#### Modelling inter-subject functional variability

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

Parietal Team, INRIA

September 26, 2017









#### Context

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

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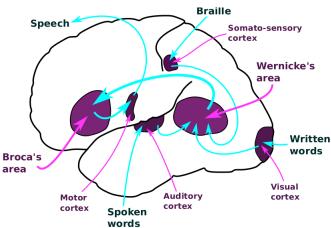
#### Introduction

Modelling inter-subject variability via dictionary-learning Concluding remarks

#### Introduction

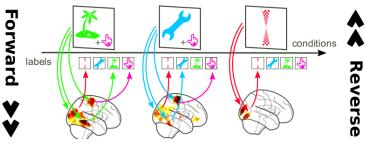
# Brain function regions and networks

#### Part of the language network



(Picture is courtesy of Gael Varoquaux)

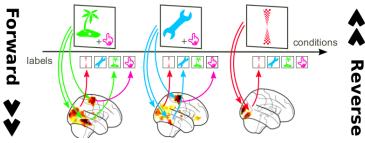
## Mapping cognitive circuits in the brain



(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

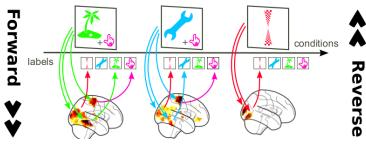
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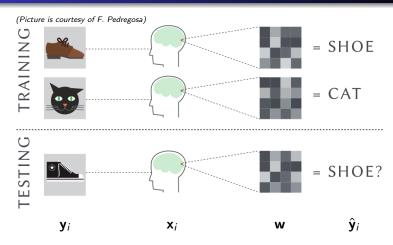
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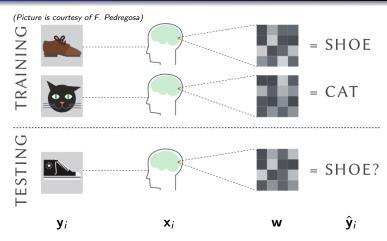
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## A zoom on brain-decoding

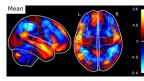


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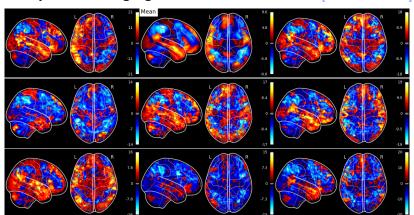


- ■This is supervised machine-learning
- ■We don't just want good predictions, we want regions

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



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



- ■Inter-subject functional variability ≠ 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
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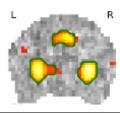
Preliminaries Spatial priors for brain decoding Contributions

# Mapping the brain with structured multi-variate models

#### What we mean by "structured"

#### **Definition:**

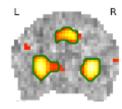
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- Clusters of active voxels smoothness



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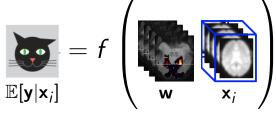
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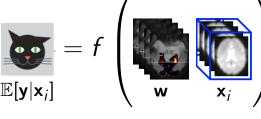
- Such a model is much more interpretable (i.e small number of regions) than classical methods like SVM, Ridge regression, Lasso
- Performs model-estimation and feature-selection jointly
- Fights the curse-of-dimensionality, via dimensionality reduction.



- Samples  $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^p$ 
  - # samples  $n \sim 10^3$
  - # features  $p \sim 10^6$  voxels



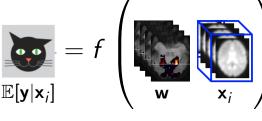
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- $\blacksquare f = "id"$  in regression

Optimization problem:

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

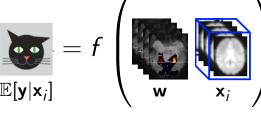


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#### data / loss term



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$$\bullet \ell(y_i, f(\mathbf{x}_i^\mathsf{T} \mathbf{w})) = \begin{cases} \frac{1}{2} (y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle)^2, & \text{in regression,} \\ \log(1 + \exp(-y_i \langle \mathbf{w}, \mathbf{x}_i \rangle)), & \text{in classif. (OvR)} \end{cases}$$

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$$\mathcal{P}(\mathbf{w}) = \begin{cases} \sum_{j \in \llbracket \rho \rrbracket} \rho |\mathbf{w}_j| + \frac{1}{2} (1-\rho) \|(\nabla \mathbf{w})_j\|_2^2, & \mathbf{GraphNet}, \\ \sum_{j \in \llbracket \rho \rrbracket} \rho |\mathbf{w}_j| + (1-\rho) \|(\nabla \mathbf{w})_j\|_2, & \mathbf{isotropic TV-L1}, \\ \sum_{j \in \llbracket \rho \rrbracket} (\rho^2 |\mathbf{w}_j|^2 + (1-\rho)^2 \|(\nabla \mathbf{w})_j\|_2^2)^{1/2}, & \mathbf{Sparse Variation}, \\ \vdots & \end{cases}$$

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■ Bayesian interpretation

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

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

## References for the penalties

- Total-Variation (TV) [Michel '11]
- ■TV-L1 [Baldassare '12, Gramfort '13]
- GraphNet / S-Lasso [Hebiri '11, Grosenick '13]
- Sparse-Variation [Eickenberg '15]

#### 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)

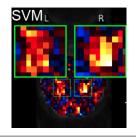
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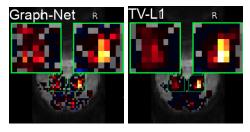
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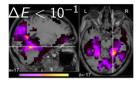
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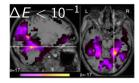
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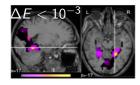
# Spatial penalties ⇒ more interpretable brain maps

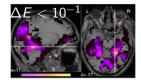


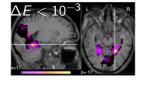


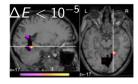




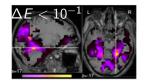


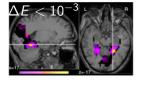


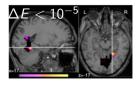




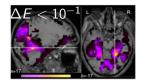
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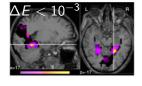


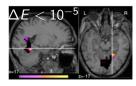




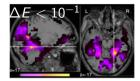
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  - high-dimensional non-smooth ill-conditioned problem

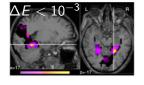


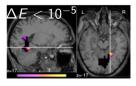




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  - high-dimensional non-smooth ill-conditioned problem
- Lack of fast solver can lead to wrong conclusions about model
- We need fast solvers!







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#### Our contributions

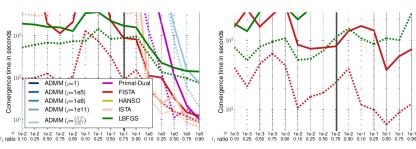
#### Faster, better, stronger!

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



# More speed via univariate feature-screening

k = 10% k = 20% k = 50%

#### [Dohmatob '15 (PRNI)]

- $\mathbf{z}_{k} := k$ th percentile of the vector  $|\mathbf{X}^{T}\mathbf{y}| := (|\mathbf{x}_{1}^{T}\mathbf{y}|, \dots, |\mathbf{x}_{p}^{T}\mathbf{y}|).$
- Discard jth voxel if  $|\mathbf{x}_i^T \mathbf{y}| < t_k$

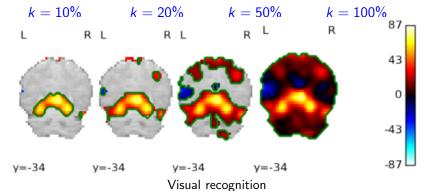
Mixed gambling

k = 100%

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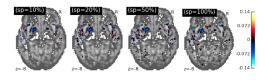
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Age prediction from gray-matter maps

## More speed via univariate feature-screening: results

#### ■ Age prediction



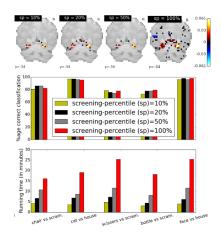
р	100%	50%	20%	10%
MSE	8.37	9.10	9.23	9.19

#### [Dohmatob '15 (PRNI)]

- Solve on subset of features
- Reduced training time

## More speed via univariate feature-screening: results

■ Visual object recognition



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## Early-stopping

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

  Training error

  Training cycles
- ■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

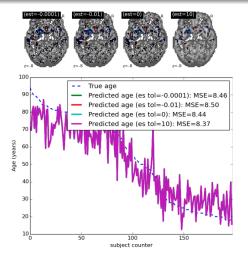
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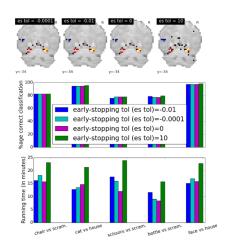


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# Early-stopping: results

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# Section wrap-up

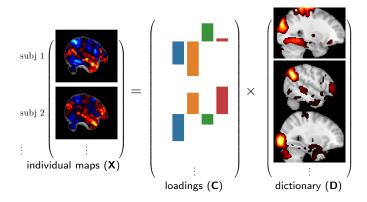
- Building on prior work, we have developed enhanced structured penalties for multi-variate brain-decoding
- Such penalties lead to more interpretable brain maps (a small number of smooth spatially localized regions)
- Focus on practical usability (fast model training)
- Our contributions are available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

eliminaries roducing the proposed mode gorithms sults

# 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)]

$$\sup_{\mathbf{z} \in \mathbb{R}^{p \times k}} 1 = \sum_{t=1}^{n} \min_{\mathbf{c}_t \in \mathbb{R}^k} \frac{1}{2} \|\mathbf{x}_t - \mathbf{D}\mathbf{c}_t\|_2^2 + \frac{1}{2}\alpha \|\mathbf{c}_t\|_2^2$$

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

 $\mathbb{R}^p \subseteq \mathbb{R}^p$  is an  $\ell_1$  ball

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[Dohmatob '16']

 $K \subseteq \mathbb{R}^p$  is an  $\ell_1$  ball

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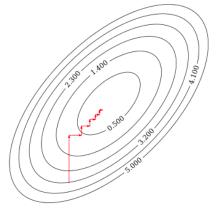
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[Dohmatob '16']

 $\mathbb{R}^p$  is an  $\ell_1$  ball

# Reminder on coordinate-descent (CD)

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





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



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- Compute loadings (i.e representation w.r.t current dict. D)

$$\mathbf{c}_t \leftarrow \mathrm{argmin}_{\mathbf{u} \in \mathbb{R}^k} \, \frac{1}{2} \|\mathbf{x}_t - \mathbf{D}\mathbf{u}\|_2^2 + \frac{1}{2} \alpha \|\mathbf{u}\|_2^2.$$



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  - Precompute  $R \leftarrow B DA$
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    - Rank-1 update:  $\mathbf{R} \leftarrow \mathbf{R} + \mathbf{d}^{j} \circ \mathbf{a}^{j}$
    - ■FISTA loop:  $\mathbf{d}^j \leftarrow \operatorname{argmin}_{\mathbf{d} \in \mathcal{K}} F_{\gamma_t}(\mathbf{d}, a_{i,j}^{-1} \mathbf{r}^j)$
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**N.B.:** 
$$F_{\gamma_t}(\mathbf{d}, \mathbf{z}) := \frac{1}{2} \|\mathbf{d} - \mathbf{z}\|_2^2 + \frac{1}{2} \gamma_t \|\nabla \mathbf{d}\|_F^2$$
,  $\gamma_t := \gamma(a_{j,j}/t)^{-1}$ 

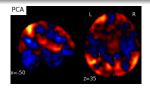


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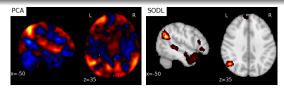
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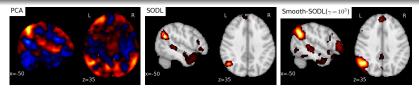
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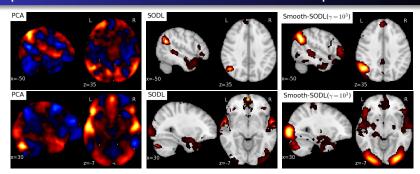
Preliminaries Introducing the proposed model Algorithms Results

## Experimental results on HCP fMRI data: qualitative

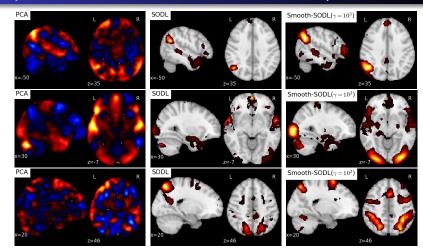




Our method produces localized and smooth decompositions



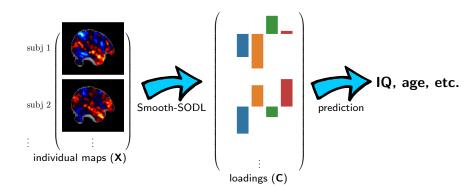
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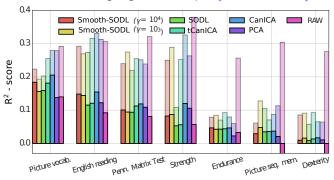
# Learned latent dimensions capture inter-subject variability

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



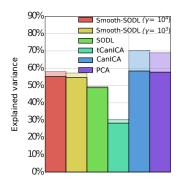
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- Thick bars  $\implies$  scores on **test** set; faint bars  $\implies$  on **train**
- Proposed Smooth-SODL overfits the least (i.e generalizes best)

# 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.

## Concluding remarks

- The goal of this thesis was to develop models for **inter-subject** variability
- "Regions" emerged as the right scale at which to work
  - A more stable representation of activity patterns across subjects, etc.

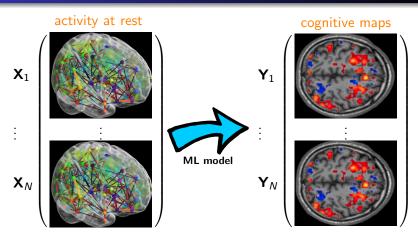
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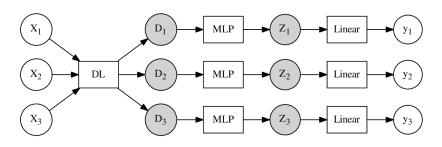
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# Can we predict task maps from resting-state data?

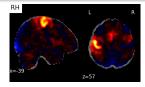


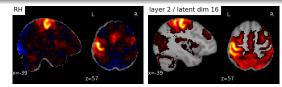
- lacktriangleX<sub>s</sub>: resting-state functional connectivity graph for subject s
- $\mathbf{Y}_s$ : task-specific activation maps for subject s

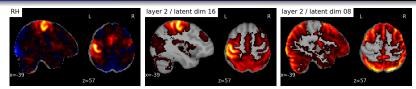
### Proposal: Deep semi-supervised voxel encoding

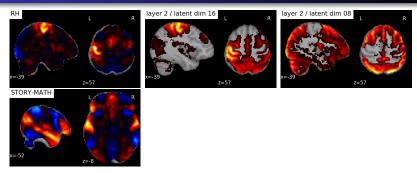


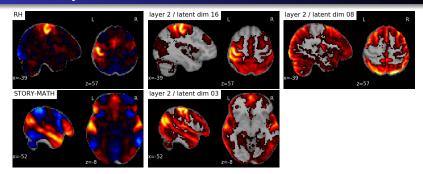
- $\mathbf{Y} \in \mathbb{R}^{p \times C}$ : subject-specific GLM maps of brain activity
- $\mathbf{X} \in \mathbb{R}^{p \times T}$ : resting-state fMRI data

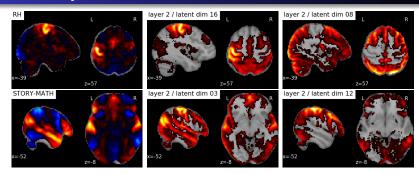


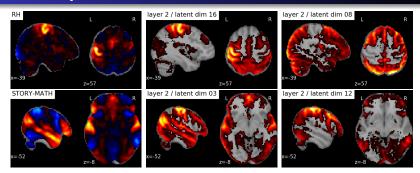






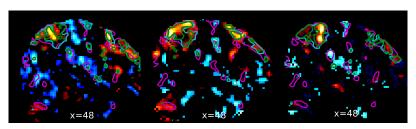






- Learned the a presentation of task activity in resting-state space!
- This is ongoing application of models developed in previous sections!

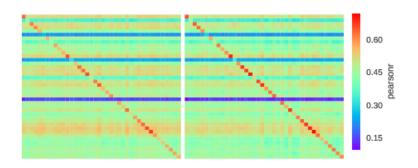
### Preliminary results: predicted individual maps



**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

Wrap-up

Perspective: predicting task activation from resting-state data

#### Relevant contributions I