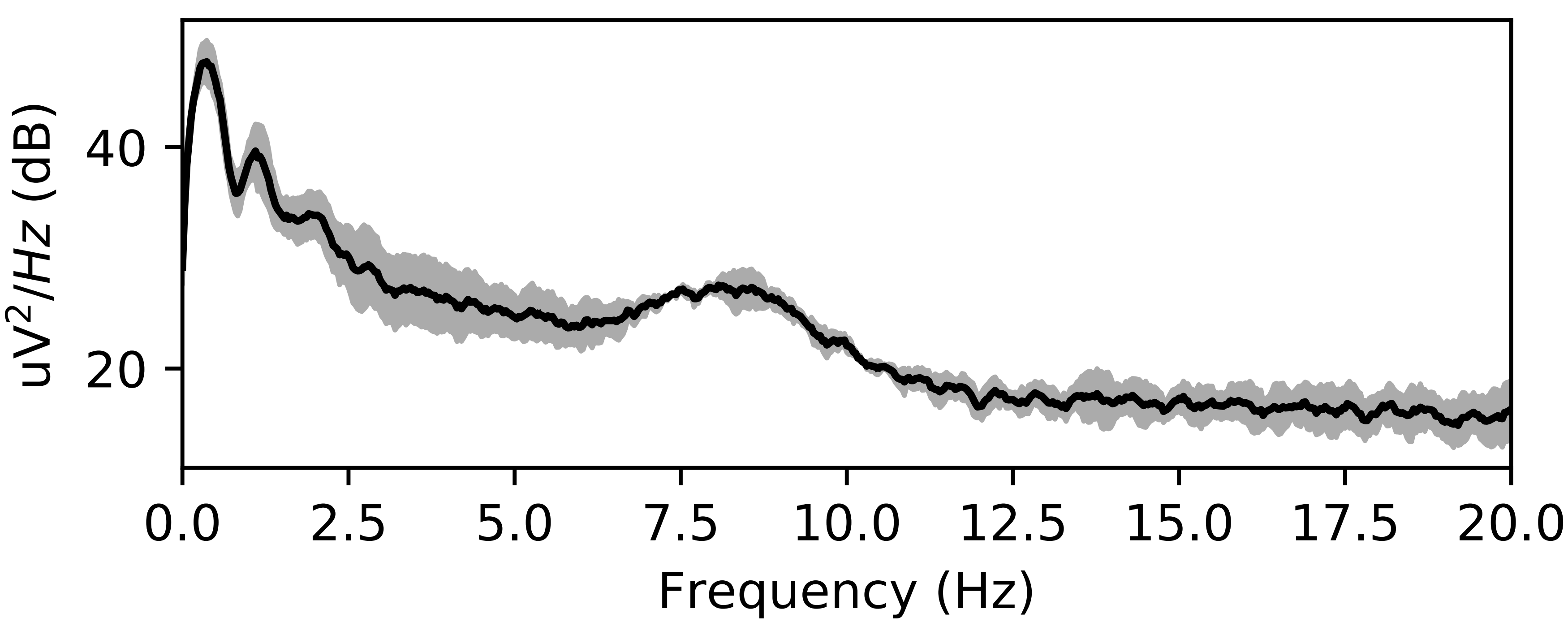
http://mne.tools



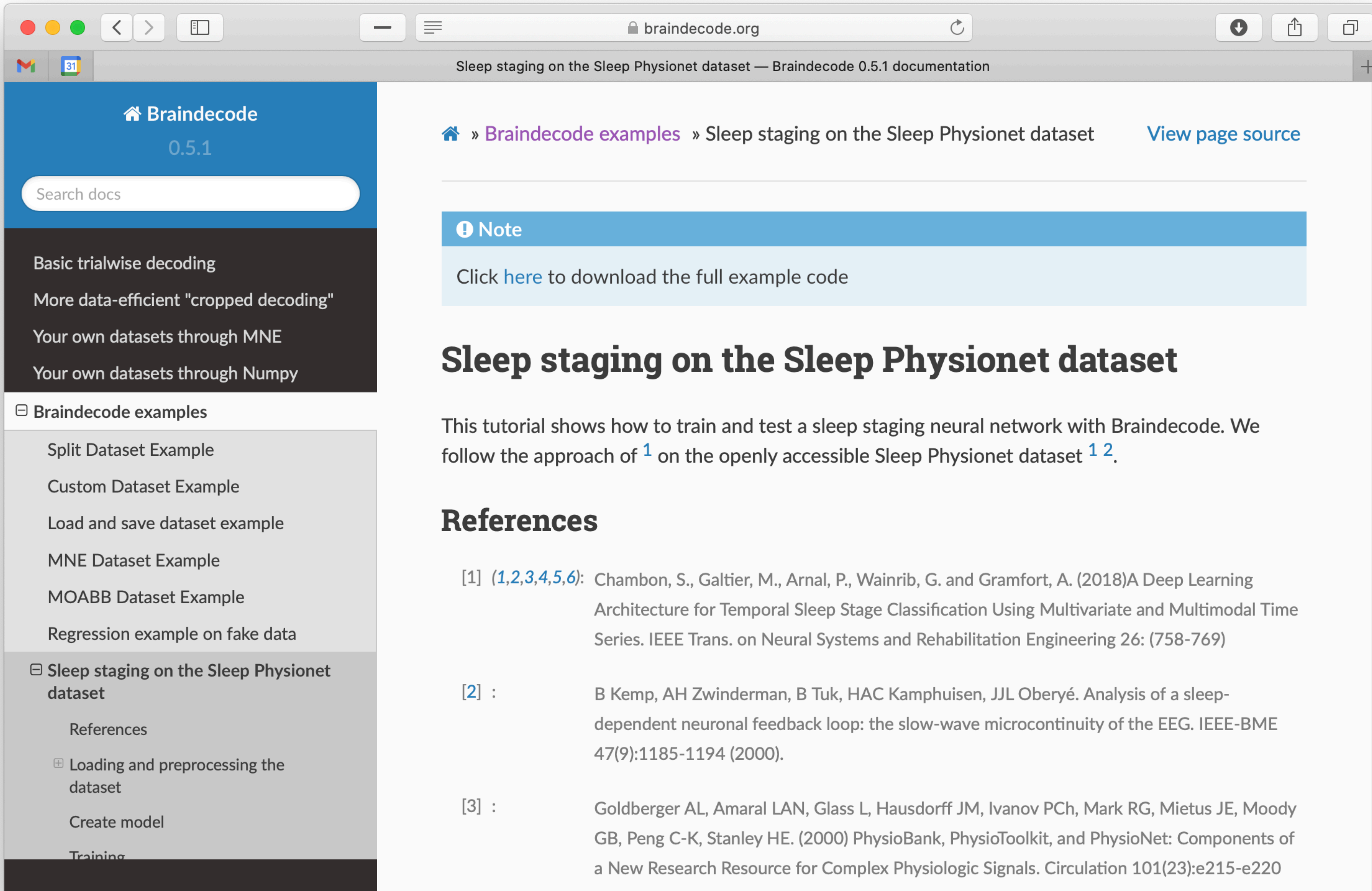
MEG + EEG ANALYSIS & VISUALIZATION

Working with EEG sleep data in 7 lines of Python code

```
>>> import mne
>>> raw = mne.io.read_raw_edf('SC4001E0-PSG.edf')
>>> annot = mne.read_annotations('SC4001EC-Hypnogram.edf')
>>> raw.set_annotations(annot)
>>> events, event_id = mne.events_from_annotations(raw)
>>> epochs = mne.Epochs(raw, events, event_id, tmin=0.,
                        tmax=30., baseline=None)
>>> epochs['Sleep stage W’].plot_psd(fmax=20., picks=[0, 1])
```



https://mne.tools/stable/auto_tutorials/clinical/60_sleep.html https://braindecode.org



https://braindecode.org

braindecode.org

Self-supervised learning on EEG with relative positioning — Braindecode 0.5.1 documentation

Note

Click here to download the full example code

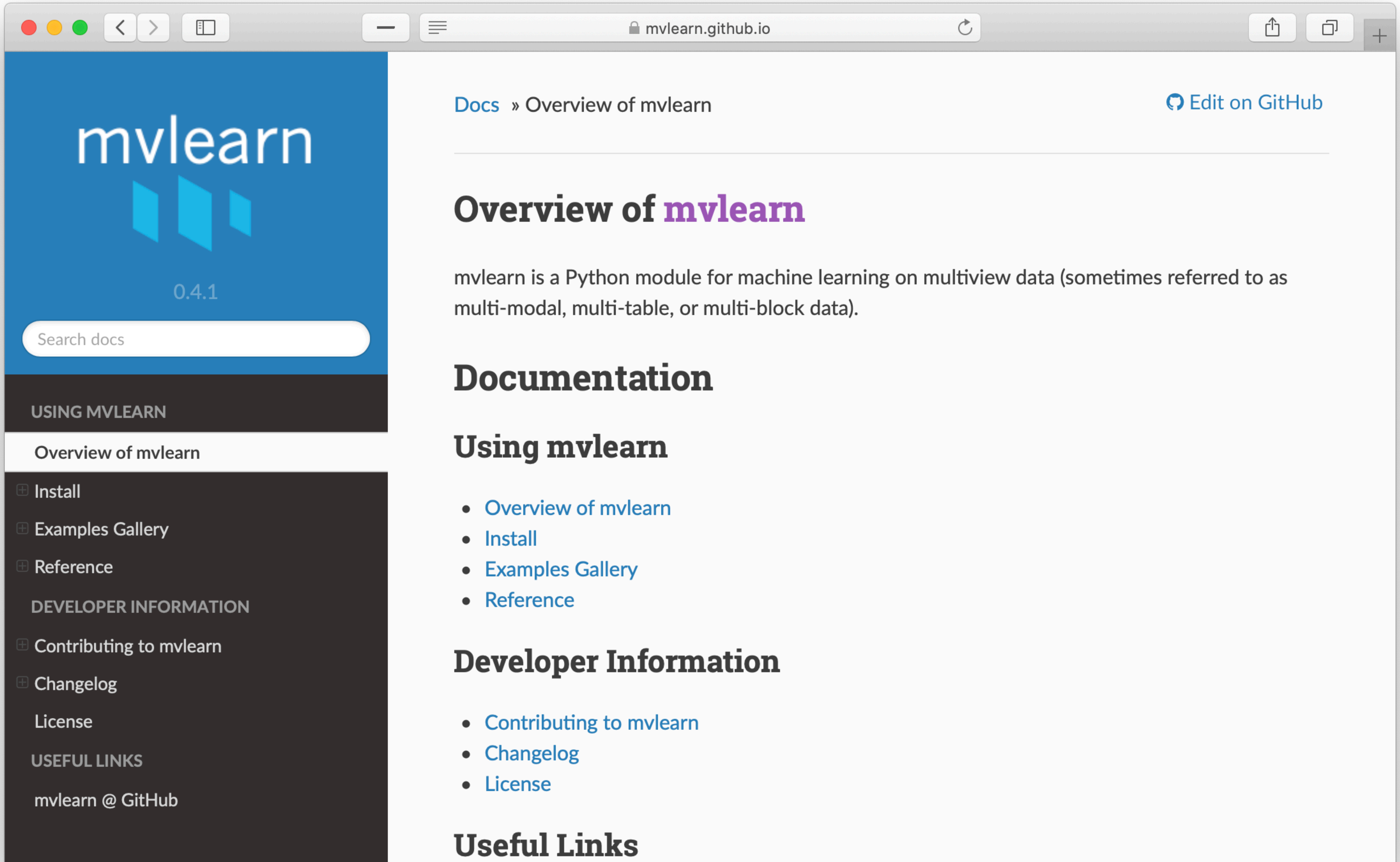
Self-supervised learning on EEG with relative positioning

This example shows how to train a neural network with self-supervision on sleep EEG data. We follow the relative positioning approach of [1] on the openly accessible Sleep Physionet dataset [2] [3].

Self-supervised learning

Self-supervised learning (SSL) is a learning paradigm that leverages unlabelled data to train neural networks. First, neural networks are trained on a “pretext task” which uses unlabelled data only. The pretext task is designed based on a prior understanding of the data under study (e.g., EEG has an underlying autocorrelation struture) and such that the processing required to perform well on this pretext task is related to the processing required to perform well on another task of interest. Once trained, these neural networks can be reused as feature extractors or weight initialization in a “downstream task”, which is the task that we are actually interested in (e.g., sleep staging). The pretext task step can help reduce the quantity of labelled data needed to perform well on the downstream task and/or improve downstream performance as compared to a strictly supervised

https://mvlearn.github.io



[Perry, Ronan, et al. "mvlearn: Multiview Machine Learning in Python." Journal of Machine Learning Research 22.109 (2021): 1-7.]

Thanks !

P. Ablin, J-F Cardoso, A. Gramfort (2017), Faster independent component analysis by preconditioning with Hessian approximations, IEEE Trans. Sig. Proc.

Richard, H., Gresele, L., Hyvärinen, A., Thirion, B., Gramfort, A., Ablin, P. (2020), Modeling Shared Responses in Neuroimaging Studies through MultiView ICA, Proc. NeurIPS

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Banville, H., Chehab, O., Hyvärinen, A., Engemann, D. and Gramfort, A. (2020), Uncovering the structure of clinical EEG signals with self-supervised learning, J. Neural Engineering

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Support

ERC SLAB, ANR-14-NEUC-0002-01
NIH R01 MH106174, ANR AI Chaire BrAIN, ANR AI-Cog