

Modelling inter-subject functional variability

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(PhD supervised by B. Thirion and G. Varoquaux)

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September 26, 2017

Context

- A major goal of human neuroscience is to understand
 - the structure,
 - function, and
 - inter-subject variability of the human brain
- We will focus on **inter-subject functional variability**

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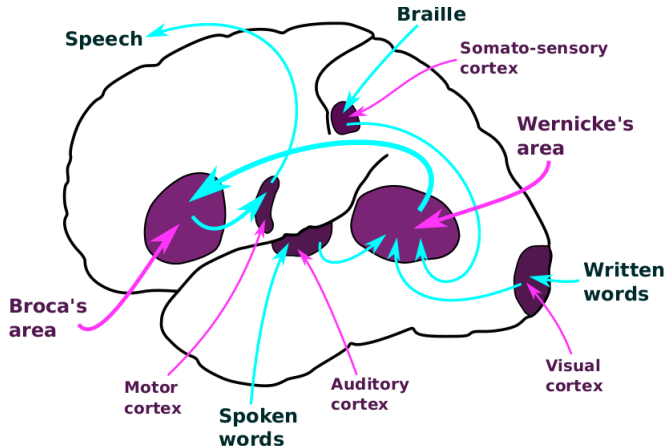
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Introduction

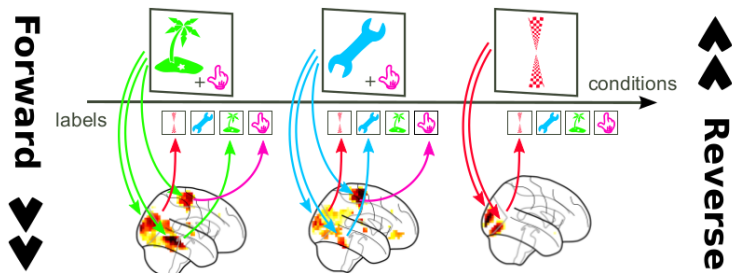
Brain function regions and networks

Part of the language network



(Picture is courtesy of Gael Varoquaux)

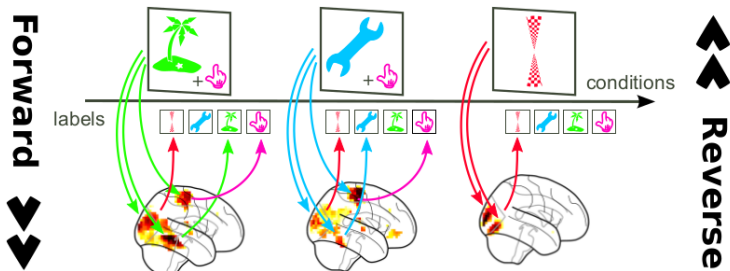
Mapping cognitive circuits in the brain



(Picture is courtesy of Yannick Schwarz)

- **Forward inference** [Friston '95] detects voxels responding to a given experimental condition
- **Reverse inference / brain-decoding** [Dehaene 98; Cox 03] predicts the experimental condition from brain signals

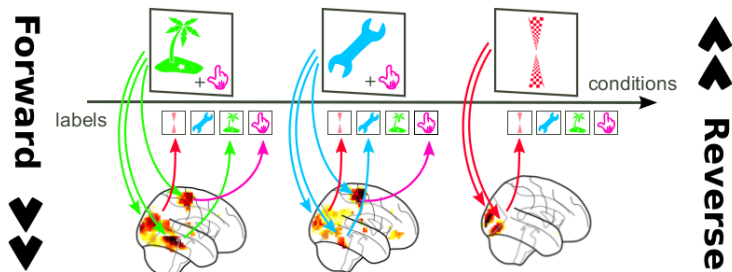
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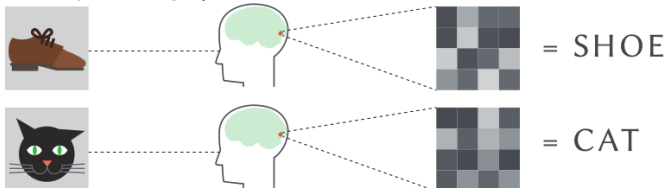
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A zoom on brain-decoding

(Picture is courtesy of F. Pedregosa)

TRAINING



TESTING



y_i

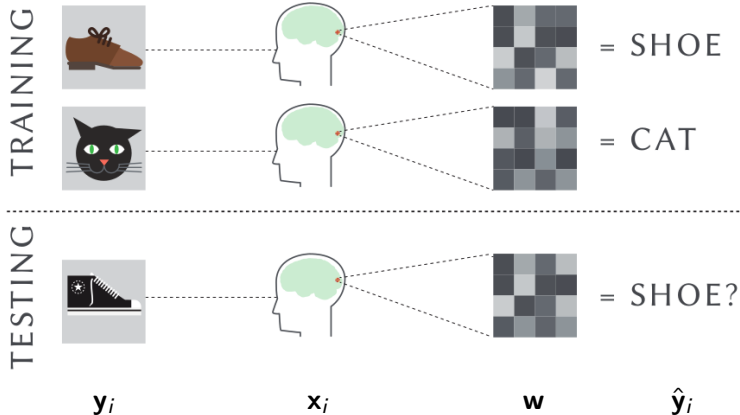
x_i

w

\hat{y}_i

A zoom on brain-decoding

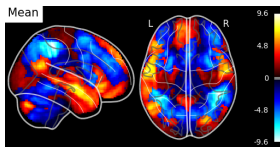
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- This is **supervised machine-learning**
- We don't just want good predictions, we want **regions**

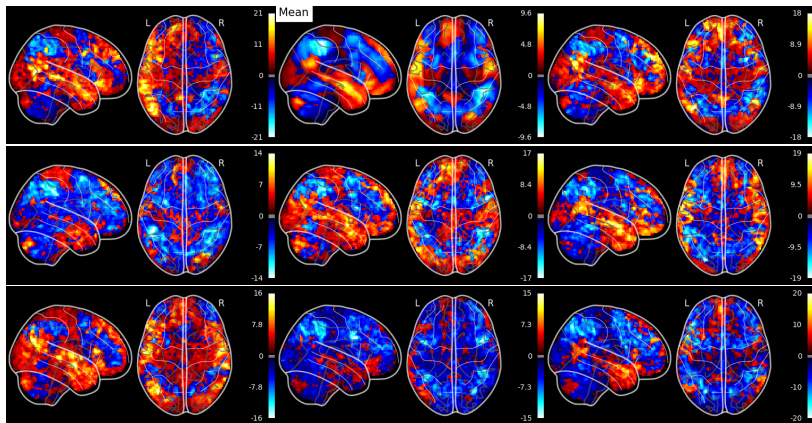
Variability in both location and magnitude of activations

- Story vs Math language contrast of HCP dataset [van Essen '12]



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Variability in both location and magnitude of activations

- Inter-subject **functional variability** \neq noise!
 - Usually (incorrectly) discarded in standard analysis
 - Is predictive of behavioral differences between individuals
- Cannot be corrected via **spatial normalization**, etc.
 - E.g spatial normalization cannot correct for differences in activation magnitude
- Driven by genetic and behavioral inter-individual differences
- Functional diseases can be seen as extremes of this variation

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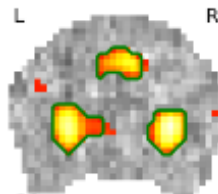
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Mapping the brain with structured multi-variate models

What we mean by “structured”

Definition:

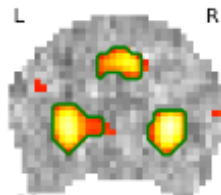
- Localized activation patterns – **sparsity**
- Clusters of active voxels – **smoothness**



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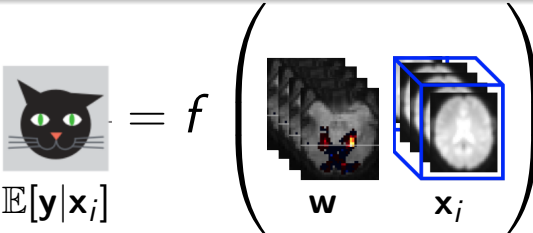
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-
- Such a model is much more **interpretable** (i.e small number of **regions**) than classical methods like SVM, Ridge regression, Lasso
 - Performs **model-estimation** and **feature-selection** jointly
 - Fights the **curse-of-dimensionality**, via dimensionality reduction.

Generalized linear models with structured penalties

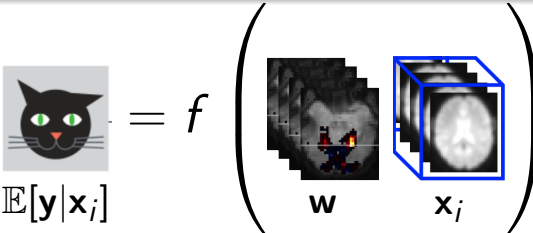


$$\mathbb{E}[y|x_i] = f \left(\begin{matrix} \mathbf{w} & \mathbf{x}_i \end{matrix} \right)$$

■ **Samples** $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^p$

- # samples $n \sim 10^3$
- # **features** $p \sim 10^6$ voxels

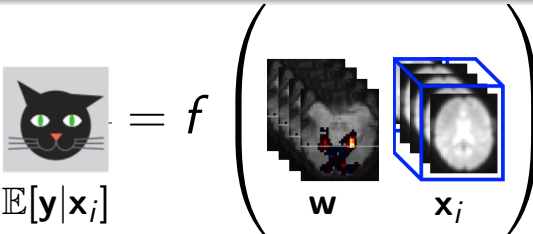
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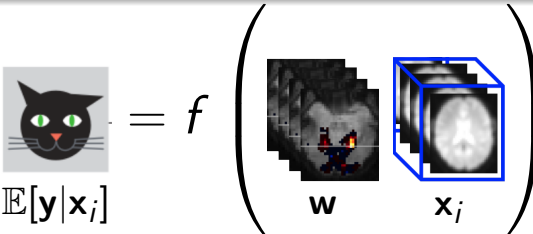
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 - $f = \text{"id"}$ in **regression**

■ Optimization problem:

$$\min_{\mathbf{w} \in \mathbb{R}^p} \underbrace{\frac{1}{n} \sum_{i=1}^n \ell(y_i, f(\langle \mathbf{w}, \mathbf{x}_i \rangle))}_{\text{data / loss term}} + \underbrace{\alpha \mathcal{P}(\mathbf{w})}_{\text{penalty}}$$

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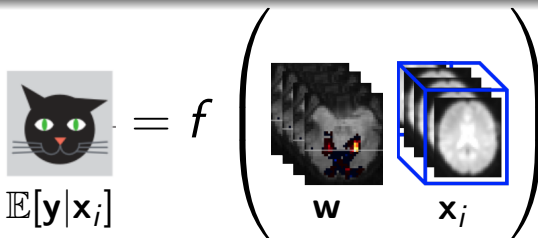
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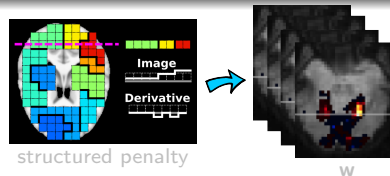
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Spatial penalties impose structure in the model

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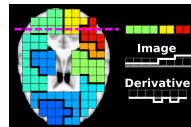


$$\mathcal{P}(\mathbf{w}) = \begin{cases} \sum_{j \in \llbracket p \rrbracket} \rho |\mathbf{w}_j| + \frac{1}{2} (1 - \rho) \|(\nabla \mathbf{w})_j\|_2^2, \\ \sum_{j \in \llbracket p \rrbracket} \rho |\mathbf{w}_j| + (1 - \rho) \|(\nabla \mathbf{w})_j\|_2, \\ \sum_{j \in \llbracket p \rrbracket} (\rho^2 |\mathbf{w}_j|^2 + (1 - \rho)^2 \|(\nabla \mathbf{w})_j\|_2^2)^{1/2}, \\ \vdots \end{cases}$$

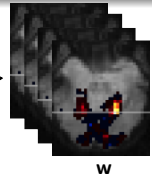
GraphNet,
 isotropic TV-L1,
 Sparse Variation,

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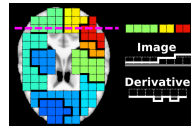
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Bayesian interpretation

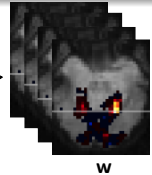
$$\underbrace{P(\mathbf{w} | \mathbf{x}_i, y_i)}_{\text{posterior}} \propto \underbrace{P(y_i | \mathbf{x}_i, \mathbf{w})}_{\text{likelihood}} \underbrace{P(\mathbf{w})}_{\text{prior}} \propto \exp(-\ell(y_i, f(\langle \mathbf{w}, \mathbf{x}_i \rangle))) \exp(-\alpha \mathcal{P}(\mathbf{w}))$$

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■ Bayesian interpretation

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Some notes

- TV is a very tight convex relaxation of Markovian prior
- GraphNet (“Dirichlet energy”) is weaker, but easier to optimize (smooth convex optimization problem)

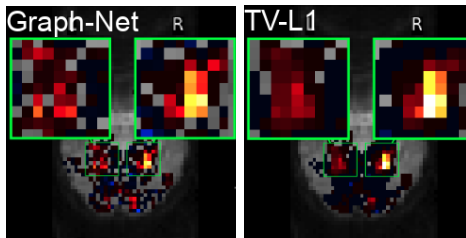
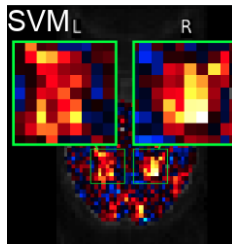
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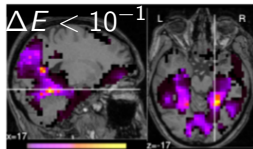
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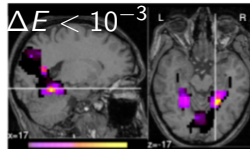
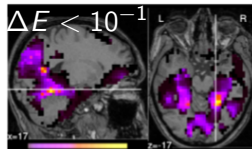
Spatial penalties \implies more interpretable brain maps



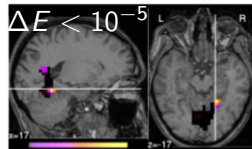
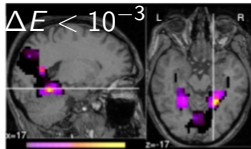
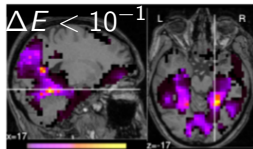
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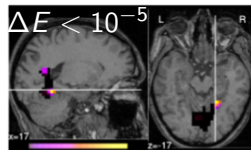
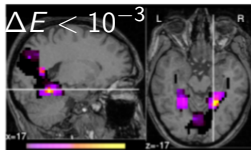
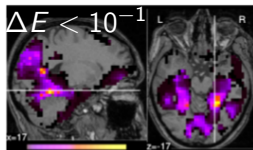


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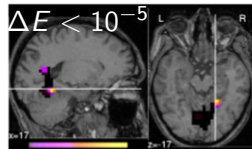
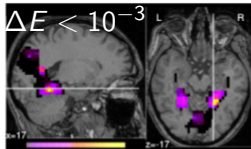
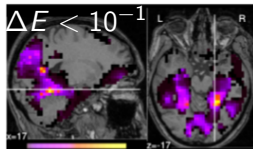
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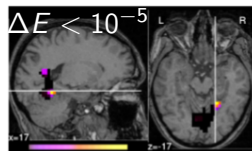
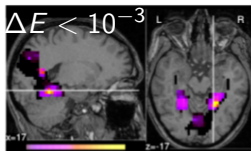
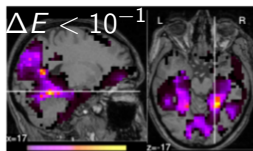
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- Corresponding optim. problem is much **harder** (than SVM, etc.)
 - **high-dimensional non-smooth ill-conditioned** problem

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- We need **fast solvers!**

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Our contributions

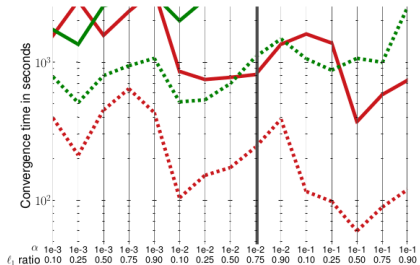
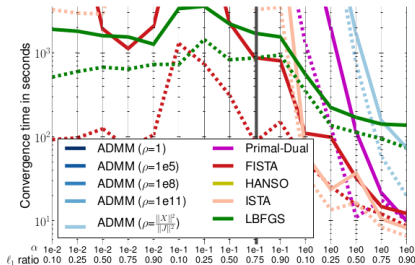
Faster, better, stronger!

We propose a combination of **algorithmic** and **implementation** improvements that make these models usable out-of-the-box

Looking for the ideal solver

[Dohmatob '14, '15 (PRNI); Varoquaux '15 (Gretsi)]

- Solver speed sensitive to hyper-parameter
- Retained strategy is nested **FISTA** [Beck '09] algorithm



Benchmarks on “mixed-gambles” task [Jimura '12]

More speed via univariate feature-screening

[Dohmatob '15 (PRNI)]

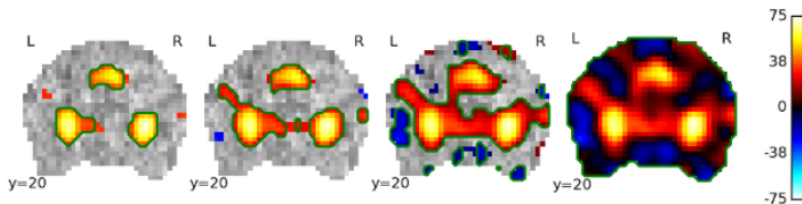
- $t_k := k$ th percentile of the vector $|\mathbf{X}^T \mathbf{y}| := (|\mathbf{x}_1^T \mathbf{y}|, \dots, |\mathbf{x}_p^T \mathbf{y}|)$.
- Discard j th voxel if $|\mathbf{x}_j^T \mathbf{y}| < t_k$

$k = 10\%$

$k = 20\%$

$k = 50\%$

$k = 100\%$

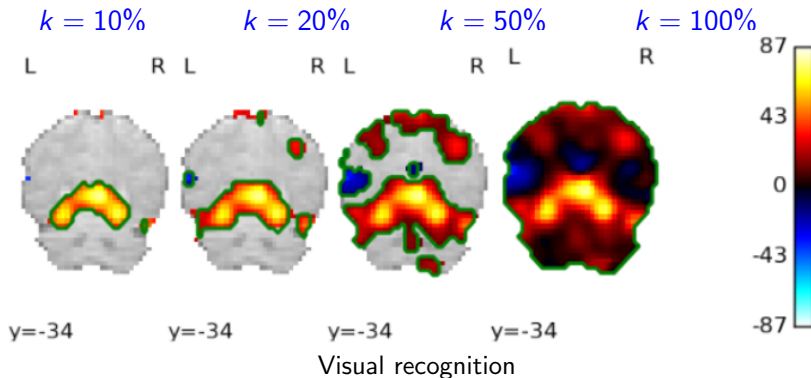


Mixed gambling

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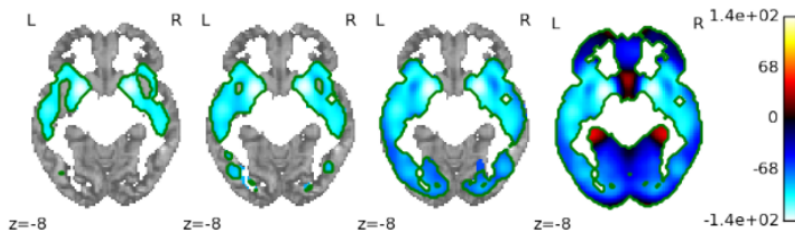
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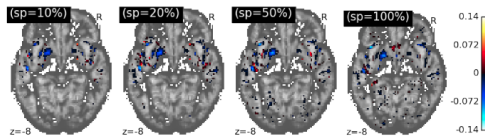
$k = 100\%$



Age prediction from gray-matter maps

More speed via univariate feature-screening: results

■ Age prediction



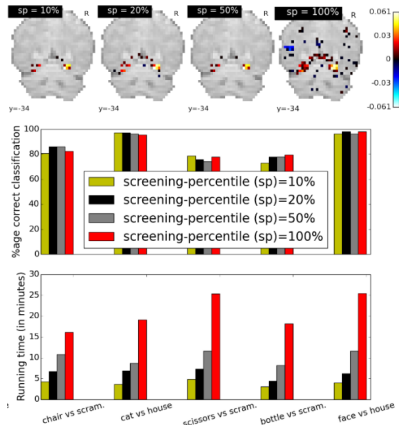
[Dohmatob '15 (PRNI)]

p	100%	50%	20%	10%
MSE	8.37	9.10	9.23	9.19

- Solve on **subset of features**
- Reduced **training time**

More speed via univariate feature-screening: results

■ Visual object recognition

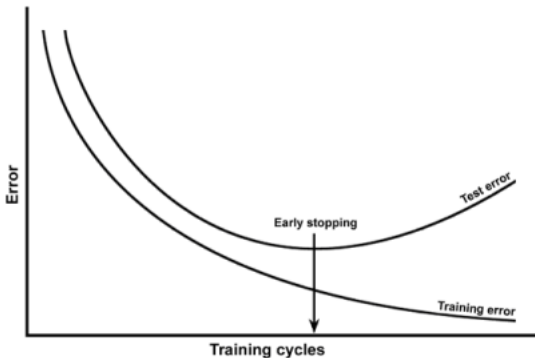


[Dohmatob '15 (PRNI)]

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Early-stopping

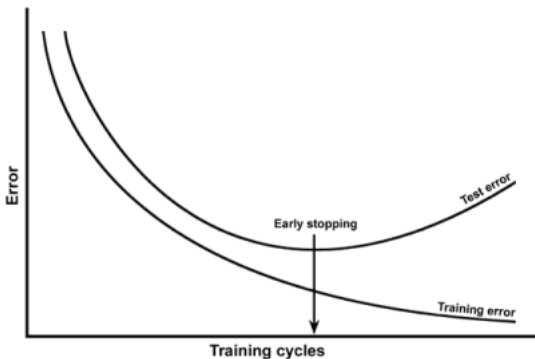
- Stop optimization if accuracy on validation data stops improving [Dohmatob '15 (PRNI)]



- old idea (e.g [Bottou '07])
- saves training time
- implicit regularization
- helps against overfitting
- it's a compromise
 - it doesn't destroy accuracy
 - but may lead to sub-optimal brain maps

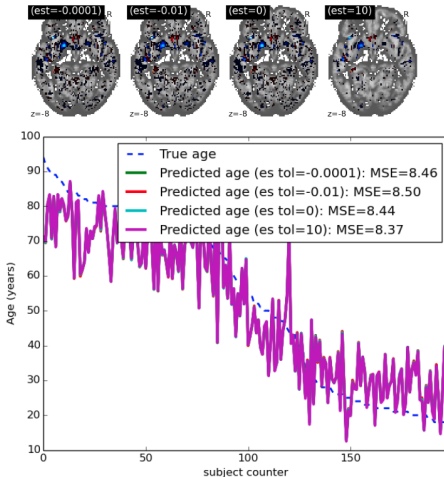
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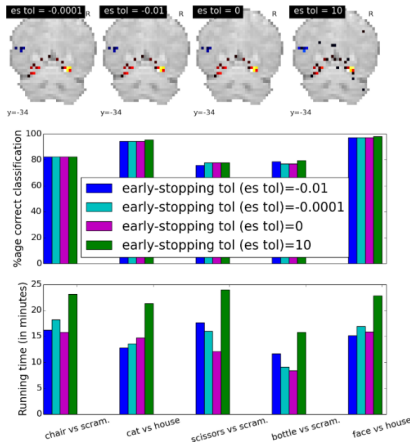


[Dohmatob '15 (PRNI)]

- Solve on subset of features
- Yields up to **x10 speedup!**
- No significant loss in accuracy

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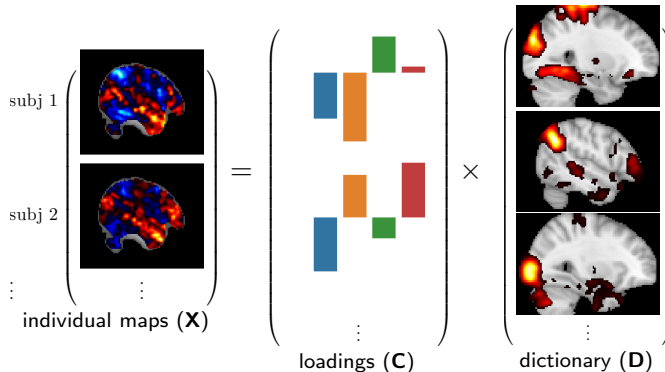
Section wrap-up

- Building on prior work, we have developed enhanced structured penalties for multi-variate brain-decoding
- Such penalties lead to more interpretable brain maps (a small number of smooth spatially localized regions)
- Focus on practical usability (fast model training)
- Our contributions are available as part of **Nilearn** toolkit.

Modelling inter-subject variability via dictionary-learning

Learn latent model for inter-subject variability

- **Goal:** Learn a latent model of inter-subject functional variability



- Each **cognitive map** \mathbf{x}_i with p voxels gets **encoded** over a **dictionary** \mathbf{D} as k **loading coefficients** \mathbf{c}_i , with $k \ll p$

The challenge

[Dohmatob '16 (NIPS)]

- **Sparsity**: spatially localized atoms
- **Smooth regions**: each atom = interpretable blobs
- **Scalable / online**: model should trainable online

Introducing the proposed model [Dohmatob '16 (NIPS)]

$$\begin{pmatrix} \text{subj 1} \\ \text{subj 2} \\ \vdots \end{pmatrix} \begin{pmatrix} \text{Brain map 1} \\ \text{Brain map 2} \\ \vdots \end{pmatrix} = \begin{pmatrix} \text{C}_1 \\ \text{C}_2 \\ \vdots \end{pmatrix} \times \begin{pmatrix} \text{D}_1 \\ \text{D}_2 \\ \vdots \end{pmatrix}$$

\mathbf{x}
 \mathbf{c}
 \mathbf{D}

$$\min_{\mathbf{D} \in \mathbb{R}^{p \times k}} \left(\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{t=1}^n \min_{\mathbf{c}_t \in \mathbb{R}^k} \frac{1}{2} \|\mathbf{x}_t - \mathbf{D} \mathbf{c}_t\|_2^2 + \frac{1}{2} \alpha \|\mathbf{c}_t\|_2^2 \right)$$

subject to $\mathbf{d}^1, \dots, \mathbf{d}^k \in \mathcal{K}$ [Mairal '09']

Introducing the proposed model [Dohmatob '16 (NIPS)]

Diagram illustrating the proposed model. The matrix \mathbf{X} (containing brain activity maps for subjects 1 and 2) is equal to the product of the coefficient matrix \mathbf{C} and the dictionary matrix \mathbf{D} .

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[Dohmatob '16']

$\mathcal{K} \subseteq \mathbb{R}^p$: $\|\mathbf{d}^j\|_1 = 1$

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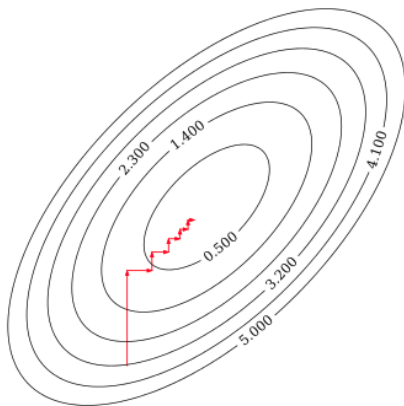
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[Dohmatob '16']

Reminder on coordinate-descent (CD)

- Optimize w.r.t a variable, and then w.r.t to another, and so on ...



The proposed algorithm



- **Draw a sample** 3D brain image (or mini-batch) $\mathbf{x}_t \in \mathbb{R}^p$

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- **Draw a sample** 3D brain image (or mini-batch) $\mathbf{x}_t \in \mathbb{R}^p$
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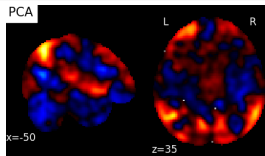
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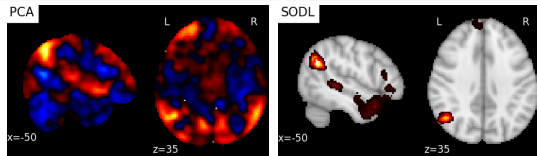
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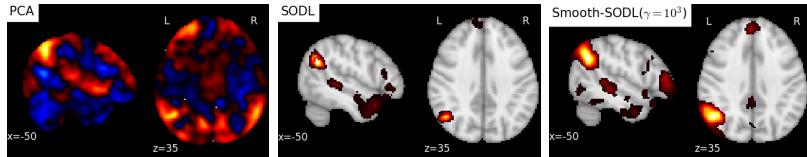
Experimental results on HCP fMRI data: qualitative



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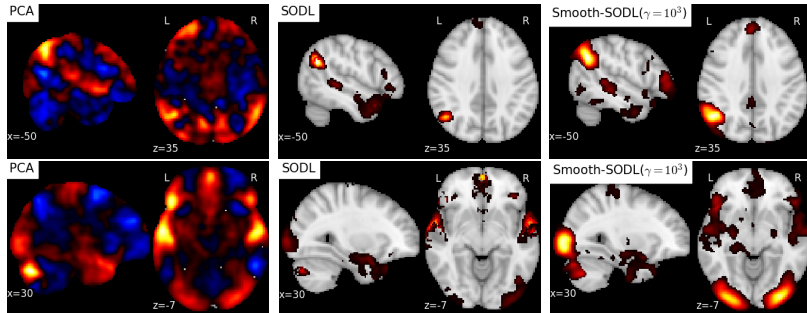


Experimental results on HCP fMRI data: qualitative



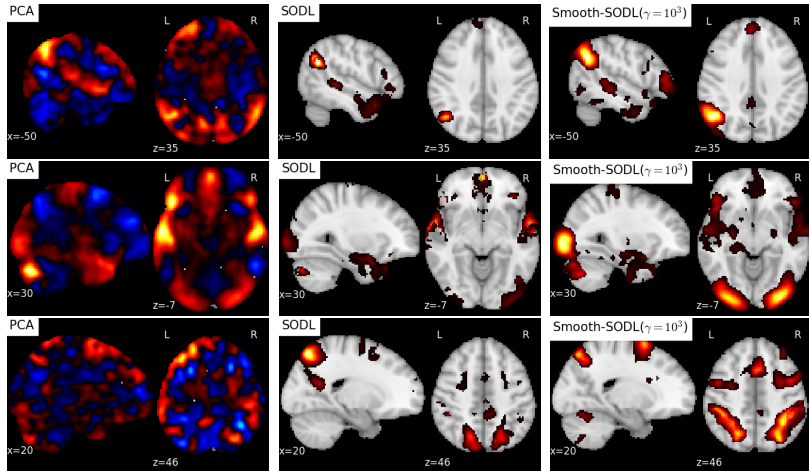
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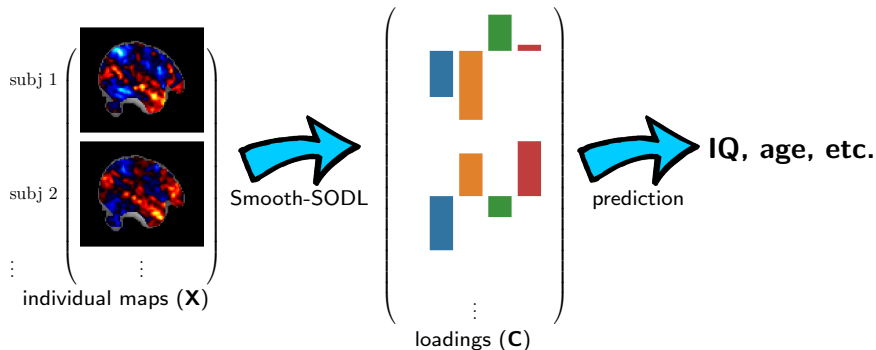
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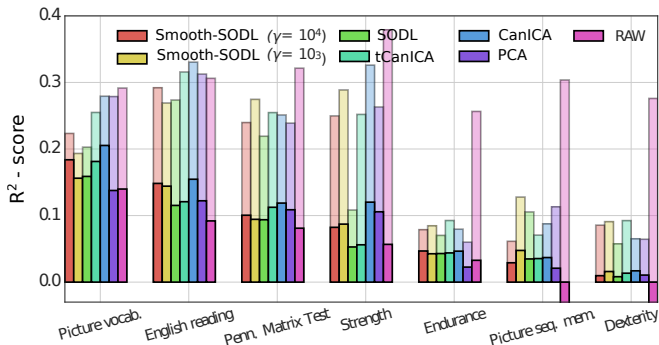
Learned latent dimensions capture inter-subject variability

- Predicting behavior from **compressed representation** of Story vs Math contrast of language task maps [van Essen '12]



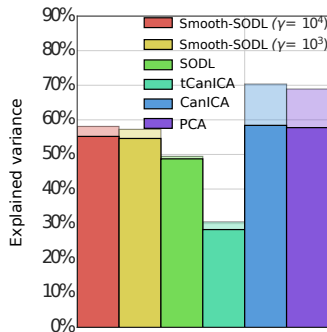
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- Thick bars \Rightarrow scores on **test set**; faint bars \Rightarrow on **train**
- Proposed **Smooth-SODL** overfits the least (i.e generalizes best)

What's happening



- Unregularized models **overfit**
- Models thresholded post-training **underfit**

Spatial prior reduces sample-complexity

Nb. subjects	vanilla [Mairal '10]	Proposed model	gain factor
17	2%	31%	13.8
92	37%	50%	1.35
167	47%	54%	1.15
241	49%	55%	1.11

Learning-curve for “boost” in explained variance of our proposed Smooth-SODL model over the reference SODL model.

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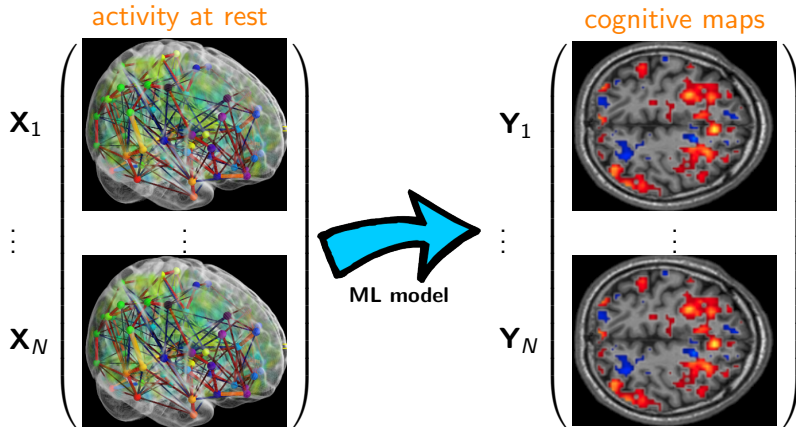
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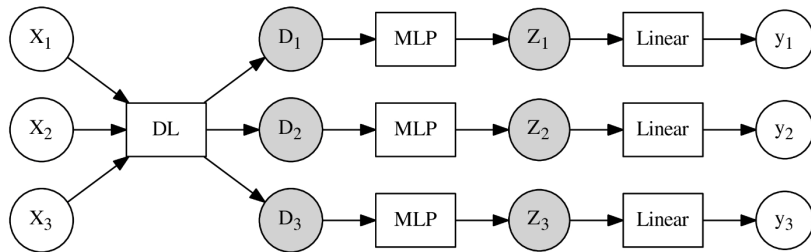
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Can we predict task maps from resting-state data ?



- \mathbf{X}_s : resting-state functional connectivity graph for subject s
- \mathbf{Y}_s : task-specific activation maps for subject s

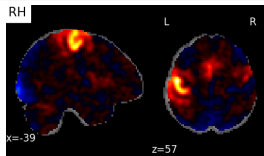
Proposal: Deep semi-supervised voxel encoding



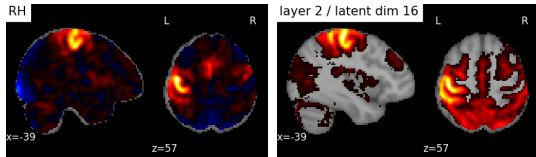
■ $\mathbf{Y} \in \mathbb{R}^{p \times C}$: subject-specific GLM maps of brain activity

■ $\mathbf{X} \in \mathbb{R}^{p \times T}$: resting-state fMRI data

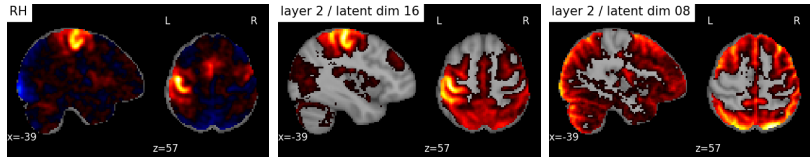
Preliminary results: learned features



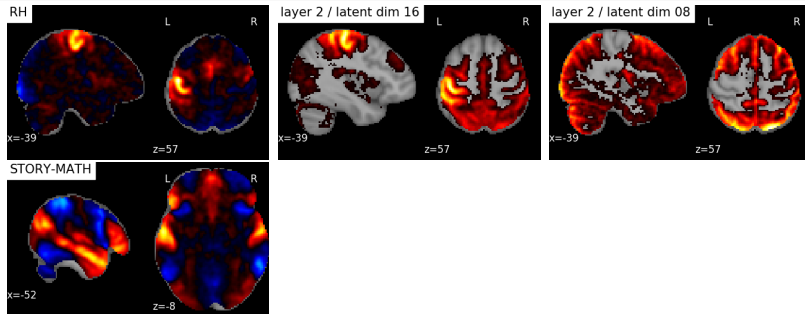
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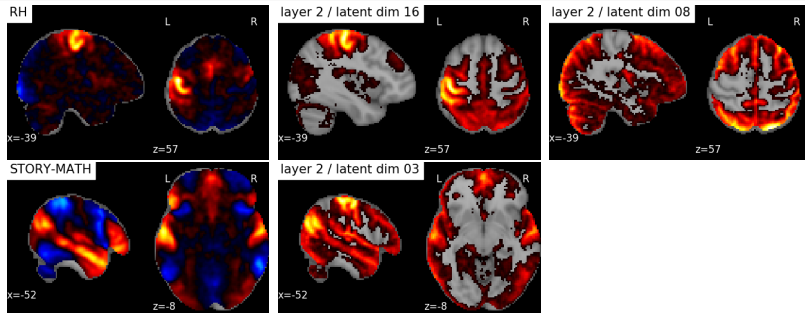
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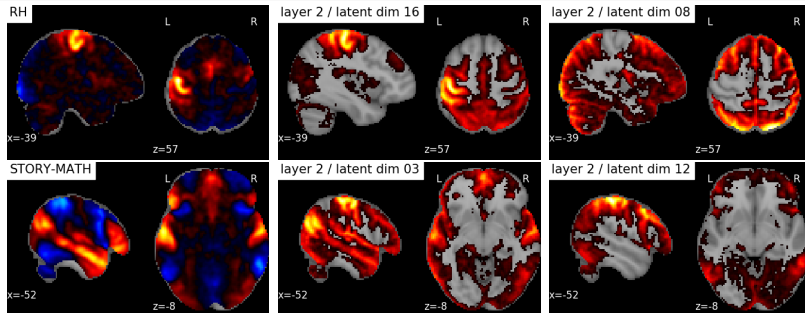
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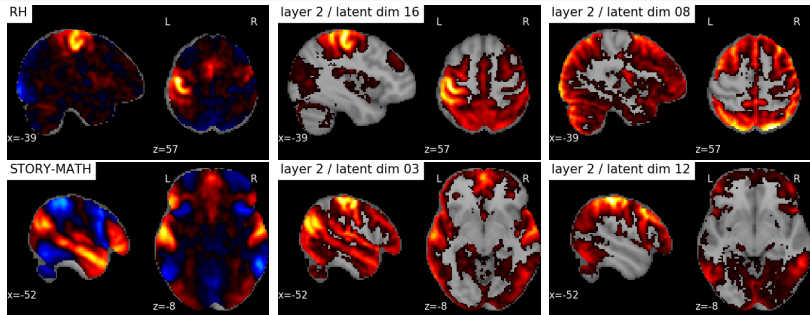
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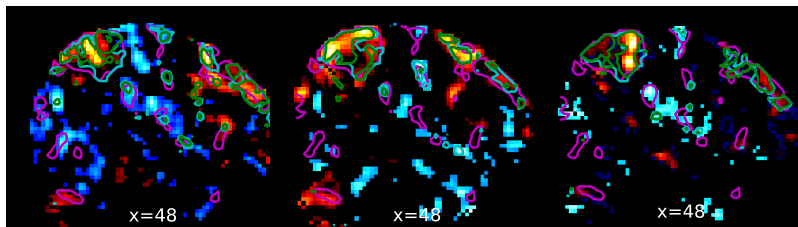


Preliminary results: learned features



- Learned the a presentation of task activity in resting-state space!
- This is ongoing application of models developed in previous sections!

Preliminary results: predicted individual maps

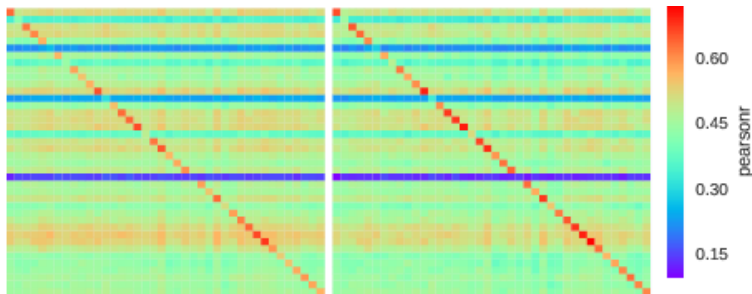


2BK vs 0BK contrast of the Working Memory task
[van Essen '12]

- magenta = population mean
- reference method [Tavor '16]
- proposed method

- Prediction agrees with subject's topography more faithfully

Preliminary results: quantitative



Confusion matrix for predicted versus true activation maps

Relevant contributions I



Alexandre Abraham, Elvis Dohmatob, Bertrand Thirion, Dimitris Samaras, and Gael Varoquaux. “Extracting brain regions from rest fMRI with Total-Variation constrained dictionary learning”. In: **MICCAI**. 2013.



Elvis Dohmatob, Michael Eickenberg, Bertrand Thirion, and Gael Varoquaux. “Local Q-Linear Convergence and Finite-time Active Set Identification of ADMM on a Class of Penalized Regression Problems”. In: **ICASSP 2016**. 2015.

Relevant contributions II



Elvis Dohmatob, Michael Eickenberg, Bertrand Thirion, and Gaël Varoquaux. “Speeding-up model-selection in GraphNet via early-stopping and univariate feature-screening”. In: **Pattern Recognition in NeuroImaging (PRNI), 2015 International Workshop on**. IEEE. 2015.



Elvis Dohmatob, Alexandre Gramfort, Bertrand Thirion, and Gaël Varoquaux. “Benchmarking solvers for TV-l1 least-squares and logistic regression in brain imaging”. In: **PRNI**. IEEE. 2014.

Relevant contributions III



Elvis Dohmatob, Arthur Mensch, Gaël Varoquaux, and Thirion Bertrand. “Learning brain regions via large-scale online structured sparse dictionary-learning”. In: **NIPS**. 2016.



Michael Eickenberg, Elvis Dohmatob, Bertrand Thirion, and Gaël Varoquaux. “Total Variation meets Sparsity: statistical learning with segmenting penalties”. In: **MICCAI**. 2015.