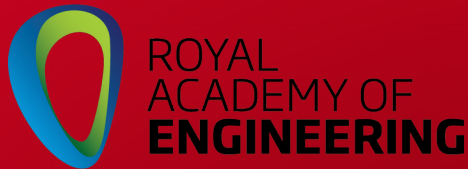


DE LA RECHERCHE À L'INDUSTRIE



Campus Paris Saclay
FONDATION DE COOPÉRATION SCIENTIFIQUE



fMRI BOLD signal decomposition using a multivariate low-rank model

Hamza Cherkaoui, *CEA Saclay, Univ. Paris-Saclay, 91191 Gif-sur Yvette, France*

Thomas Moreau, *Parietal Team, INRIA Saclay, Université Paris-Saclay, Saclay, France*

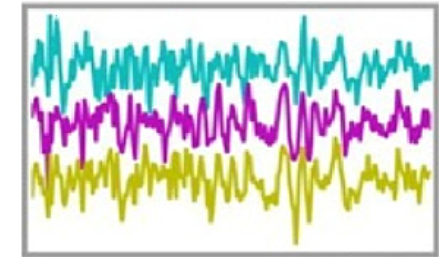
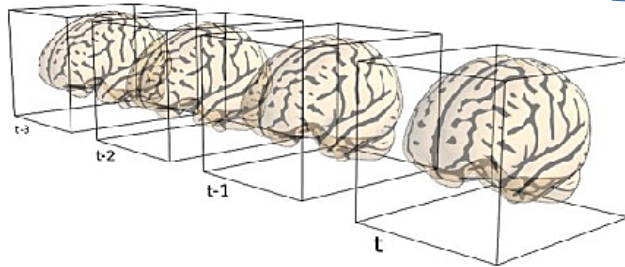
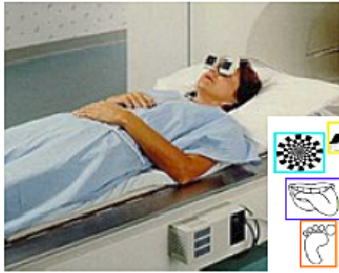
Abderrahim Halimi, *School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh UK*

Philippe Ciuciu, *CEA Saclay, Univ. Paris-Saclay, 91191 Gif-sur Yvette, France*

FUNCTIONAL MAGNETIC RESONANCE IMAGING

fMRI acquisition:

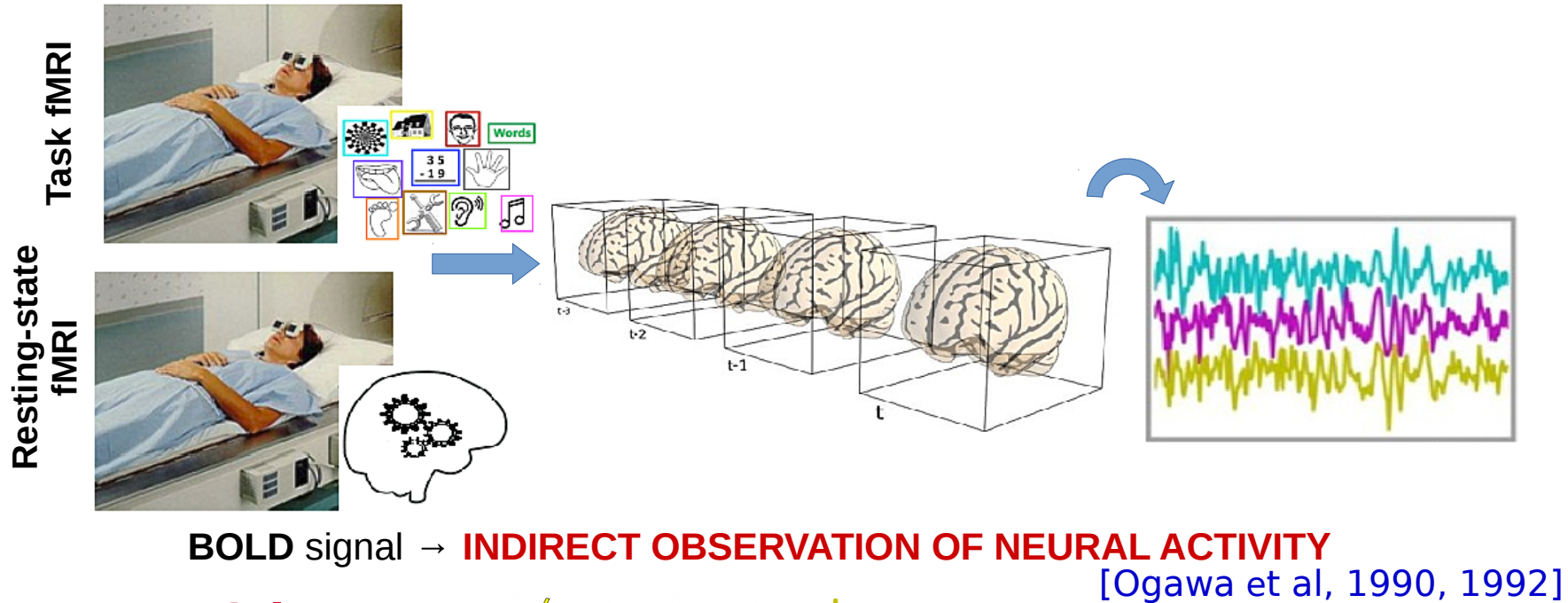
Task fMRI
Resting-state fMRI



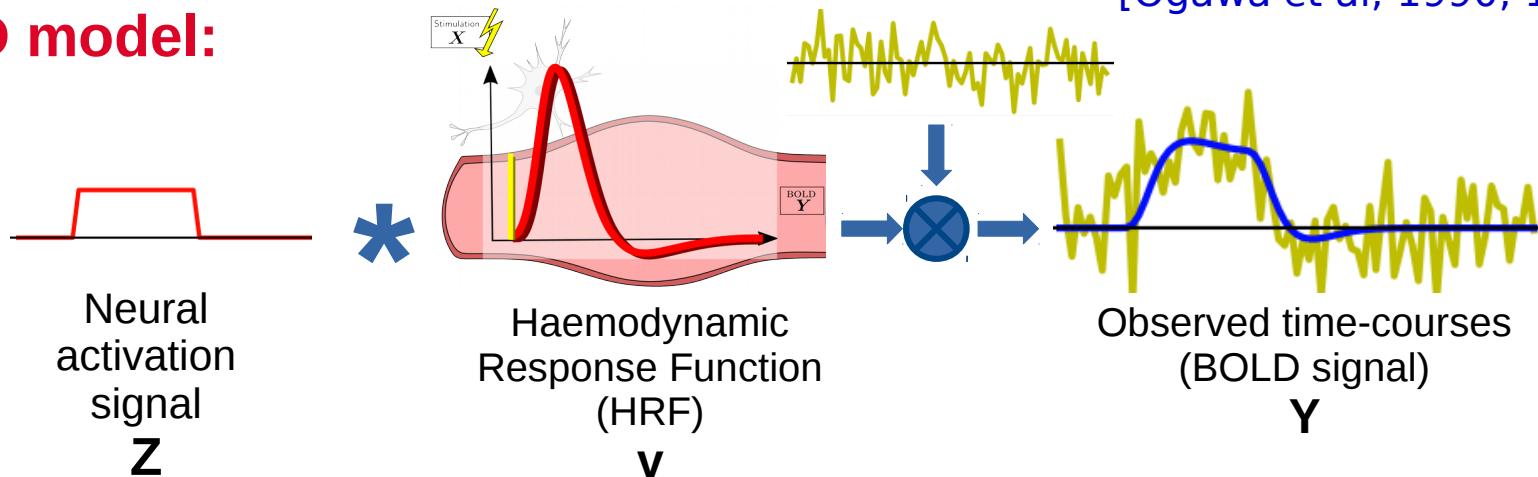
BOLD signal → INDIRECT OBSERVATION OF NEURAL ACTIVITY

[Ogawa et al, 1990, 1992]

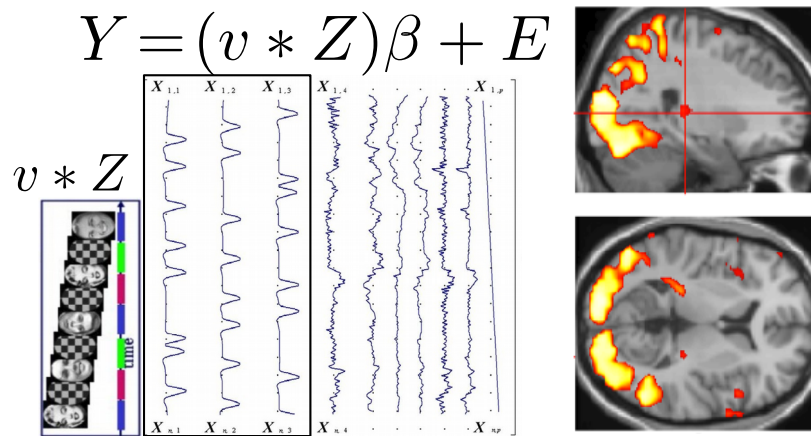
fMRI acquisition:



BOLD model:

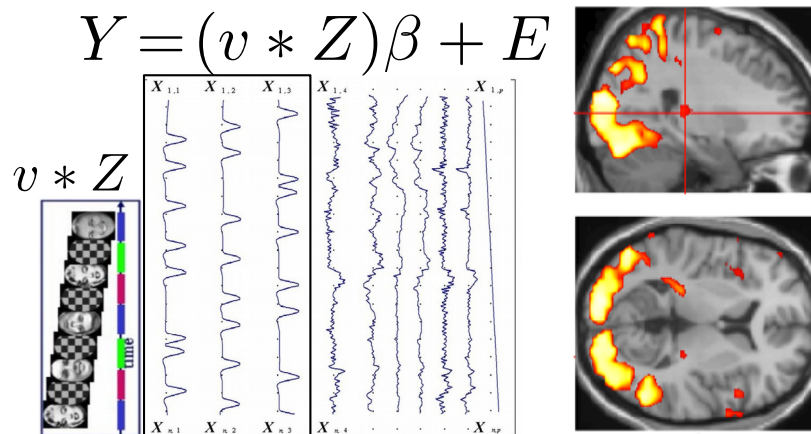


Task fMRI:



[Poldrack et al, Handbook of Functional MRI Data Analysis, 2013]

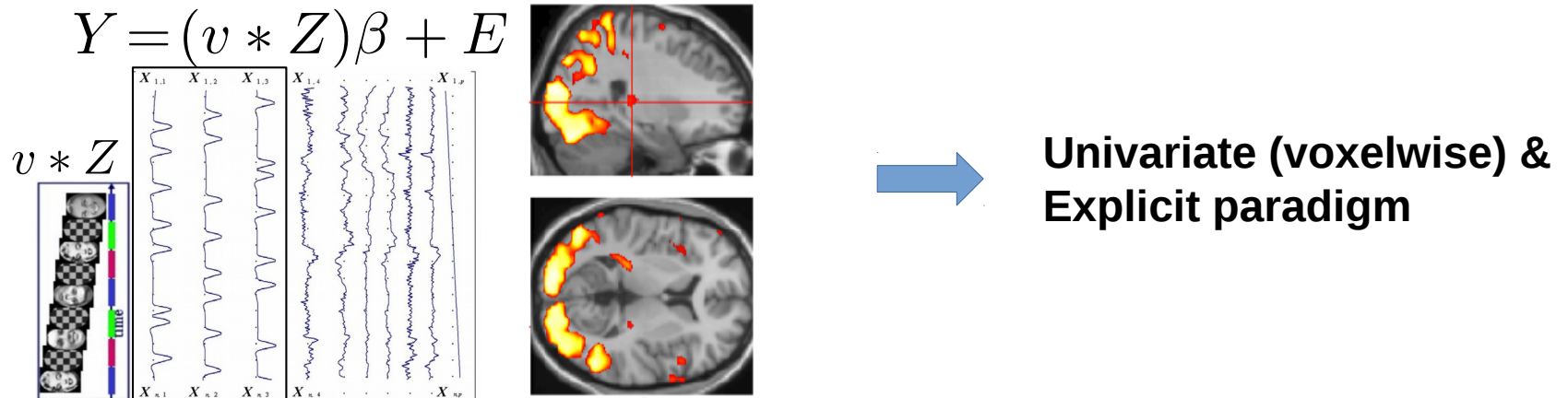
Task fMRI:



**Univariate (voxelwise) &
Explicit paradigm**

[Poldrack et al, Handbook of Functional
MRI Data Analysis, 2013]

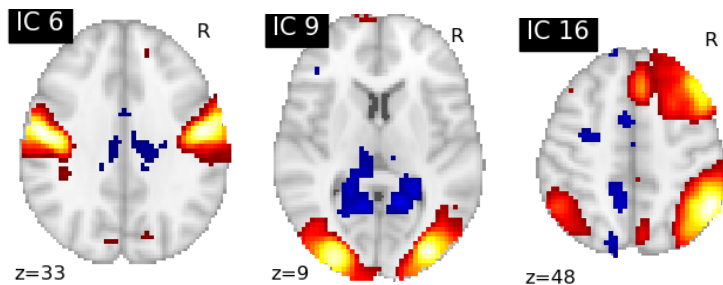
Task fMRI:



Univariate (voxelwise) & Explicit paradigm

[Poldrack et al, Handbook of Functional MRI Data Analysis, 2013]

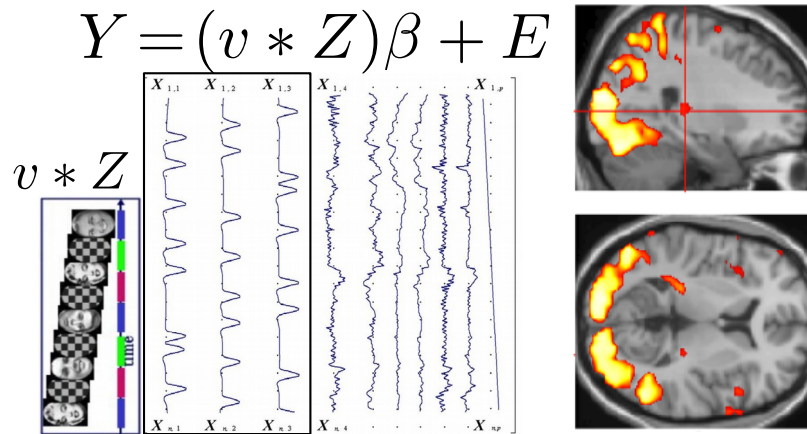
Resting-state fMRI:



3 independent components of the ICA on resting-state data (ADHD dataset)

[Varoquaux et al, 2009]

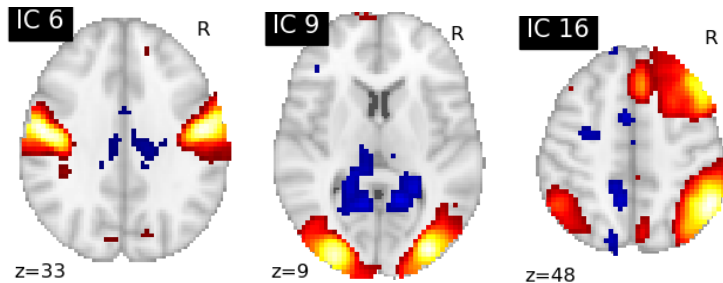
Task fMRI:



Univariate (voxelwise) & Explicit paradigm

[Poldrack et al, Handbook of Functional MRI Data Analysis, 2013]

Resting-state fMRI:



3 independent components of the ICA on resting-state data (ADHD dataset)

[Varoquaux et al, 2009]



Multivariate & Paradigm free

Our objective:

- Develop a multivariate deconvolution approach for functional connectivity analysis of **neural activation** signals
 - Accommodate both task and rs-fMRI data
- Multivariate extension of the 'Total Activation' framework [[Karahanoğlu et al, 2013](#)]

OBSERVATION MODEL OF THE BOLD DATA

Model: multivariate approach (temporal components and corresponding spatial maps) with predefined HRF

$$Y = \sum_{k=1}^K u_k^\top (v * z_k) + E$$

P number of voxels

L HRF length

T number of scans

$\tilde{T} = T - L + 1$ the number of time points in the temporal atoms

K the number of atoms (model rank)

E additive Gaussian noise

Parameters to estimate: z_k, u_k

OBSERVATION MODEL OF THE BOLD DATA

Model: multivariate approach (temporal components and corresponding spatial maps) with predefined HRF

$$Y = \sum_{k=1}^K u_k \top (v * z_k) + E$$

P number of voxels

L HRF length

T number of scans

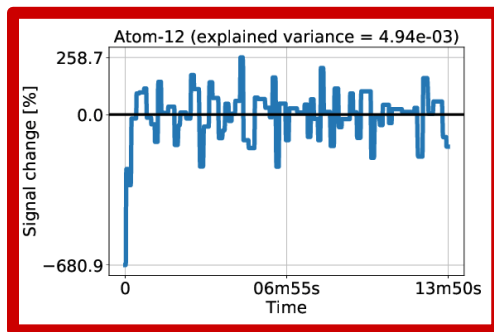
$\tilde{T} = T - L + 1$ the number of time points in the temporal atoms

K the number of atoms (model rank)

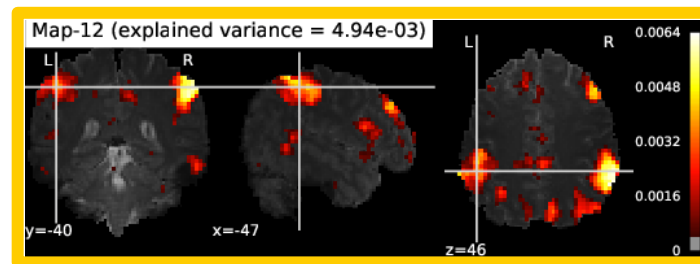
E additive Gaussian noise

Parameters to estimate: z_k, u_k

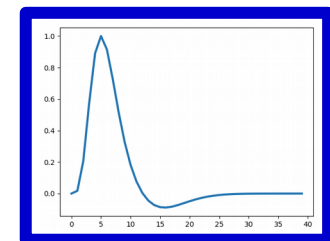
z_k



u_k



v



[Friston et al, 2000]

Spatio-temporal constrained optimization problem:

$$J((\mathbf{u}_k)_k, (\mathbf{z}_k)_k) = \frac{1}{2} \left\| Y - \sum_{k=1}^K \mathbf{u}_k^\top (v * \mathbf{z}_k) \right\|_F^2 + \lambda \sum_{k=1}^K \|D\mathbf{z}_k\|_1$$

subject to $\|\mathbf{u}_k\|_1 = \eta$ and $u_{jk} \geq 0$ (1)

- **Data fidelity term:**

- The Gaussian noise leads to a quadratic loss

- **Temporal components:**

- TV regularization: promote sparsity of the 1st order derivative [Karahanoglu et al, 2013]

- **Spatial constraints:**

- Positivity of each entry in each spatial map to avoid sign ambiguity with the corresponding temporal component

- L1 norm of each spatial map fixed to a certain level to avoid any scale ambiguity

Spatio-temporal constrained optimization problem:

$$J((\mathbf{u}_k)_k, (\mathbf{z}_k)_k) = \frac{1}{2} \left\| Y - \sum_{k=1}^K \mathbf{u}_k^\top (v * \mathbf{z}_k) \right\|_F^2 + \lambda \sum_{k=1}^K \|D\mathbf{z}_k\|_1$$

subject to $\|\mathbf{u}_k\|_1 = \eta$ and $u_{jk} \geq 0$ (1)

- **Strategy of minimization:**

- The global cost function is bi-convex in $(\mathbf{z}_k, \mathbf{u}_k)$: Each sub-problem is convex
- We propose to alternate the minimization between the \mathbf{z}_k and the \mathbf{u}_k .
- The \mathbf{z}_k are initialized to zero and \mathbf{u}_k to a truncated Gaussian random vector (to ensure positive values for \mathbf{u}_k)

Minimization of the cost-function: different possible approaches

- z_k estimation step:

$$J_z((z_k)_k) = \frac{1}{2} \left\| Y - \sum_{k=1}^K u_k^\top (v * z_k) \right\|_F^2 + \lambda \sum_{k=1}^K \|Dz_k\|_1$$

Analysis formulation

ISTA [Daubechies et al. 2004]

FISTA [Beck, Teboulle, 2009]

Restarting-FISTA [Liang et al, 2013]

Greedy FISTA [Liang et al, 2013]

Condat-Vu [Condat, 2016]

Minimization of the cost-function: different possible approaches

- \mathbf{z}_k estimation step:

$$J_z((z_k)_k) = \frac{1}{2} \left\| Y - \sum_{k=1}^K u_k^\top (v * z_k) \right\|_F^2 + \lambda \sum_{k=1}^K \|D z_k\|_1$$

Analysis formulation

ISTA [Daubechies et al. 2004]

FISTA [Beck, Teboulle, 2009]

Restarting-FISTA [Liang et al, 2013]

Greedy FISTA [Liang et al, 2013]

Condat-Vu [Condat, 2016]

$$J'_z((z_k)_k) = \frac{1}{2} \left\| Y - \sum_{k=1}^K u_k^\top (v * L z_k) \right\|_F^2 + \lambda \sum_{k=1}^K \|z_k\|_1$$

Synthesis formulation

ISTA [Daubechies et al. 2004]

FISTA [Beck, Teboulle, 2009]

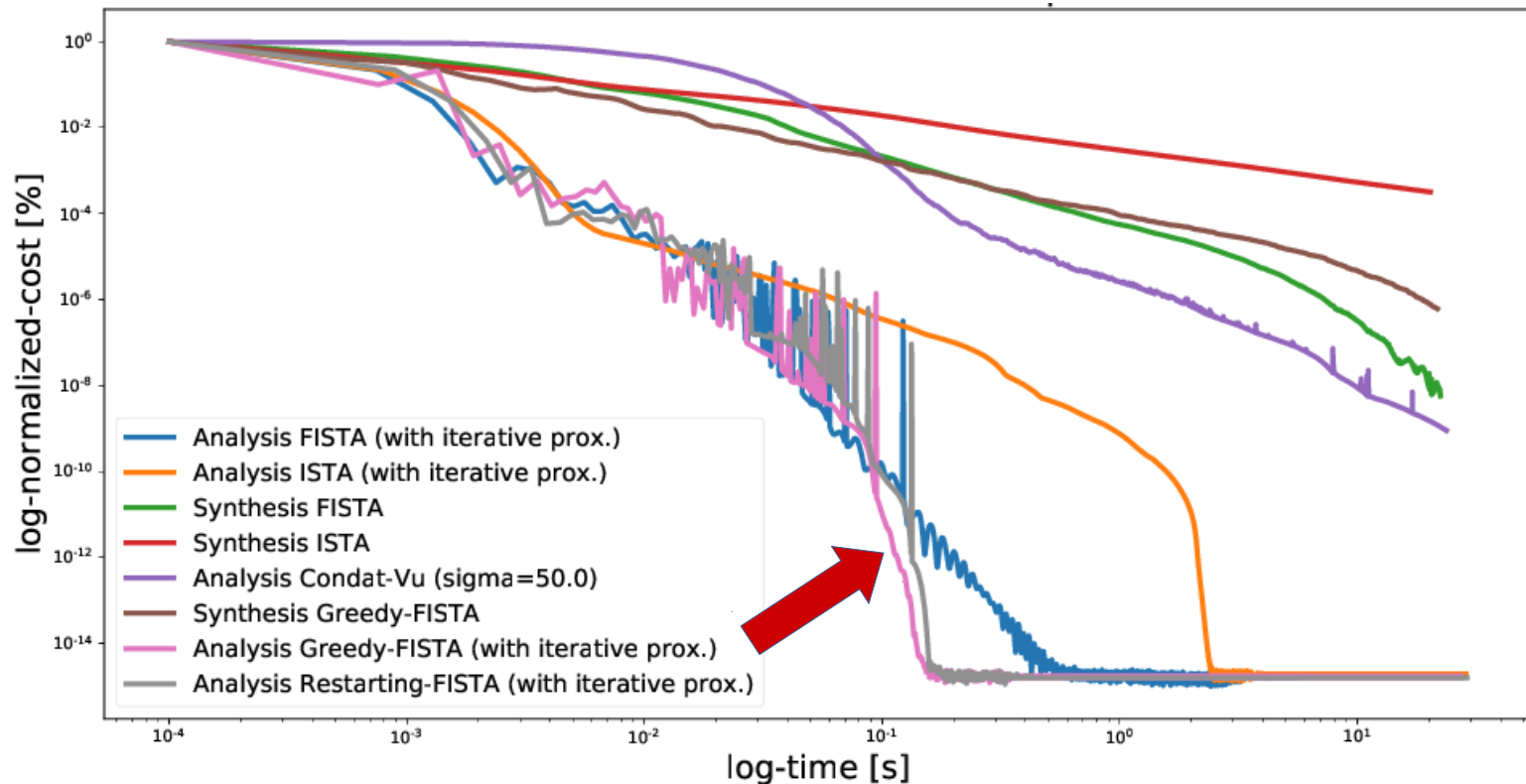
Restarting-FISTA [Liang et al, 2013]

Greedy FISTA [Liang et al, 2013]

CONVERGENCE RATE COMPARISON FOR THE RECOVERY OF NEURAL ACTIVATION SIGNALS

Convergence rate comparison:

Convergence rate comparison for the temporal components estimation problem



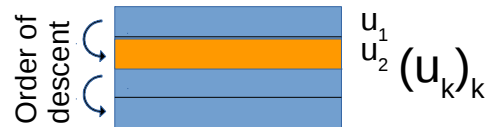
Minimization of the cost-function: different possible approaches

- u_k estimation step:

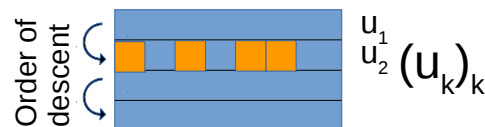
$$\begin{aligned}
 J_u((u_k)_k) &= \frac{1}{2} \left\| Y - \sum_{k=1}^K u_k^\top (v * z_k) \right\|_F^2 \\
 \text{subject to } & \|u_k\|_1 = \eta \quad \text{and} \quad u_{jk} \geq 0
 \end{aligned} \tag{1}$$

ISTA, FISTA, Greedy FISTA: (cf. previous slide)

Mairal: coordinate descent with optimal step-size in the context of online learning [Mairal et al, 2009]



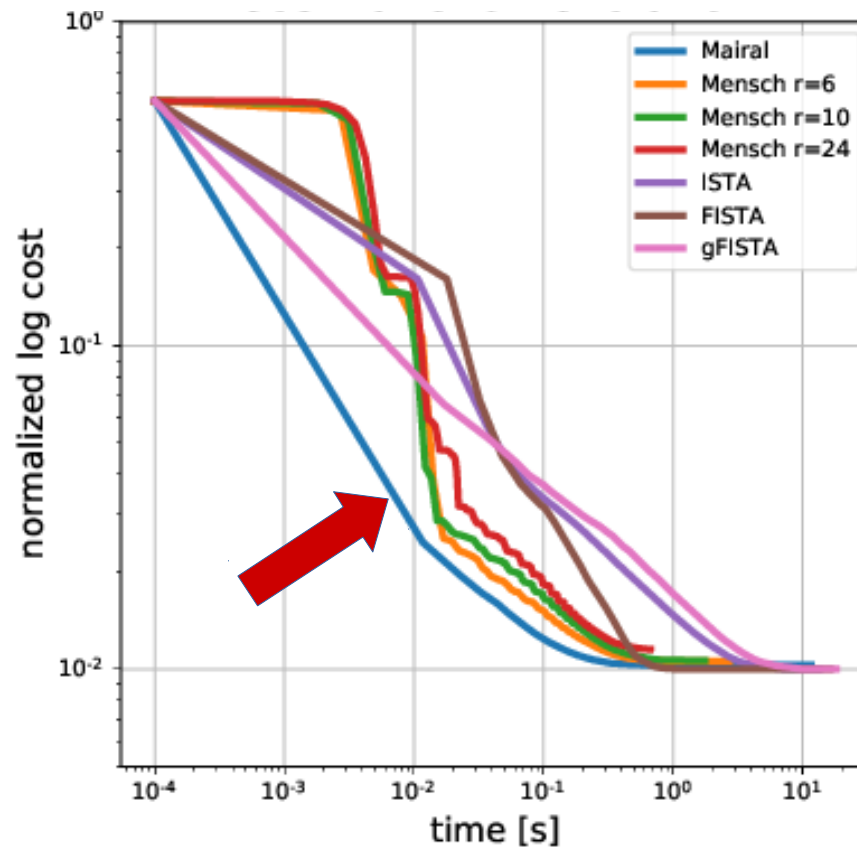
Mensch: based on Mairal's algorithm with a subsampling along a dimension of the problem [Mensch et al, 2016]



CONVERGENCE RATE COMPARISON FOR THE RECOVERY OF SPATIAL ACTIVATION MAPS

Convergence rate comparison:

Convergence rate comparison
for the spatial maps estimation
problem



The final algorithm:

Algorithm 1: Low rank decomposition of the BOLD signal.

Input: BOLD signal \mathbf{Y} , ϵ

1 initialization: $\mathbf{z}_k^{(0)} = \mathbf{0}_{\tilde{T}}$, $\mathbf{u}_k^{(0)} = \mathbf{u}_k^{(init)}$, $i = 1$;

2 repeat

3 Estimate the temporal atoms $\mathbf{z}_k^{(i)}$ with fixed $\mathbf{u}_k^{(i-1)}$:

$$\arg \min_{(\mathbf{z}_k)_k} \frac{1}{2} \left\| \mathbf{Y} - \sum_{k=1}^K \mathbf{u}_k^{(i-1)\top} (v * \mathbf{z}_k) \right\|_F^2 + \lambda \sum_{k=1}^K \|\mathbf{D} \mathbf{z}_k\|_1$$

4 Estimate the spatial maps $\mathbf{u}_k^{(i)}$ with fixed $\mathbf{z}_k^{(i)}$:

$$\arg \min_{(\mathbf{u}_k)_k} \frac{1}{2} \left\| \mathbf{Y} - \sum_{k=1}^K \mathbf{u}_k^\top (v * \mathbf{z}_k^{(i)}) \right\|_F^2$$

subject to $\|\mathbf{u}_k\|_1 = \eta$ and $u_{kj} \geq 0$

5 until $\frac{J((\mathbf{z}_k^{(i-1)})_k, (\mathbf{u}_k^{(i-1)})_k) - J((\mathbf{z}_k^{(i)})_k, (\mathbf{u}_k^{(i)})_k)}{J((\mathbf{z}_k^{(i-1)})_k, (\mathbf{u}_k^{(i-1)})_k)} \leq \epsilon$;

Restarting-FISTA

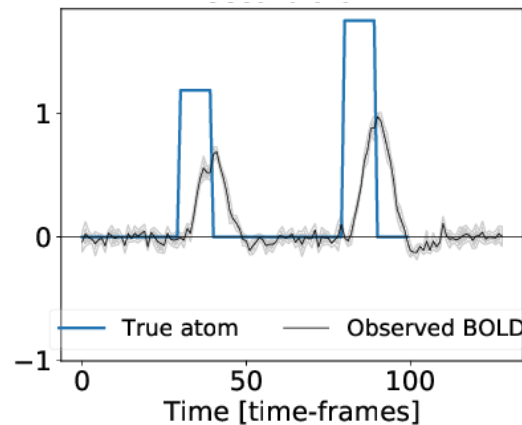
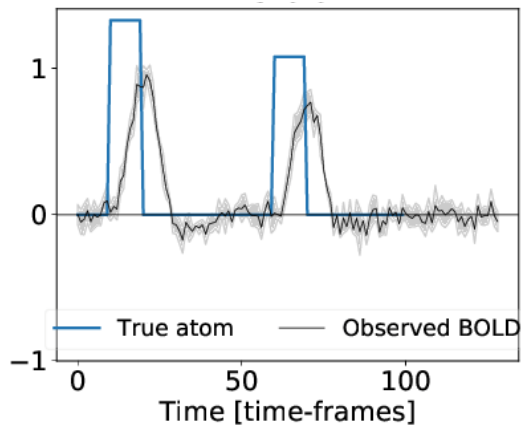
Mairal's algorithm

Simulated paradigm: two activation blocks

Data:

- $K_{\text{true}} = 2$
- $T = 100$
- $TR = 1.0\text{s}$
- $P = 100$
- Each true spatial maps contains a single square regions of 'activity'
- Signal-to-noise ratio: 0.1, 0.5, 1.0, 5.0, 10.0, 15.0, 20.0 dB $\text{SNR} = 10 \log_{10} \left(\frac{\|\sum_{k=1}^K u_k^\top (v * z_k)\|_2^2}{\|E\|_2^2} \right)$
- Each temporal component contains 2 blocks whose duration was fixed to 10 s and the magnitude was randomly drawn from a Gaussian distribution centred on 1.0.

z_{true}



u_{true}



In **yellow-purple** maps define the spatial ground truth

In **blue**, the true temporal atoms

In **black**, the observed BOLD signal (*here* SNR = 1.0 dB)

In **grey**, the standard deviation across voxels encoded by transparency around mean curves

Simulated paradigm: two activation blocks

Data:

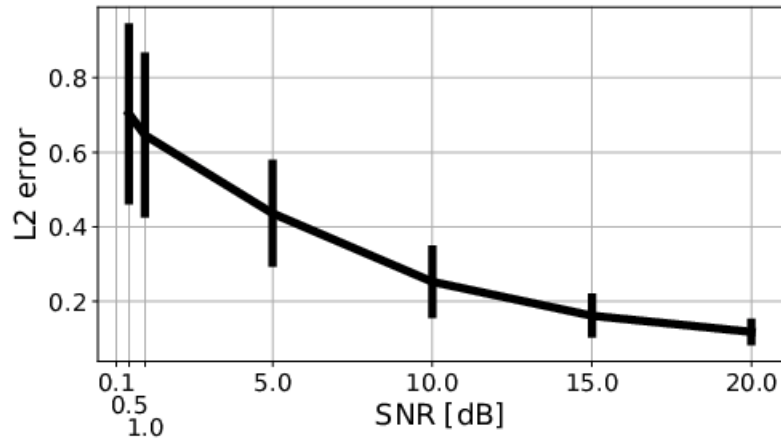
- $K_{\text{true}} = 2$
- $T = 100$
- $TR = 1.0\text{s}$
- $P = 100$
- Each true spatial maps contains a single square regions of 'activity'
- Signal-to-noise ratio: 0.1, 0.5, 1.0, 5.0, 10.0, 15.0, 20.0 dB $\text{SNR} = 10 \log_{10} \left(\frac{\|\sum_{k=1}^K u_k^\top (v * z_k)\|_2^2}{\|E\|_2^2} \right)$
- Each temporal component contains *2 blocks* whose duration was fixed to *10 s* and the magnitude was randomly drawn from a Gaussian distribution centred on 1.0.

Algorithm parameters for estimation:

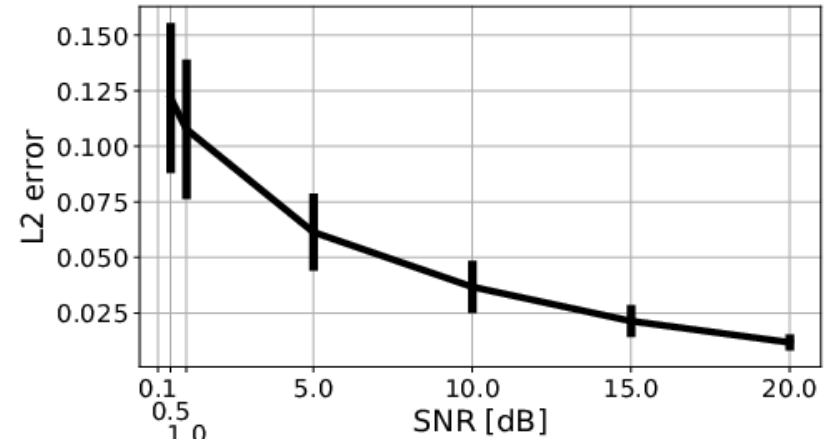
- $K = 2$
- $\eta = 10.0$
- $\lambda =$ grid-search for each SNR scenario
- Max-iteration = 30
- 3 initializations tested

Simulation: two activation blocks case

(z_k, u_k) Evolution of the estimation error



Evolution of the z_k -estimation error
w.r.t the SNR



Evolution of the u_k -estimation error
w.r.t the SNR

→ The estimation error decreases while the SNR increases

Motor task: Human Connectome Project (HCP) dataset

Data:

- HCP release: HCP-1200 [www.humanconnectome.org]
- Motor task fMRI data
- One subject (randomly chosen)
- ~3min30s of acquisition
- Spatial resolution: 2x2x2mm
- $P = 57790$
- $T = 284$
- $TR = 0.72s$

Motor task: Human Connectome Project (HCP) dataset

Data:

- HCP release: HCP-1200 [www.humanconnectome.org]
- Motor task fMRI data
- One subject (randomly chosen)
- ~3min30s of acquisition
- Spatial resolution: 2x2x2mm
- P = 57790
- T = 284
- TR = 0.72s

Motor task:

- Each condition were preceded by a *visual cue* of 3 s
- The motor tasks consisted of a sequence of *right/left hands clenching* and *right/left foot squeezing*
- Each condition lasted 12 s

Motor task: Human Connectome Project (HCP) dataset

Data:

- HCP release: HCP-1200 [www.humanconnectome.org]
- Motor task fMRI data
- One subject (randomly chosen)
- ~3min30s of acquisition
- Spatial resolution: 2x2x2mm
- $P = 57790$
- $T = 284$
- $TR = 0.72s$

Motor task:

- Each condition were preceded by a *visual cue* of 3 s
- The motor tasks consisted of a sequence of *right/left hands clenching* and *right/left foot squeezing*
- Each condition lasted 12 s

Decomposition parameters:

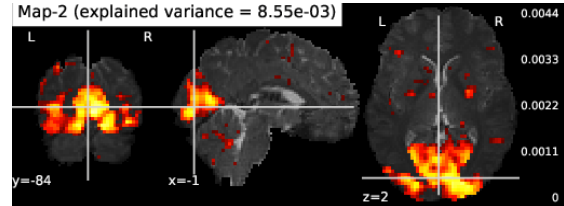
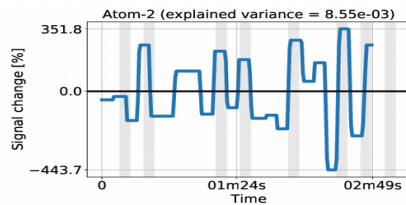
- $K = 40$
- $\eta = 10.0$
- $\lambda = 1.0e-2$
- Max-iteration = 30
- 3 initializations tested

Data were provided (in part) by the Human Connectome Project, WU-Minn Consortium (Principal Investigators: David Van Essen and Kamil Ugurbil; 1U54MH091657) funded by the 16 NIH Institutes and Centers that support the NIH Blueprint for Neuroscience Research; and by the McDonnell Center for Systems Neuroscience at Washington University.

Motor task: Human Connectome Project (HCP) dataset

Temporal activation 10%-thresholded spatial map

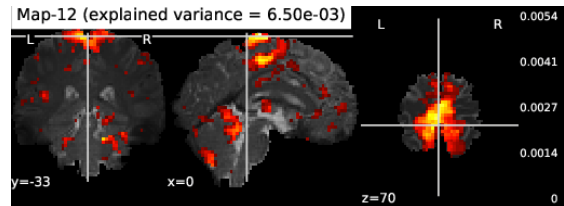
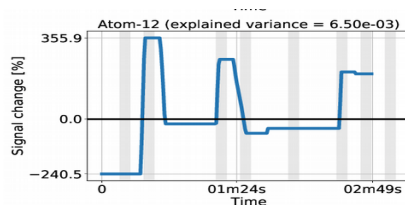
Component #2



Visual cortex

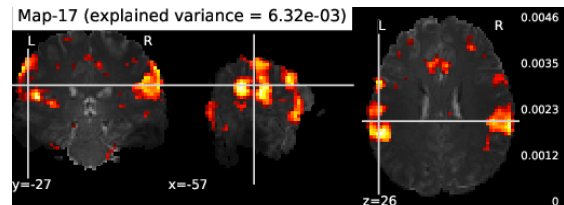
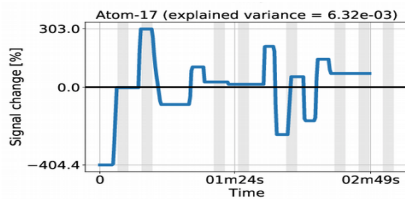
Each motor task was cued by a visual instruction

Component #12



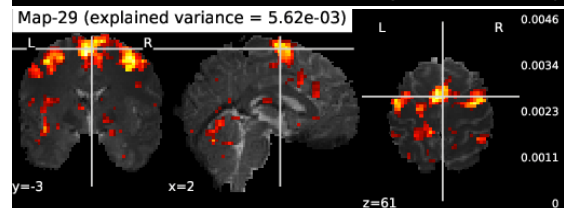
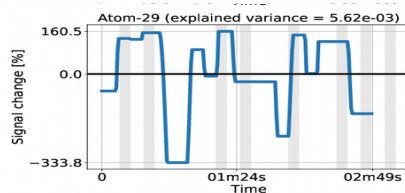
Primary somatosensory cortex

Component #17



Primary motor cortex

Component #29



Supplementary motor area

c.t = 33 min

Resting state: Human Connectome Project (HCP) dataset

Data:

- HCP release: HCP-1200 [www.humanconnectome.org]
- Resting-state fMRI data
- One subject (randomly chosen)
- ~14min of acquisition
- Spatial resolution: 2x2x2mm
- $P = 57790$
- $T = 1200$
- $TR = 0.72s$

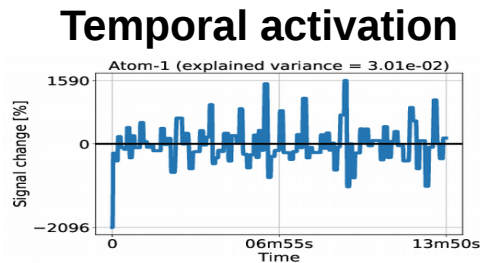
Decomposition parameters:

- $K = 10$
- $\eta = 10.0$
- $\lambda = 5.0e-3$
- Max-iteration = 30
- 3 initializations tested

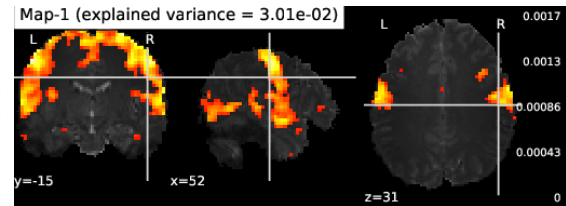
Data were provided (in part) by the Human Connectome Project, WU-Minn Consortium (Principal Investigators: David Van Essen and Kamil Ugurbil; 1U54MH091657) funded by the 16 NIH Institutes and Centers that support the NIH Blueprint for Neuroscience Research; and by the McDonnell Center for Systems Neuroscience at Washington University.

Resting state: Human Connectome Project (HCP) dataset

Component #1

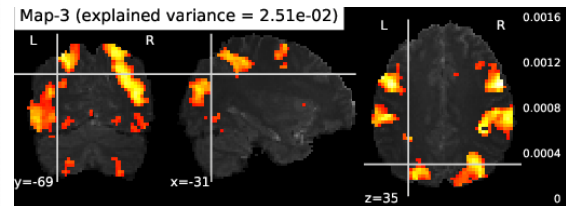
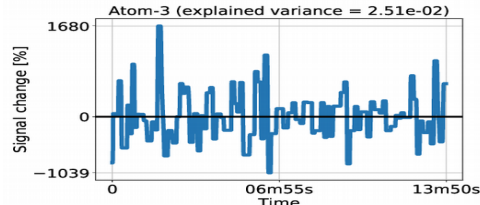


10%-thresholded spatial map



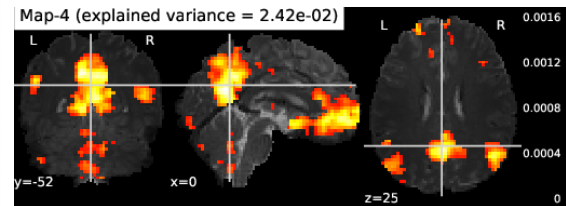
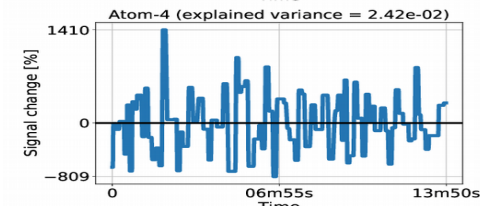
Motor cortex

Component #3



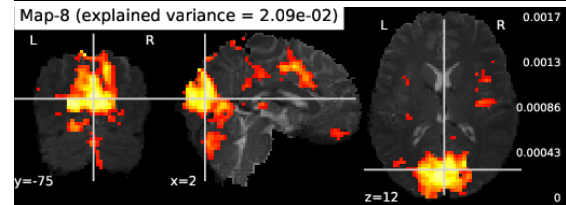
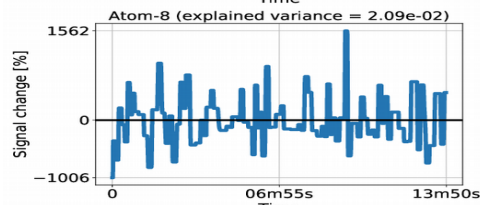
Attention network

Component #4



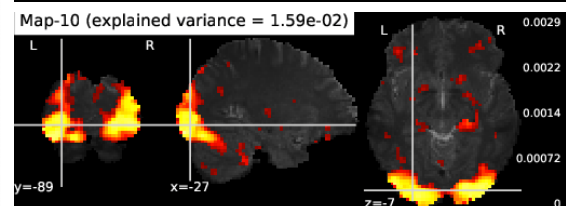
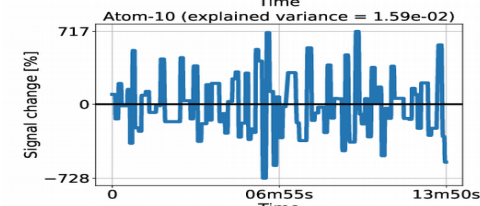
Default Mode Network

Component #8



Visual cortex (V2)

Component #10



Visual cortex (V1)

c.t = 6 min

REAL RESTING-STATE DATA DECOMPOSITION

Resting state: Human Connectome Project (HCP) dataset

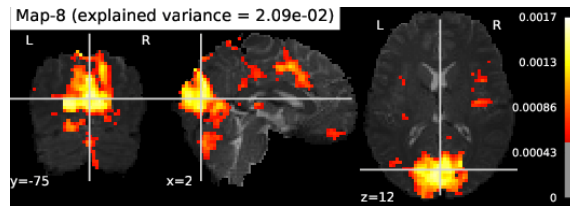
K = 10

10%-thresholded spatial map

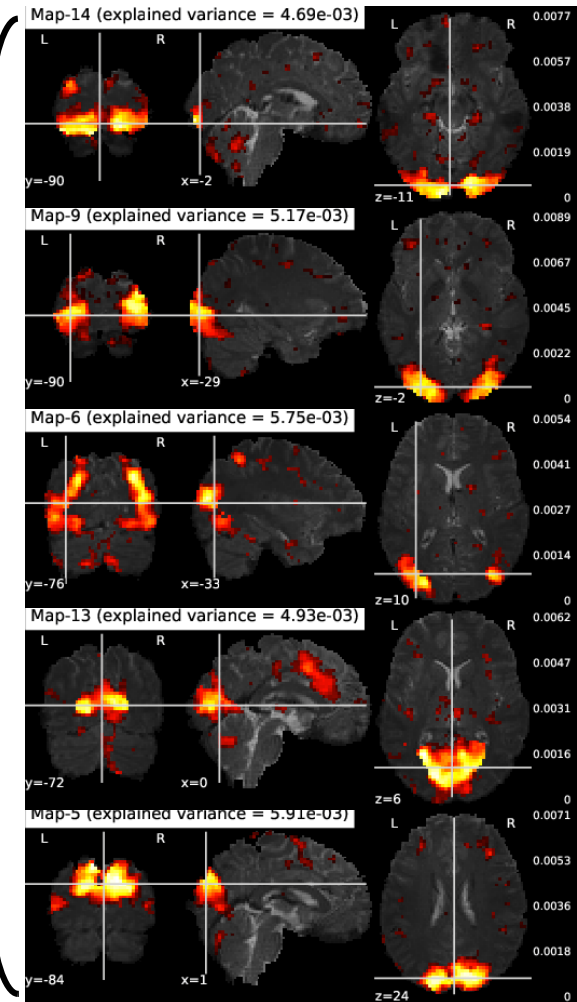
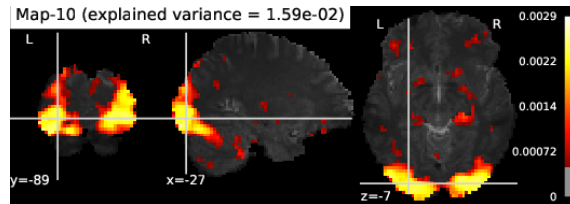
K = 40

10%-thresholded spatial map

Visual cortex
(V2)



Visual cortex
(V1)





Resting state: Human Connectome Project (HCP) dataset

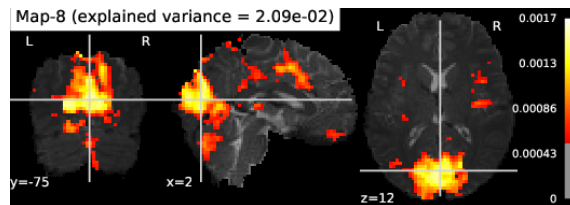
K = 10

10%-thresholded spatial map

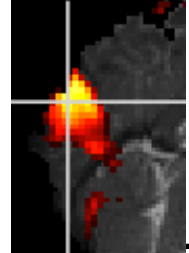
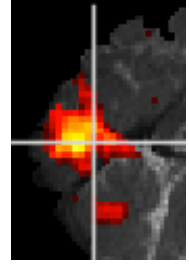
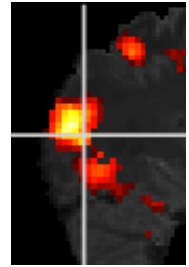
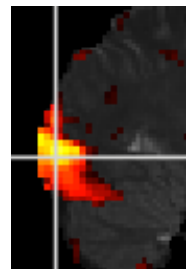
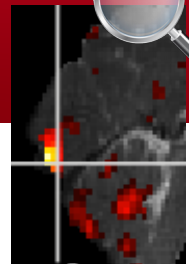
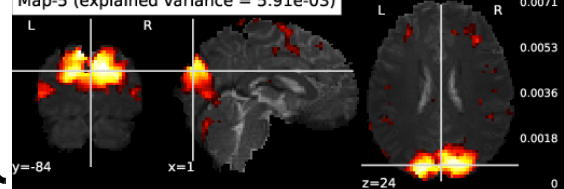
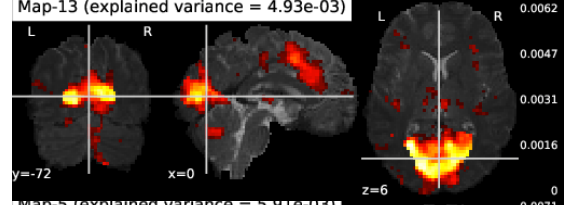
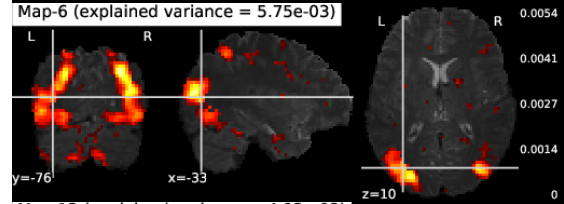
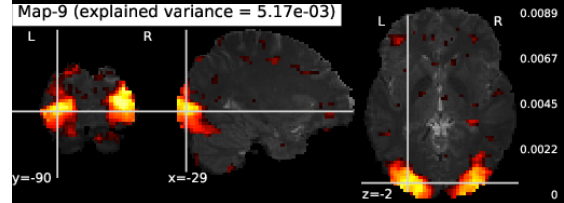
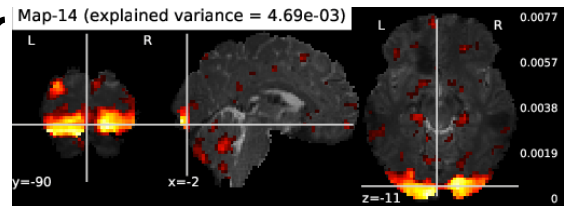
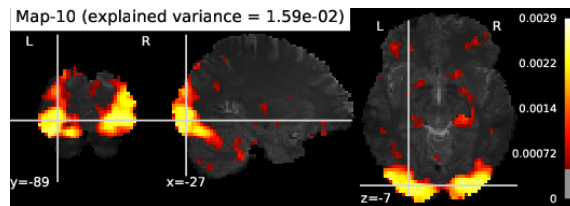
K = 40

10%-thresholded spatial map

Visual cortex (V2)



Visual cortex (V1)



Summary:

- We provided a new low-rank decomposition of the BOLD signal which yields deconvolved neural activity signals and their corresponding spatial maps
- The proposed algorithm performs this decomposition in a reasonable computing time
- We showed that our method provides meaningful decomposition on the neural activity in resting-state and task fMRI

Future works:

- Blind deconvolution: estimate one HRF for each predefined brain region
- Unsupervised estimation: estimate λ , K (model comparison: r^2 score, etc)
- Characterize the statistical properties of the decomposition (neural activity signals)
- Validation on large scale datasets (HCP, Synchropioïd, etc)

Summary:

- We provided a new low-rank decomposition of the BOLD signal which yields deconvolved neural activity signals and their corresponding spatial maps
- The proposed algorithm performs this decomposition in a reasonable computing time
- We showed that our method provides meaningful decomposition on the neural activity in resting-state and task fMRI



<https://github.com/CherkaouiHamza/seven>

Future works:

- Blind deconvolution: estimate one HRF for each predefined brain region
- Unsupervised estimation: estimate λ , K (model comparison: r^2 score, etc)
- Characterize the statistical properties of the decomposition (neural activity signals)
- Validation on large scale datasets (HCP, Synchropioïd, etc)

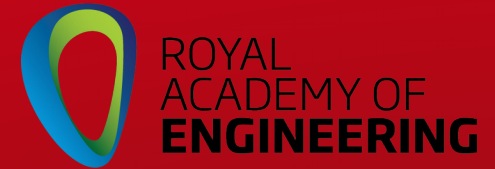


Hamza Cherkaoui, CEA Saclay, Univ. Paris-Saclay, 91191 Gif-sur Yvette, France

Thomas Moreau, Parietal Team, INRIA Saclay, Université Paris-Saclay, Saclay, France

Abderrahim Halimi, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh UK

Philippe Ciuciu, CEA Saclay, Univ. Paris-Saclay, 91191 Gif-sur Yvette, France



- Ogawa S, Lee TM, Kay AR and Tank DW, « Brain magnetic resonance imaging with contrast dependent on blood oxygenation », Proc Natl Acad Sci U S A, 1990
- K. J. Friston, A. Mechelli, R. Turner and C. J. Price, « Nonlinear Responses in fMRI: The Balloon Model Volterra Kernels, and Other Hemodynamics », NeuroImage, 2000
- Logothetis NK, Pauls J, Augath M, Trinath T and Oeltermann A, « Neurophysiological investigation of the basis of the fMRI signal », Nature, 2001
- M. A. Lindquist and T. D. Wager, « Validity and power in hemodynamic response modeling: a comparison study and a new approach », Humain brain mapping, 2007
- F. Pedregosa, M. Eickenberg, P. Ciuciu, B. Thirion, and A. Gramfort, « Data-driven HRF estimation for encoding and decoding models », NeuroImage, 2015
- F. I. Karahanoglu, C. Caballero-Gaudes, C., Lazeyras, F., and Van De Ville, « Total Activation: FMRI Deconvolution Through Spatio-Temporal Regularization », Neuroimage, vol. 73, 2013
- Younes Farouj, F. Işık Karahanoğlu and Dimitri Van De Ville, « BOLD signal deconvolution under uncertain haemodynamics: a semi-blind approach », IEEE International Symposium on Biomedical Imaging, April 2019
- TD La Tour, T Moreau, M Jas and A Gramfort, « Multivariate convolutional sparse coding for electromagnetic brain signals », Advances in Neural Information Processing Systems, 2018
- Arthur Mensch, Julien Mairal, Bertrand Thirion and Gaël Varoquaux, « Dictionary Learning for Massive Matrix Factorization », International Conference on Machine Learning, Jun 2016