Analyzing brain function: decoding and reverse inference

Deep learning summer school

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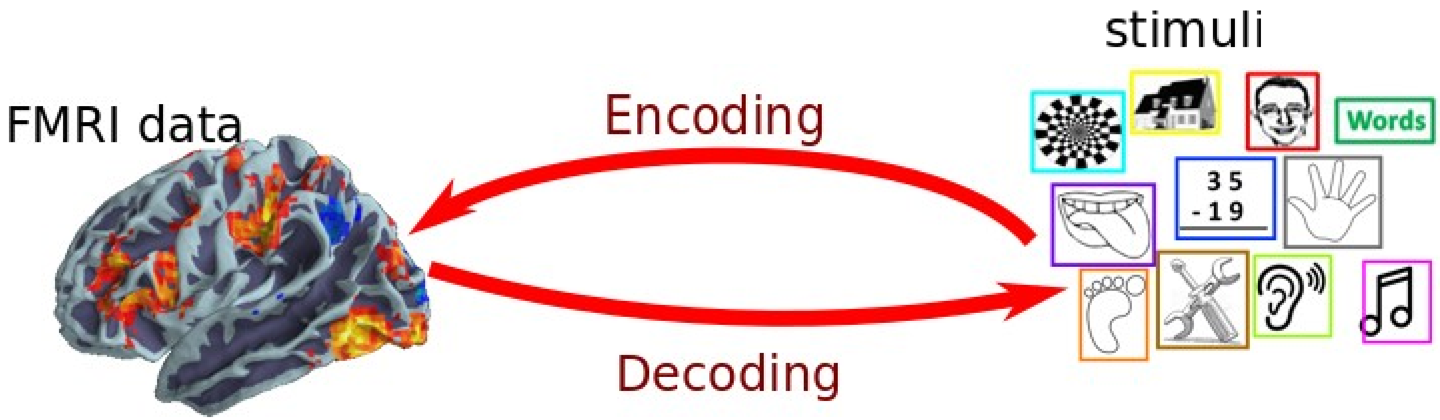
Introduction



- Encoding and decoding brain activity: why are both interesting ?
- Decoding with pre-defined categories of decoding at large scale ? Functional specificity
- Decoding as an inverse problem: ill-posedness and (some) solution
-

Outline

- Why is decoding important ? A causal perspective
- Intermezzo: Learning representations for brain images with dictionary learning
- Large-scale brain activity decoding
  - coordinated decoding
  - Joint decoding
- Decoding an in inverse problem: what can we learn from it ?

What analysis is necessary to gain insights into brain-function relationships ?

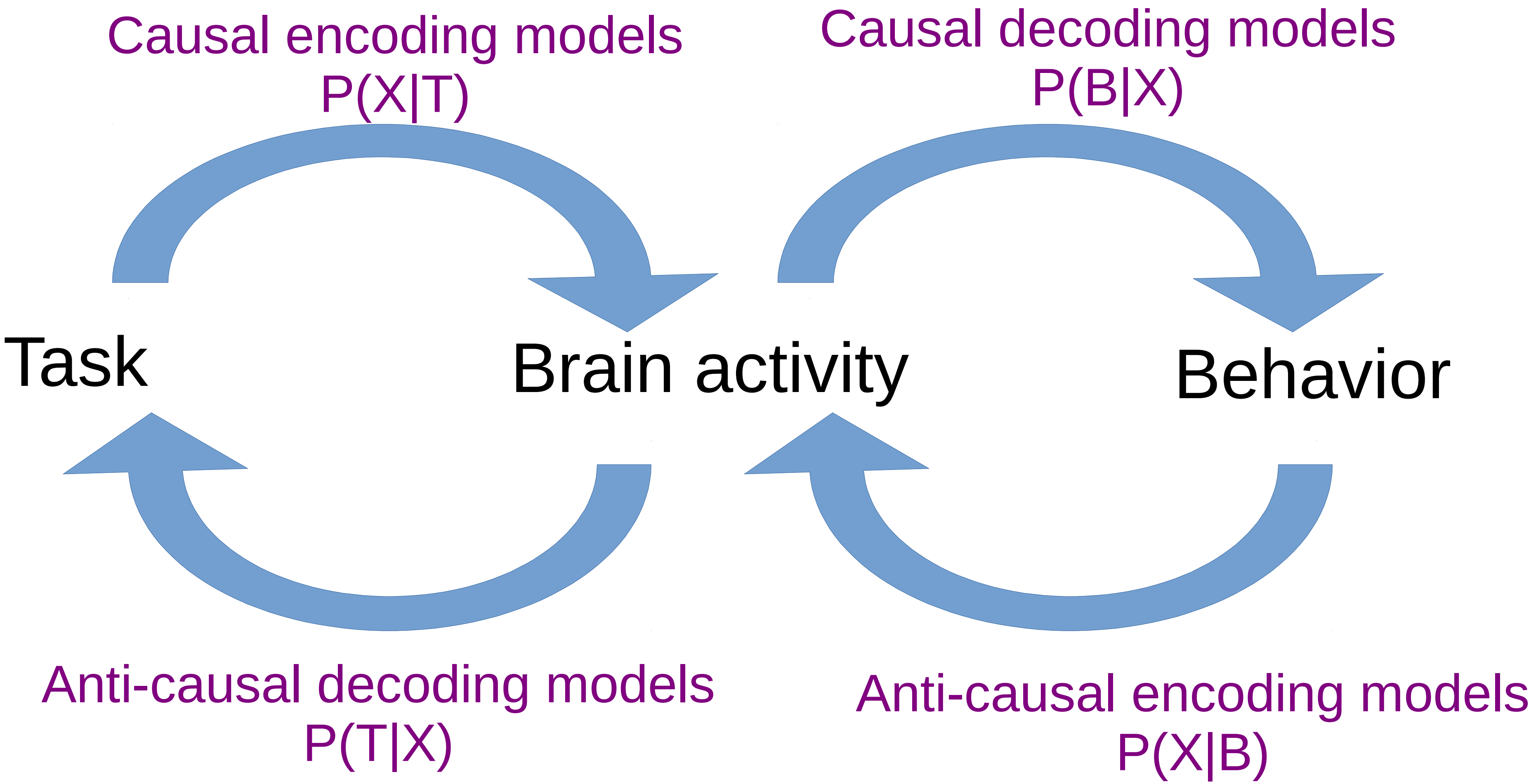
A) Encoding: study the association of brain activity in any given region with the stimuli/tasks

B) Decoding: assess whether a regions is important or not in the prediction of stimulus occurrence

C) Both

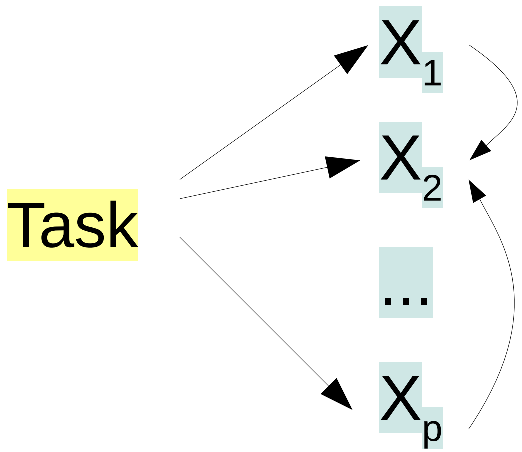
D) Other suggestions

Causal reasoning on encoding/decoding



[Weichwald et al Nimg 2015]

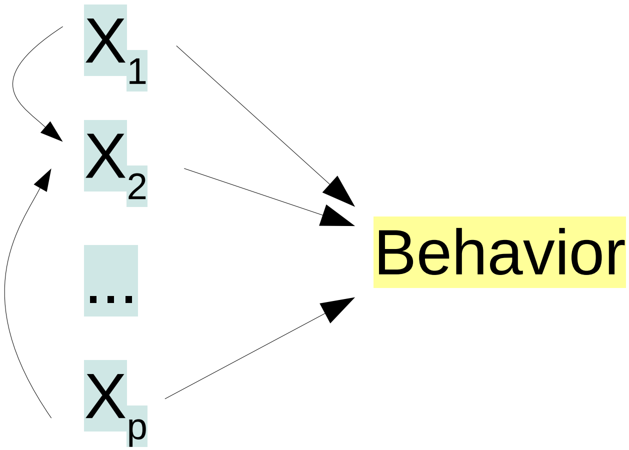
Causal interpretation



$$\mathbf{X_i} \perp\!\!\!\perp \mathbf{T}$$

Encoding: causal
Decoding: anti-causal

$$\mathbf{X_i} \perp\!\!\!\perp \mathbf{T} | (\mathbf{X_j}, \mathbf{j} \neq \mathbf{i})$$



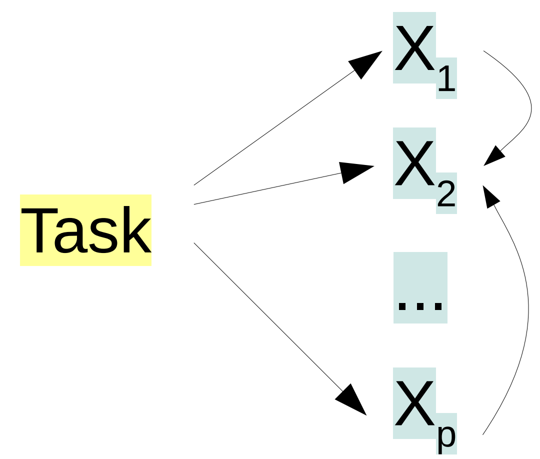
$$\mathbf{X_i} \perp\!\!\!\perp \mathbf{B}$$

Encoding: anti-causal
Decoding: causal

$$\mathbf{X_i} \perp\!\!\!\perp \mathbf{B} | (\mathbf{X_j}, \mathbf{j} \neq \mathbf{i})$$

Causal reasoning on encoding/decoding

		Feature X_i relevant?		
		Encoding	Decoding	Causal interpretation
Experimental setting	Task	$\times$		$T \perp\!\!\!\perp X_i \Rightarrow X_i$ is no effect of T
		$\surd$		$T \not\perp\!\!\!\perp X_i \Rightarrow X_i$ is an effect of T
	Behaviour			



[Weichwald et al. NIMG 2015]

Causal reasoning on encoding/decoding

Experimental setting		Feature X_i relevant? Encoding	Decoding	Causal interpretation
	Task	$\times$		$T \perp\!\!\!\perp X_i \Rightarrow X_i$ is no effect of T
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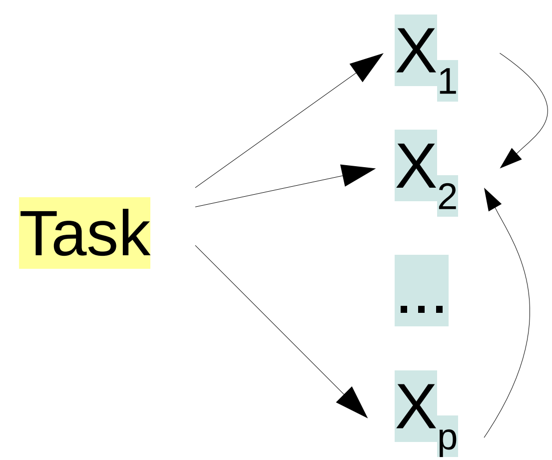
	Task		$\times$	$T \perp\!\!\!\perp X_i \mid \boldsymbol{X} \setminus X_i \Rightarrow$ inconclusive
	Task		$\surd$	$T \not\!\perp\!\!\!\perp X_i \mid \boldsymbol{X} \setminus X_i \Rightarrow$ inconclusive
	Behaviour			
	Behaviour			



[Weichwald et al. NIMG 2015]

Causal reasoning on encoding/decoding

Experimental setting		Feature X_i relevant? Encoding	Decoding	Causal interpretation
Experimental setting	Task	$\times$		$T \perp\!\!\!\perp X_i \Rightarrow X_i$ is no effect of T
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	Task		$\surd$	$T \not\!\perp\!\!\!\perp X_i \mid \boldsymbol{X} \setminus X_i \Rightarrow$ inconclusive
	Behaviour	$\times$		$B \perp\!\!\!\perp X_i \Rightarrow X_i$ is no cause of B
	Behaviour	$\surd$		$B \not\!\perp\!\!\!\perp X_i \Rightarrow$ inconclusive
	Behaviour		$\times$	$B \perp\!\!\!\perp X_i \mid \boldsymbol{X} \setminus X_i \Rightarrow$ inconclusive
	Behaviour		$\surd$	$B \not\!\perp\!\!\!\perp X_i \mid \boldsymbol{X} \setminus X_i \Rightarrow$ inconclusive

[Weichwald et al. NIMG 2015]

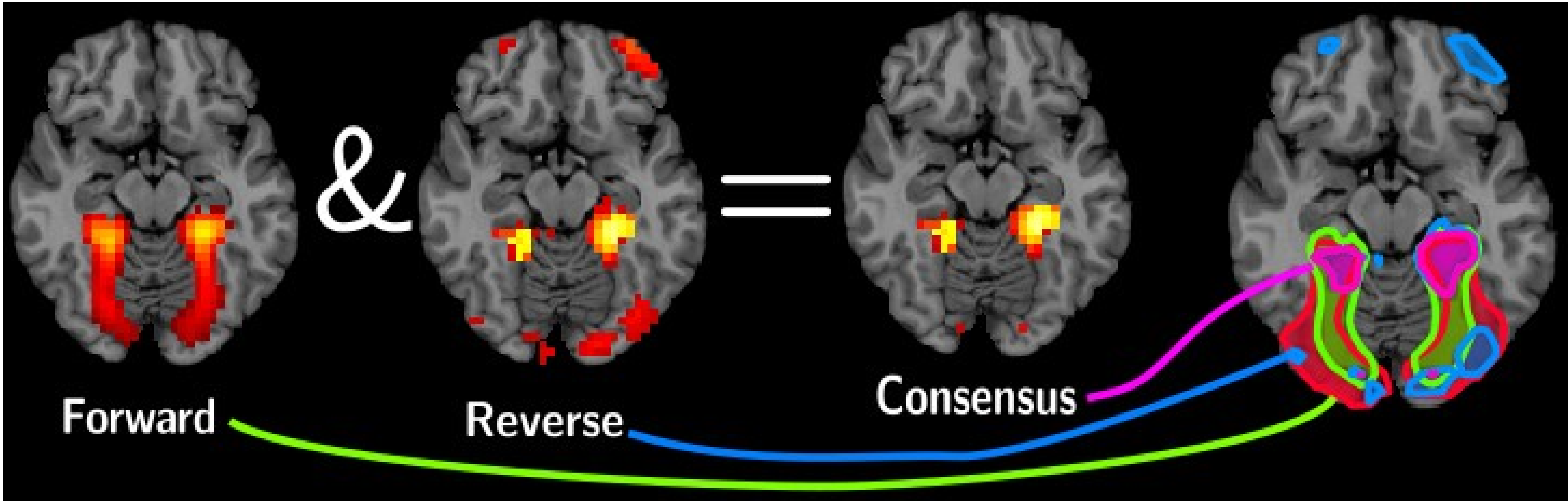
Causal reasoning on encoding/decoding

		Feature X_i relevant? Encoding	Decoding	Causal interpretation
Experimental paradigm	Task	$\times$	$\times$	X_i is no effect of T
		$\surd$	$\times$	X_i is an indirect effect of T
		$\times$	$\surd$	X_i provides context
		$\surd$	$\surd$	X_i is an effect of T
	Behaviour	$\times$	$\times$	X_i is no cause of B
		$\surd$	$\times$	X_i is no direct cause of B
		$\times$	$\surd$	X_i provides context
		$\surd$	$\surd$	inconclusive

[Weichwald et al. NIMG 2015]

Joint encoding and decoding

Brain response to the task: “view a place image”



“Encoding” “Decoding”

Decoding solves a difficult inverse problem: noisy estimates [Haufe et al. Nimg 2014, Chevalier et al. MICCAI 2018]

[Schwartz et al. NIPS 2013, Varoquaux et al. PCB 2018]

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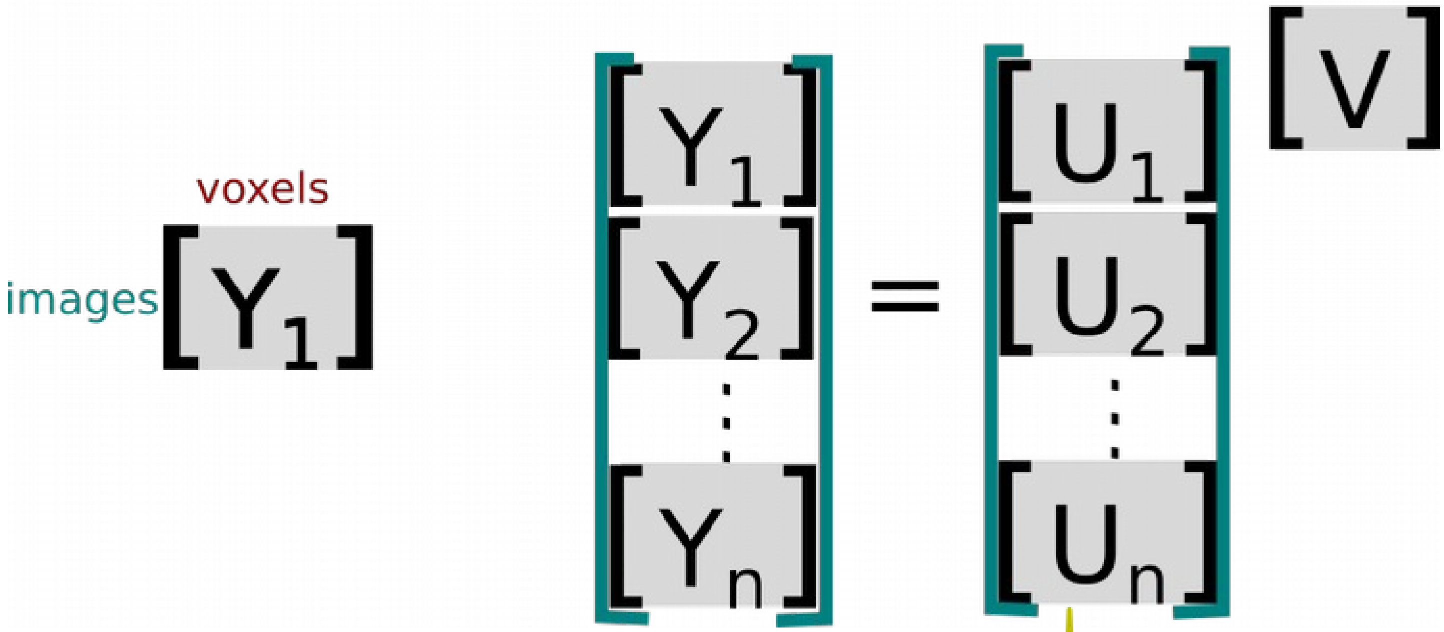
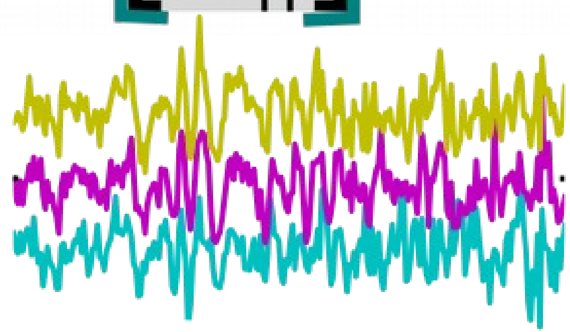
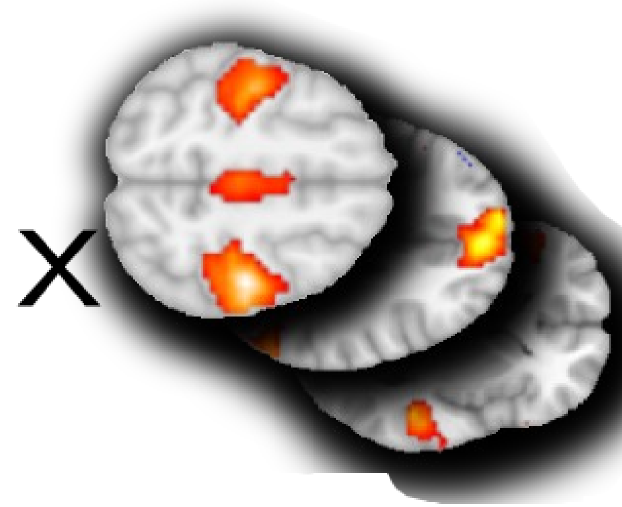
Learning representation of fMRI data







$$\min_{\mathbf{V},\mathbf{U}:\|\mathbf{U}_k\|\leq 1,\forall k} \|\mathbf{Y} - \mathbf{U}\mathbf{V}^T\|^2 + \lambda\|\mathbf{V}\|_1$$

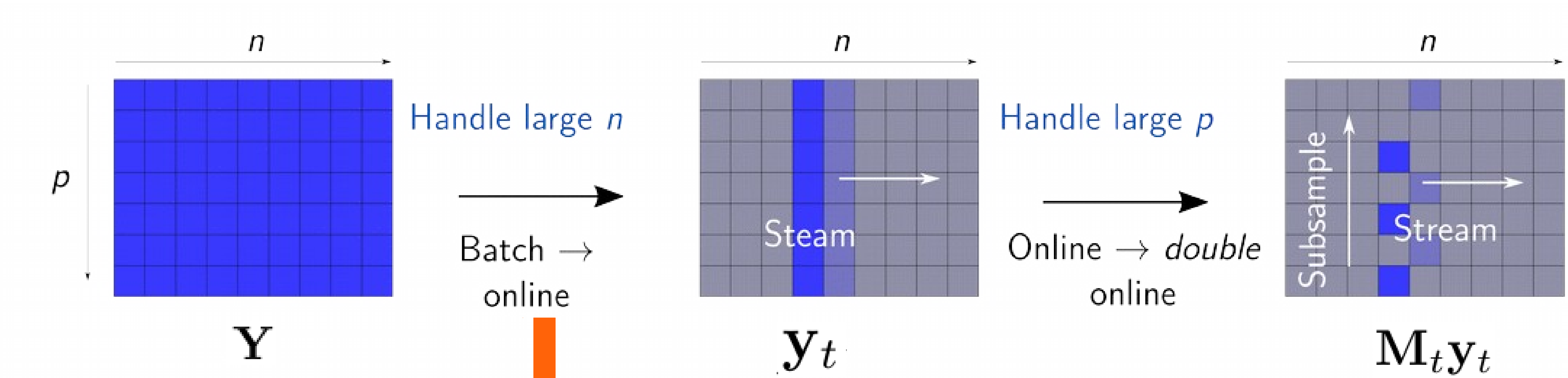
Concatenation mode for multi-subject → long “time courses”

Huge ?

- Human Connectome project $n=4.10^6$, $p=2.10^5$, 4**TB** of data
- Spatially-concatenated DL [varoquaux IPMI 2013] does not scale well:
  - Requires loading the data [Mensch et al. ISBI 2016]
- Solution
  - Work on batches of images **and** voxels
    - Online method in both samples and feature dimensions

Stochastic gradient approaches

http://amensch.fr/research/2016/06/10/modl.html



$$\mathbf{u}_t(\mathbf{V}) = \operatorname{argmin}_{\mathbf{u}\in\mathbb{R}^{n\times k}} \|\mathbf{y}_t - \mathbf{u}\mathbf{V}\|_F^2 + \lambda\Omega(\mathbf{u})$$

$$\mathbf{V}_t = \operatorname{argmin}_{\mathbf{V}\in\mathcal{C}} \sum_{i=1}^{t} \|\mathbf{y}_i - \mathbf{u}_i\mathbf{V}\|_F^2$$

$$\mathbf{u}_t(\mathbf{V}) = \operatorname{argmin}_{\mathbf{u}\in\mathbb{R}^{n\times k}} \|\mathbf{M}_t\left(\mathbf{y}_t - \mathbf{u}\mathbf{V}\right)\|_F^2$$
$$\lambda\frac{s}{p}\Omega(\mathbf{u})$$

Stochastic gradient approaches

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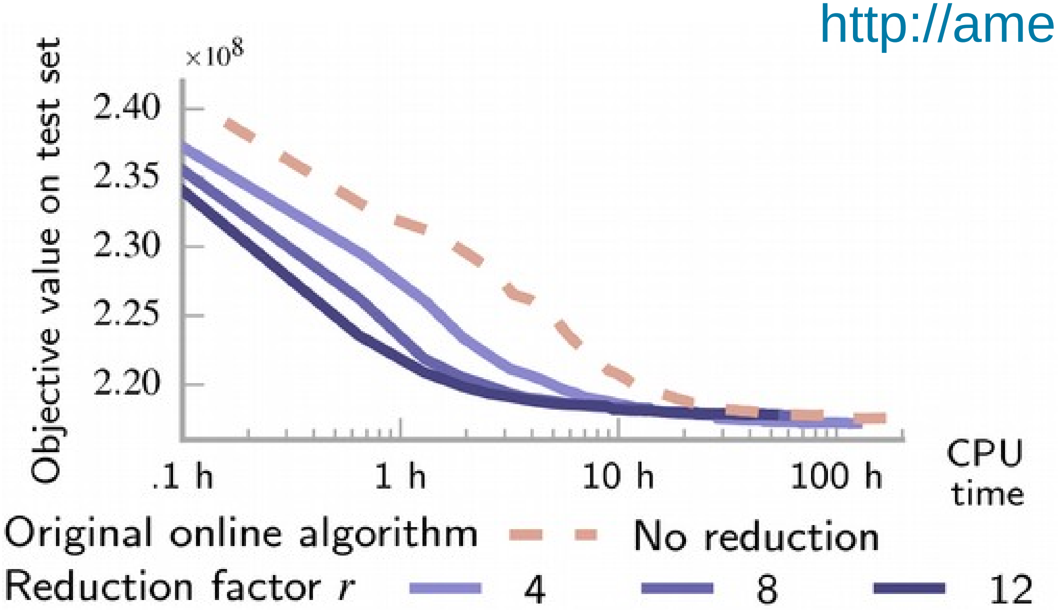
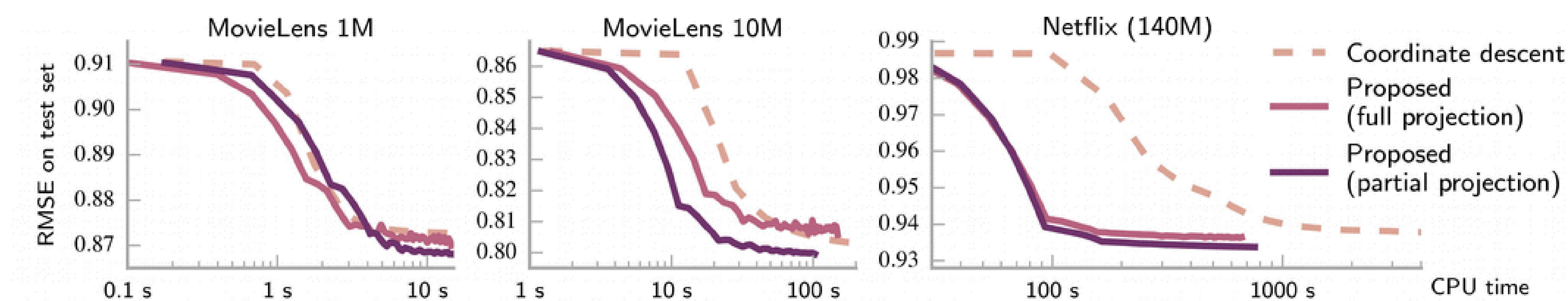


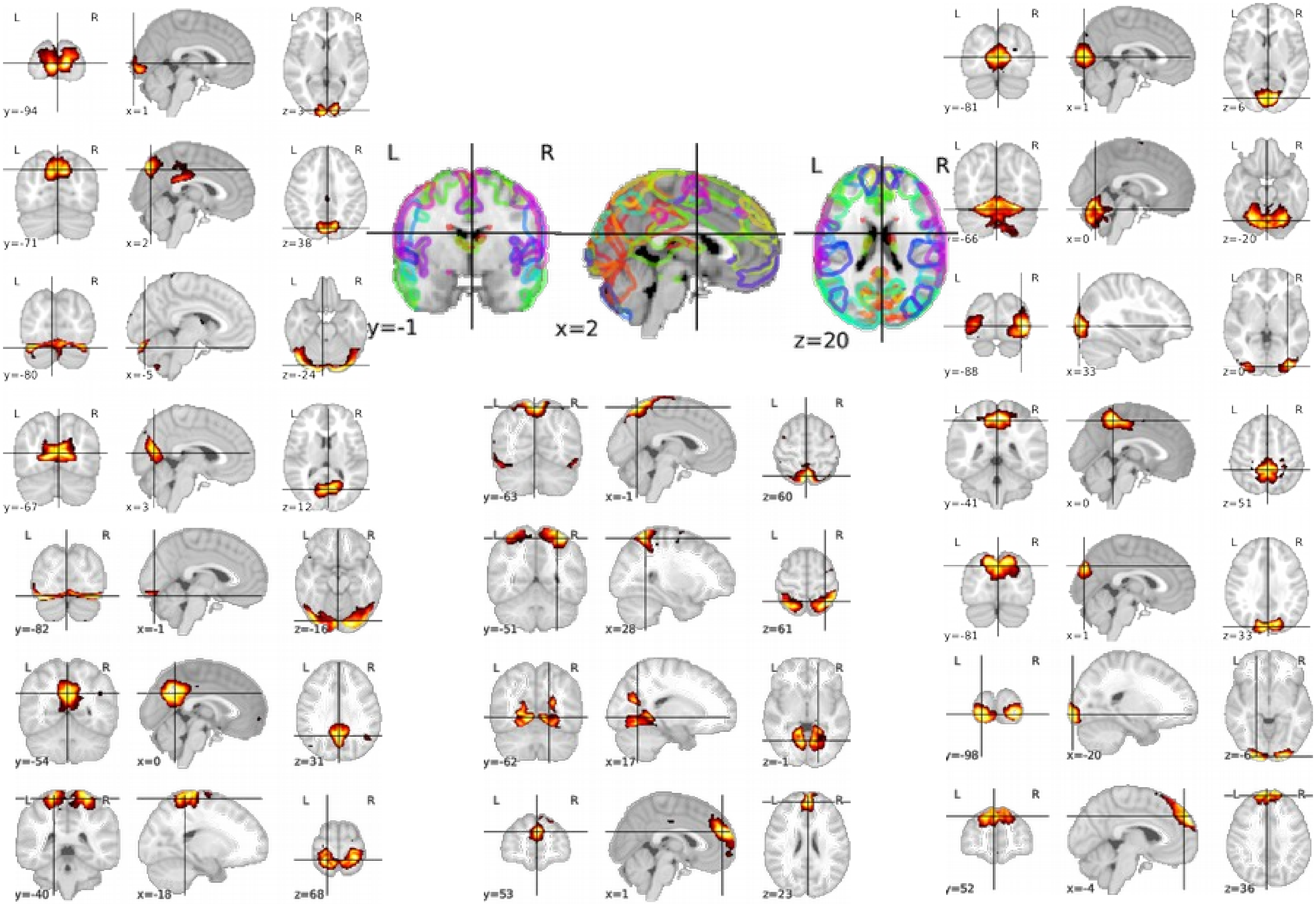
10-fold gain in CPU time
without loss in accuracy

[Mensch et al. IEEE TSP 2018]

Can be used for recommender systems



Brain atlases



[Mensch et al. ICML 2016]

Brain atlases from fMRI data

- Relax clustering into spatio-temporal decompositions
- Sparse-/smooth- PCA algorithms perform well
  - Fine-tuning to individual configuration is expensive
  - Sophisticated penalties (TV + l1…) are expensive
- Development of online methods to scale to large data [Mairal et al. JMLR 2010, Mensch et al. ICML 2016, IEEE TSP 2018]

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The big data revolution is ongoing – in neuroimaging also !

Nature Reviews Neuroscience | AOP, published online 10 April 2013; doi:10.1038/nrn3475

nature REVIEWS

Power failure: why small sample size undermines the reliability of neuroscience

Katherine S. Button[1,2], John P. A. Ioannidis[3], Claire Mokrysz[1], Brian A. Nosek[4], Jonathan Flint[5], Emma S. J. Robinson[6] and Marcus R. Munafò[1]

https://en.wikipedia.org/wiki/Replication_crisis

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nature REVIEWS NEUROSCIENCE

Analysis | Published: 05 January 2017

Scanning the horizon: towards transparent and reproducible neuroimaging research

Russell A. Poldrack, Chris I. Baker, Joke Durnez, Krzysztof J. Gorgolewski, Paul M. Matthews, Marcus R. Munafò, Thomas E. Nichols, Jean-Baptiste Poline, Edward Vul & Tal Yarkoni

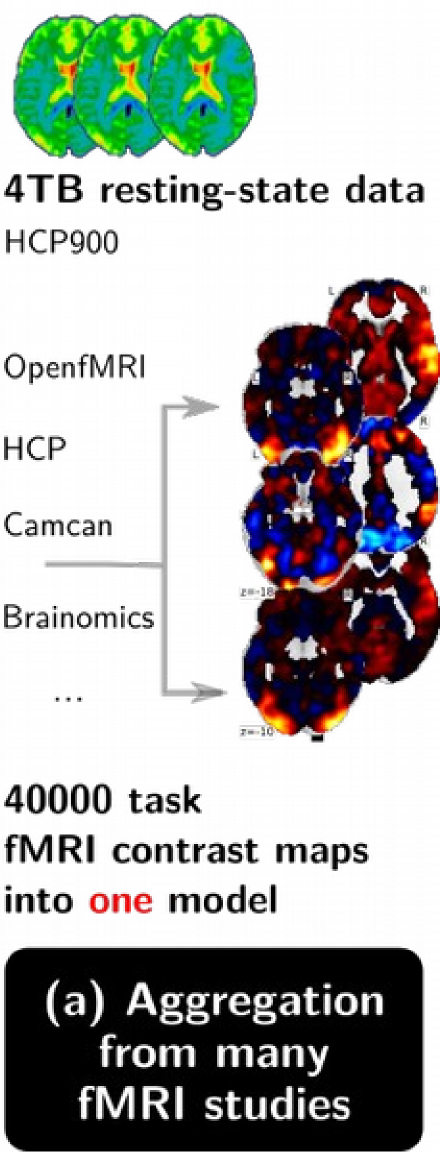
Problem: generalization across studies

"You cannot play 20 questions with nature and win"

- Coordinated analysis: Use large studies to inform small studies ("transfer learning")
  - Principle: co-analyse studies, leverage joint representations
- joint/mega-analysis: find semantic commonalities across studies
  - Difficulty: what common vocabulary across studies?

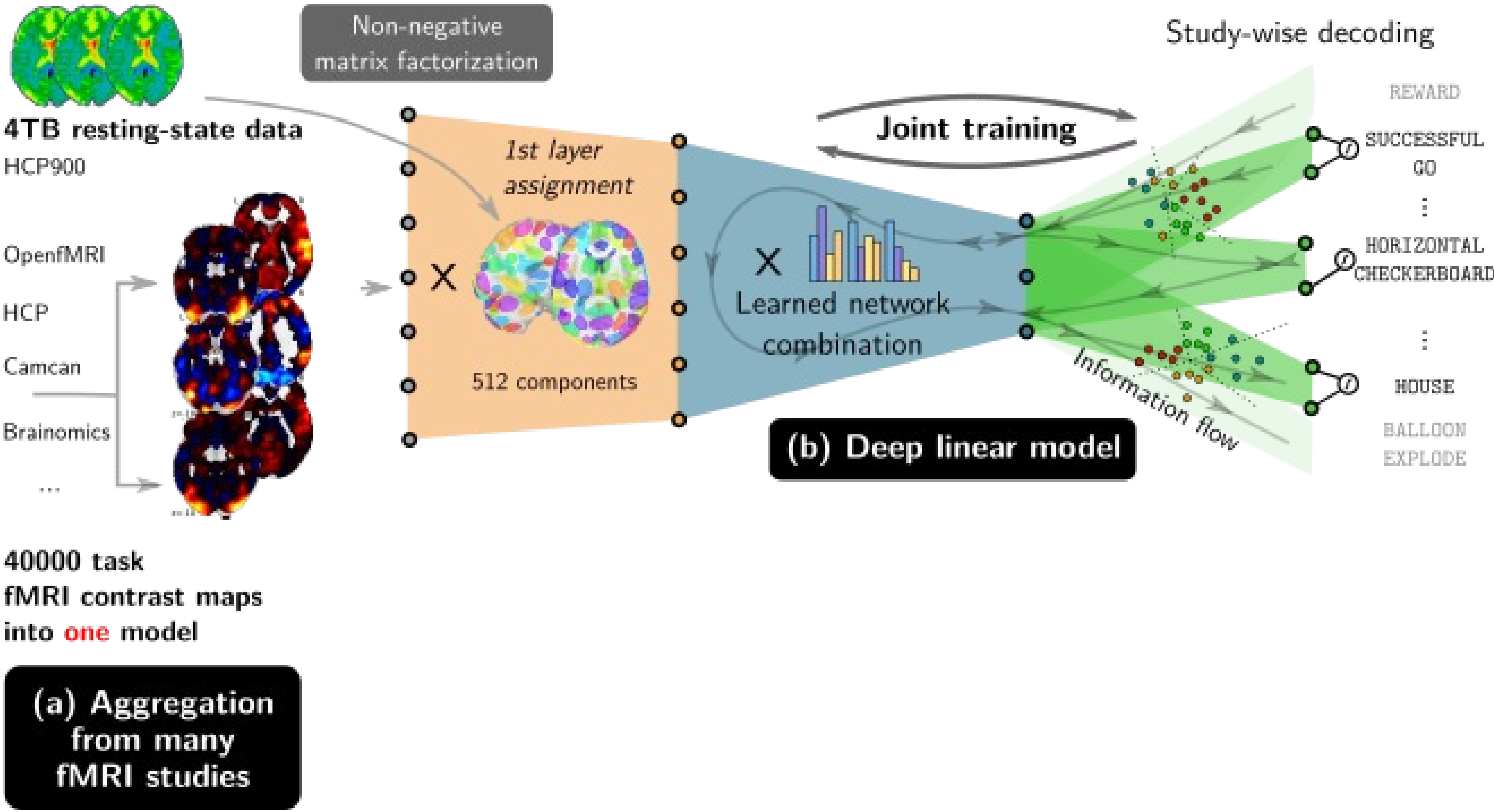
Large studies to inform analysis of small studies: coordinated decoding

Predictive modeling across datasets



[Bzdok et al. Plos Comp Biol 2016, Mensch et al NIPS 2017]

Predictive modeling across datasets



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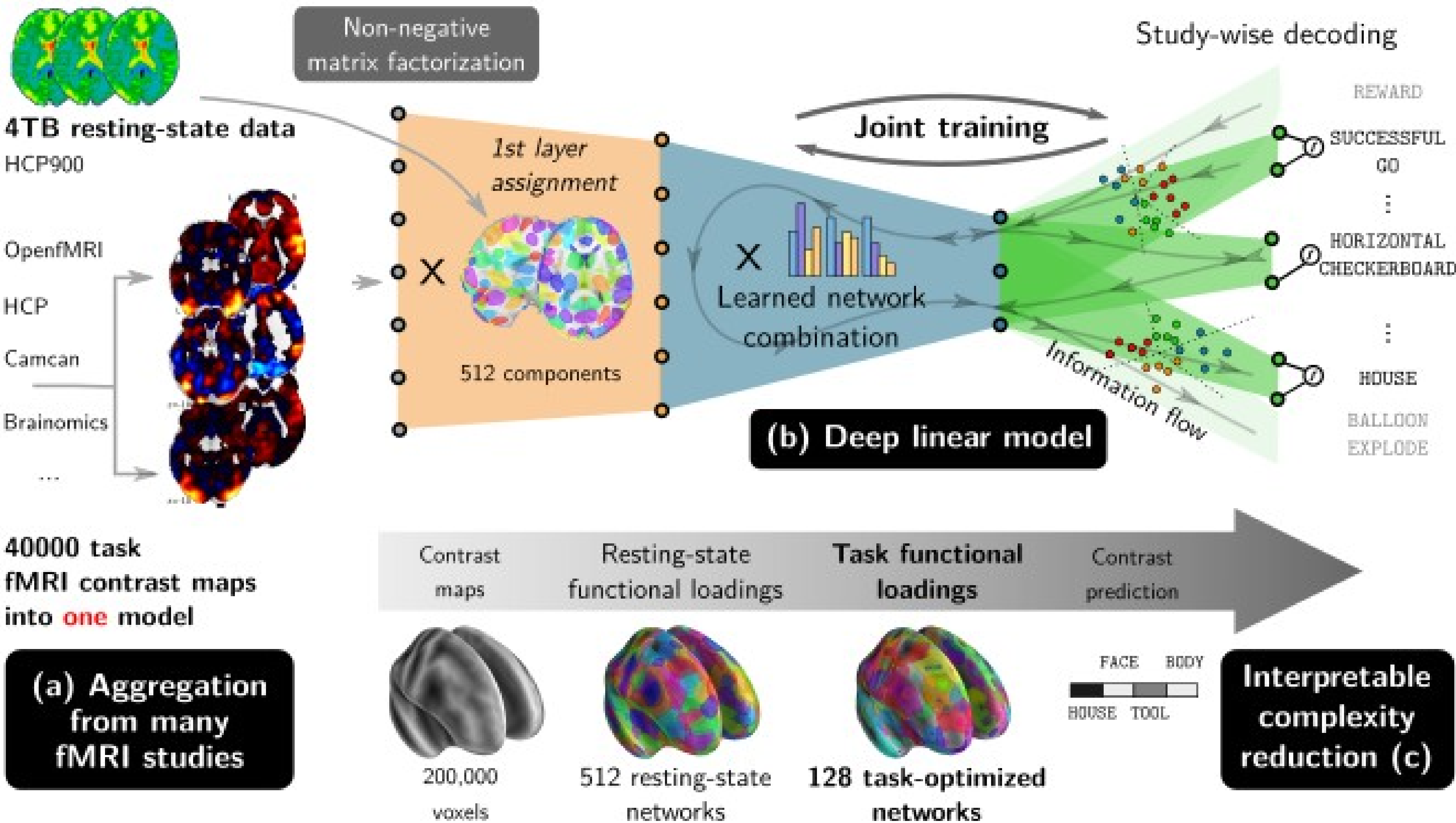
Predictive modeling across datasets



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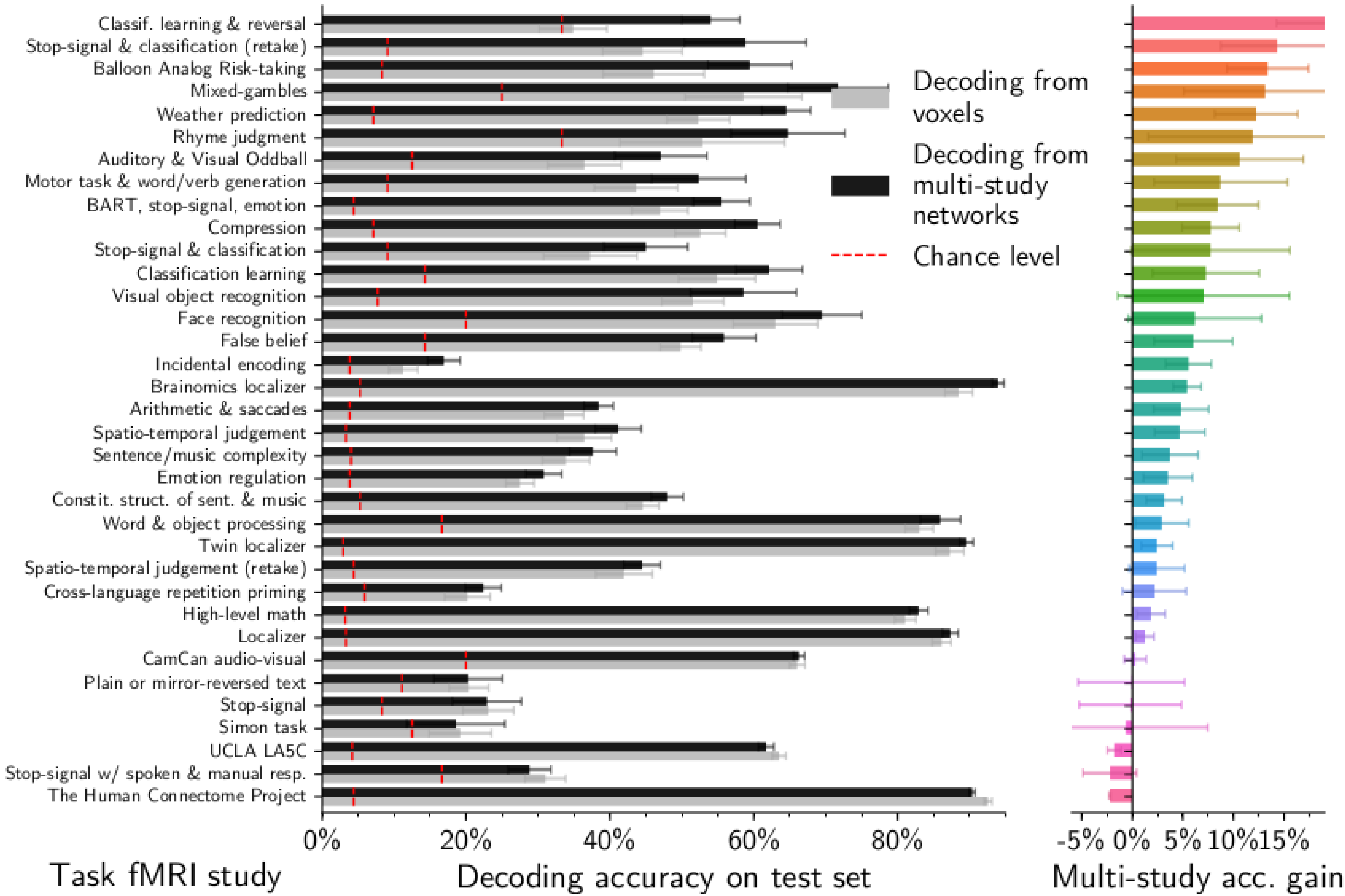
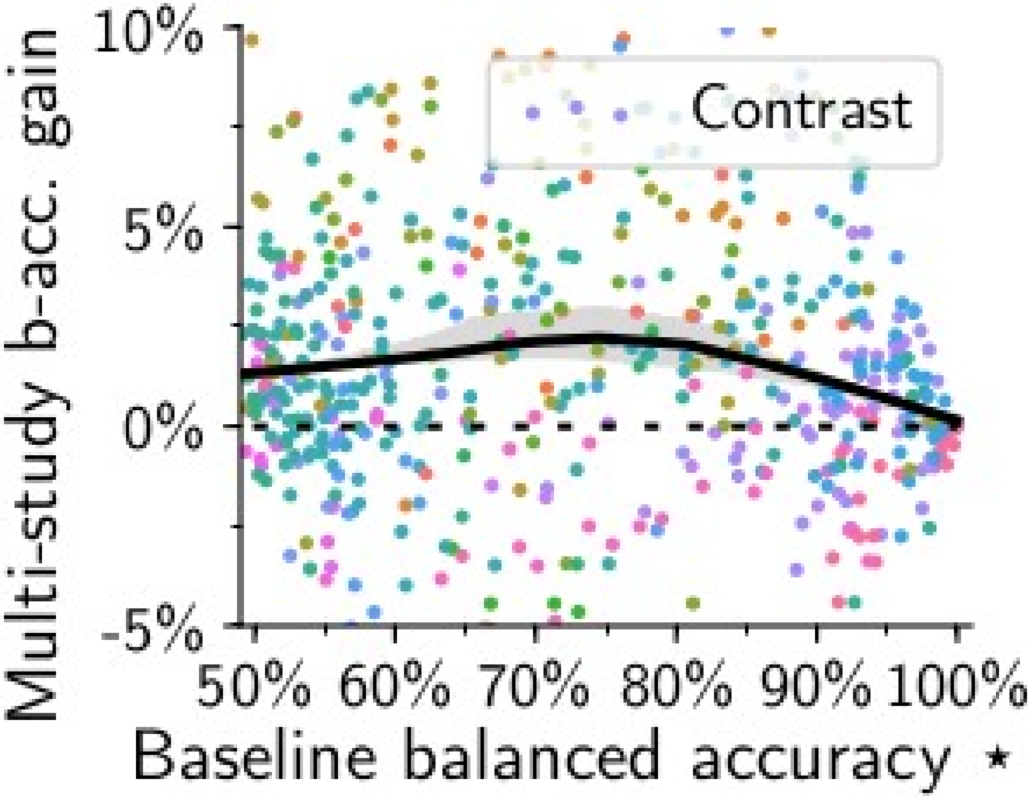
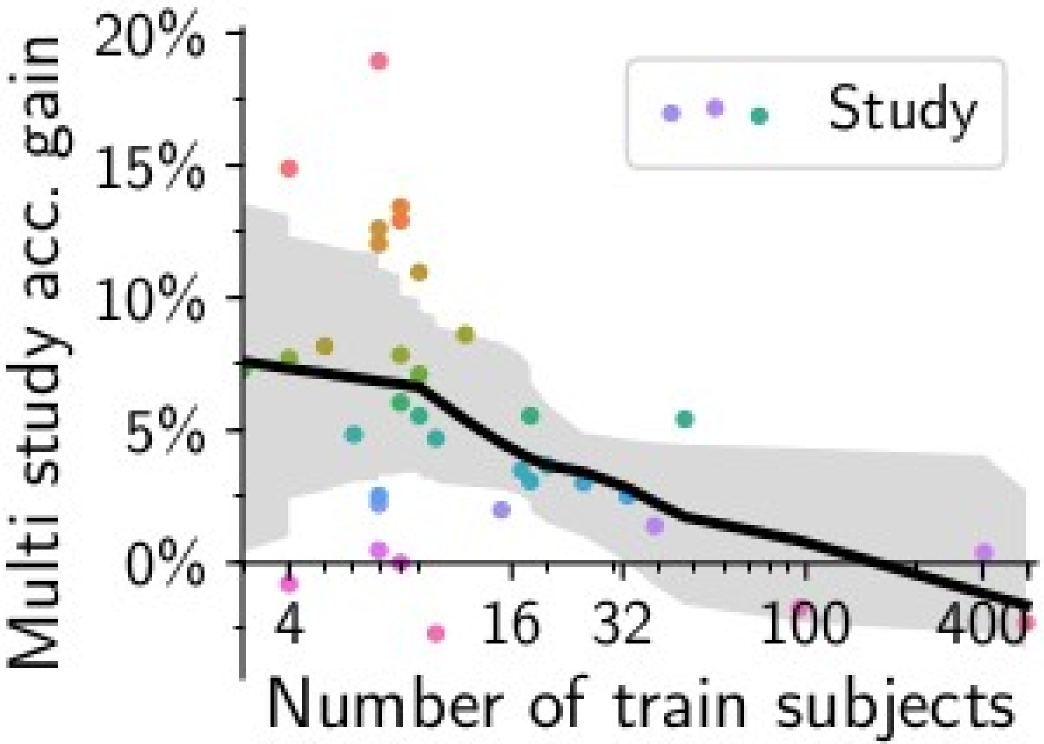
Transfer learning

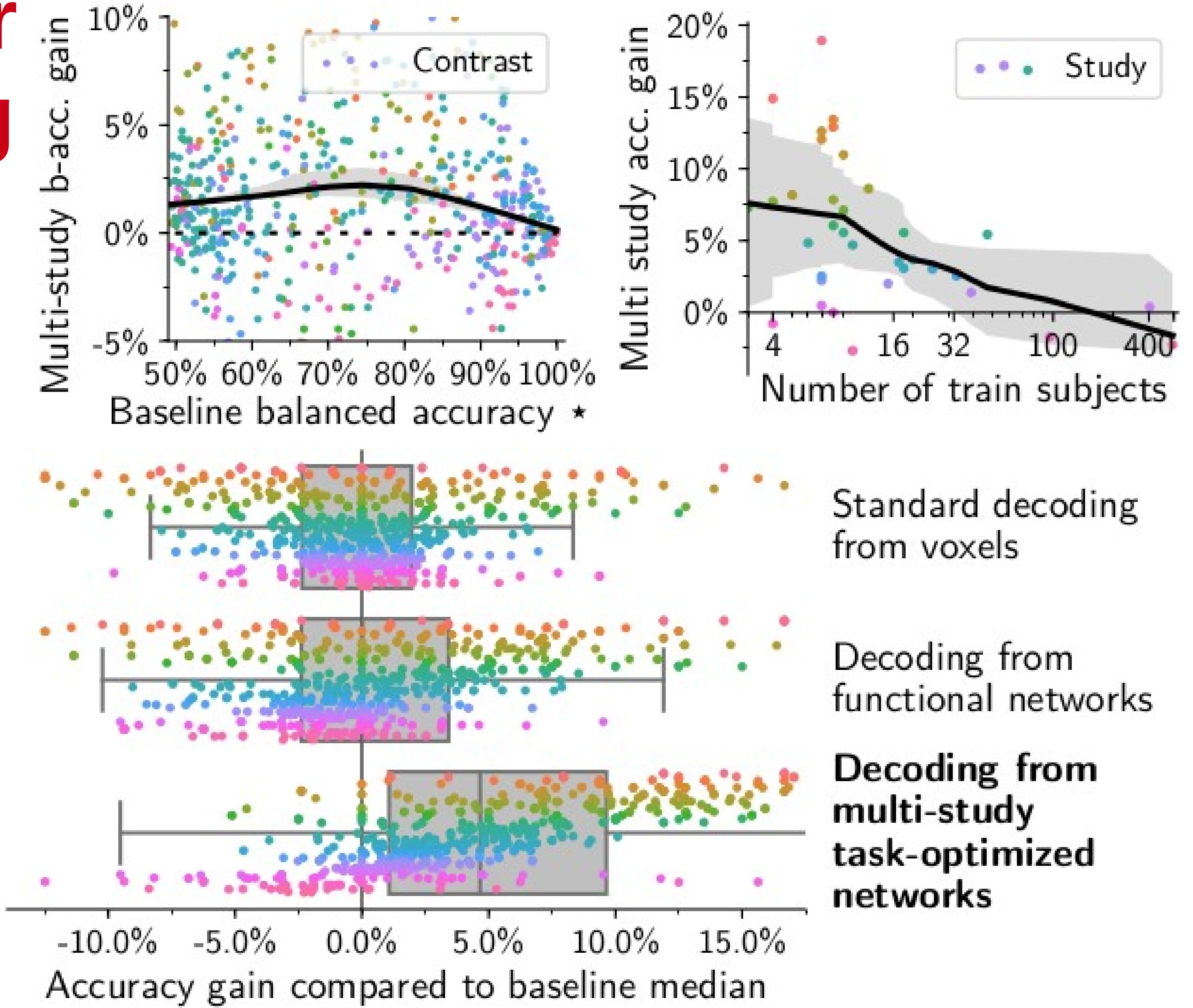


Transfer learning

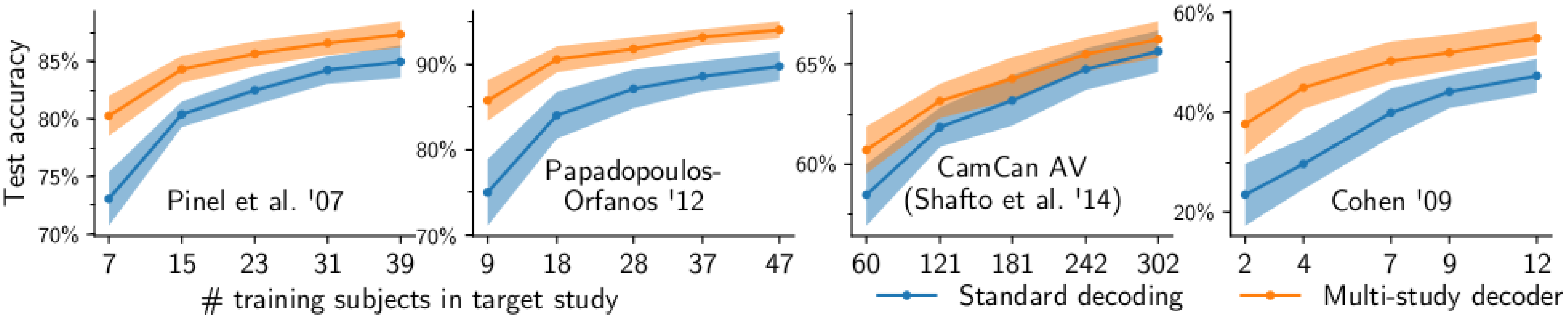




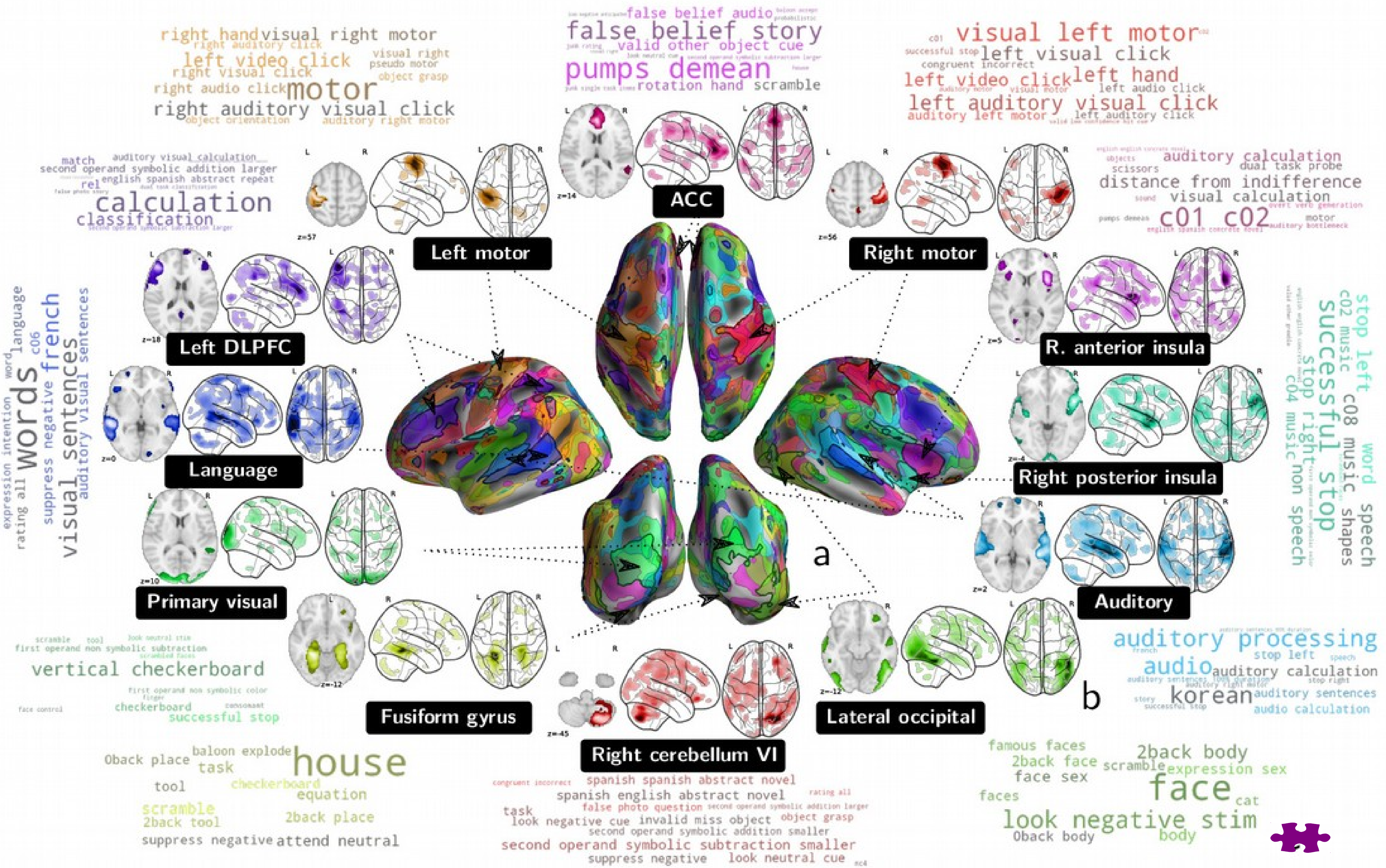
Transfer learning



Small studies benefit more than large studies



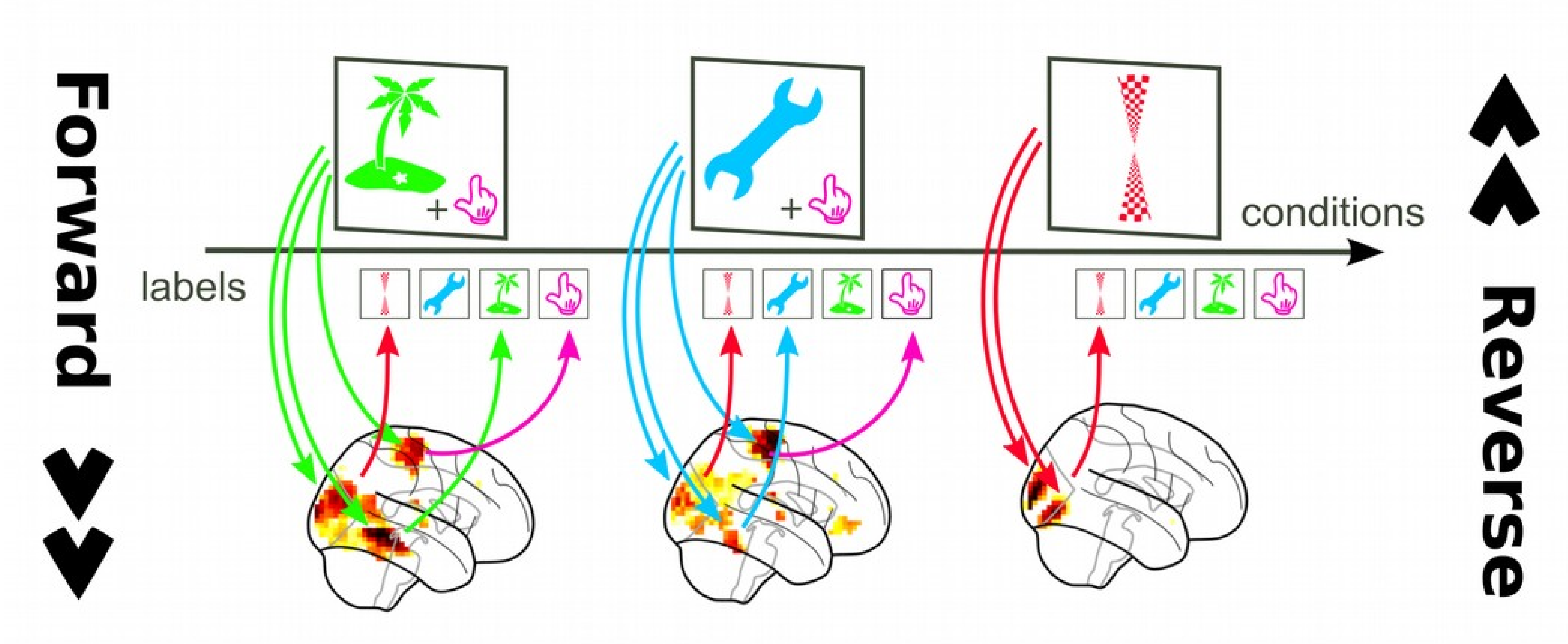
Resulting atlas



Joint decoding aka Mega-analyses

[Costafreda et al. Front. Neuroinf. 2009]

Indentifying cognitive tasks in brain activity



An image database

Task fMRI repository
[Gorgolewski et al. 2015]

Currently 48k independent usable fMRIs

[Poldrack 2011], knowledge-base

- *concepts*: cognitive activity/state (e.g. working memory)
- *tasks*: standard experiment to probe it (e.g. n-back task)

Forward inference

What is the brain response common to these stimuli?

Which regions are recruited by tasks containing a given term?

- Linear Model for terms effects

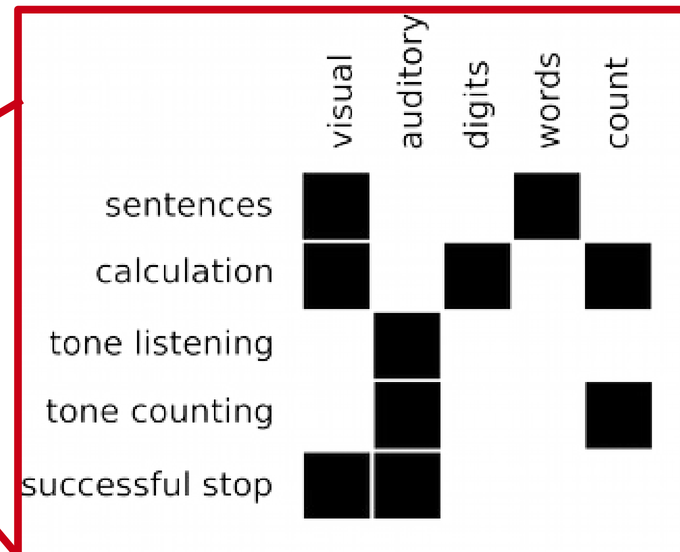
$$X = Y\beta + \varepsilon$$

X Conditions images

Y Design matrix

β Terms effect

ε Error

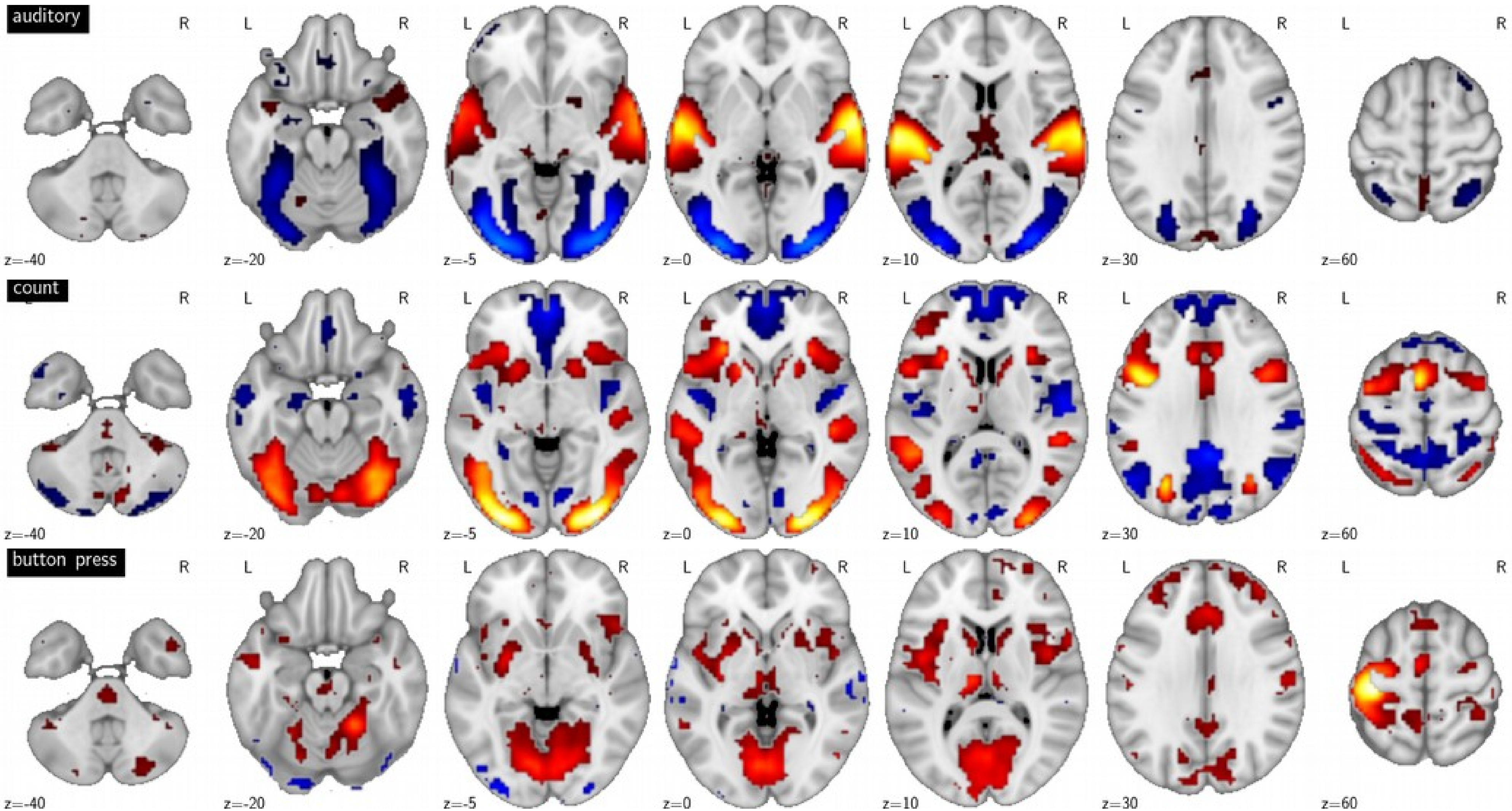


Forward inference

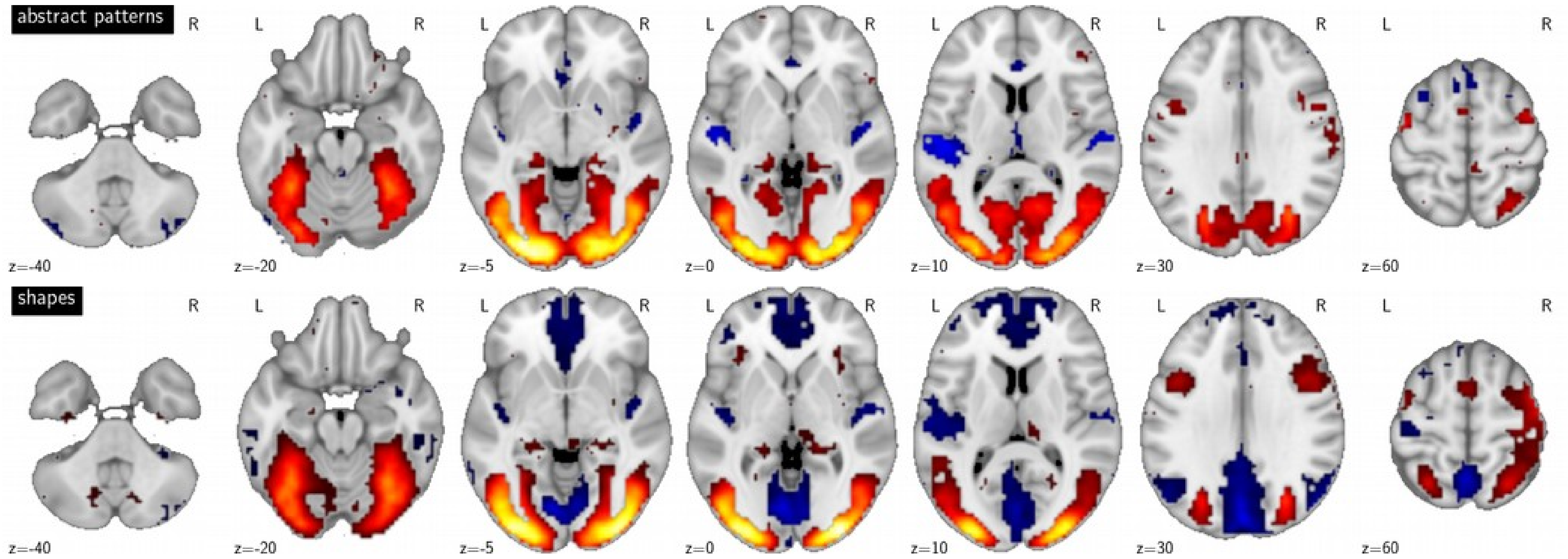
Correlation of the design matrix: difficulties from the heavily correlated terms (database bias)

	visual	auditory	digits	face	patterns	scramble	saccades	none	button press	count	inhibit	discriminate	read	move	track	sounds	shapes	attend	words
visual	+1.0	-0.9	+0.0	+0.1	+0.1	+0.1	+0.1	-0.1	+0.1	-0.1	-0.0	+0.2	+0.4	-0.2	+0.1	-0.3	+0.2	-0.3	-0.1
auditory	-0.9	+1.0	-0.0	-0.1	-0.2	-0.1	-0.1	+0.1	-0.2	+0.0	+0.2	-0.3	-0.2	+0.2	-0.1	+0.4	-0.2	+0.3	+0.2
digits	+0.0	-0.0	+1.0	-0.1	-0.1	-0.1	-0.1	+0.3	-0.3	+0.8	-0.1	-0.2	-0.1	-0.2	-0.1	-0.1	-0.1	-0.2	-0.4
face	+0.1	-0.1	-0.1	+1.0	-0.1	-0.0	-0.0	+0.1	-0.1	-0.0	-0.0	-0.0	-0.1	-0.1	-0.0	-0.0	-0.0	+0.2	-0.1
patterns	+0.1	-0.2	-0.1	-0.1	+1.0	-0.1	-0.1	-0.0	+0.1	-0.1	+0.1	+0.3	-0.2	-0.2	-0.1	+0.0	-0.1	+0.1	-0.4
scramble	+0.1	-0.1	-0.1	-0.0	-0.1	+1.0	-0.0	-0.0	+0.0	-0.1	-0.0	+0.1	-0.1	-0.1	-0.0	-0.1	-0.1	+0.1	-0.2
saccades	+0.1	-0.1	-0.1	-0.0	-0.1	-0.0	+1.0	-0.2	-0.1	-0.1	-0.0	-0.1	-0.1	-0.1	+0.9	-0.1	+0.5	-0.1	-0.2
none	-0.1	+0.1	+0.3	+0.1	-0.0	-0.0	-0.2	+1.0	-0.9	+0.2	-0.0	-0.5	+0.1	-0.5	-0.2	+0.1	-0.1	+0.6	-0.2
button press	+0.1	-0.2	-0.3	-0.1	+0.1	+0.0	-0.1	-0.9	+1.0	-0.2	-0.1	+0.6	-0.1	+0.5	-0.1	-0.2	+0.0	-0.5	+0.2
count	-0.1	+0.0	+0.8	-0.0	-0.1	-0.1	-0.1	+0.2	-0.2	+1.0	-0.1	-0.1	-0.2	-0.1	-0.1	+0.0	-0.1	-0.2	-0.4
inhibit	-0.0	+0.2	-0.1	-0.0	+0.1	-0.0	-0.0	-0.0	-0.1	-0.1	+1.0	+0.1	+0.1	-0.1	-0.0	+0.5	-0.1	-0.1	+0.0
discriminate	+0.2	-0.3	-0.2	-0.0	+0.3	+0.1	-0.1	-0.5	+0.6	-0.1	+0.1	+1.0	+0.0	-0.2	-0.1	-0.0	+0.1	-0.4	-0.1
read	+0.4	-0.2	-0.1	-0.1	-0.2	-0.1	-0.1	+0.1	-0.1	-0.2	+0.1	+0.0	+1.0	-0.2	-0.1	-0.0	-0.2	-0.4	+0.5
move	-0.2	+0.2	-0.2	-0.1	-0.2	-0.1	-0.1	-0.5	+0.5	-0.1	-0.1	-0.2	-0.2	+1.0	-0.1	-0.1	-0.1	-0.3	+0.4
track	+0.1	-0.1	-0.1	-0.0	-0.1	-0.0	+0.9	-0.2	-0.1	-0.1	-0.0	-0.1	-0.1	-0.1	+1.0	-0.1	+0.5	-0.1	-0.2
sounds	-0.3	+0.4	-0.1	-0.0	+0.0	-0.1	-0.1	+0.1	-0.2	+0.0	+0.5	-0.0	-0.0	-0.1	-0.1	+1.0	-0.1	+0.2	-0.2
shapes	+0.2	-0.2	-0.1	-0.0	-0.1	-0.1	+0.5	-0.1	+0.0	-0.1	-0.1	+0.1	-0.2	-0.1	+0.5	-0.1	+1.0	+0.0	-0.3
attend	-0.3	+0.3	-0.2	+0.2	+0.1	+0.1	-0.1	+0.6	-0.5	-0.2	-0.1	-0.4	-0.4	-0.3	-0.1	+0.2	+0.0	+1.0	-0.2
words	-0.1	+0.2	-0.4	-0.1	-0.4	-0.2	-0.2	-0.2	+0.2	-0.4	+0.0	-0.1	+0.5	+0.4	-0.2	-0.2	-0.3	-0.2	+1.0

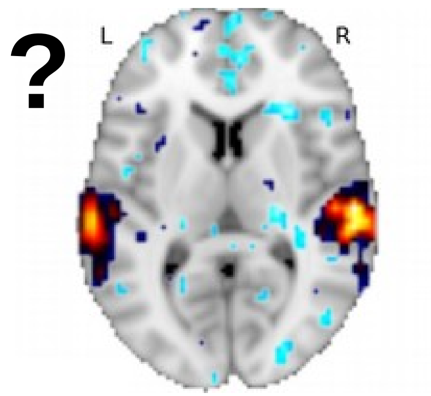
Results of forward inference



Limittaions of forward inference



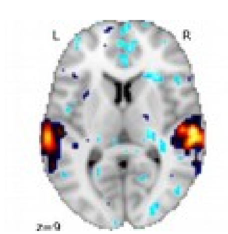
Open-ended brain decoding



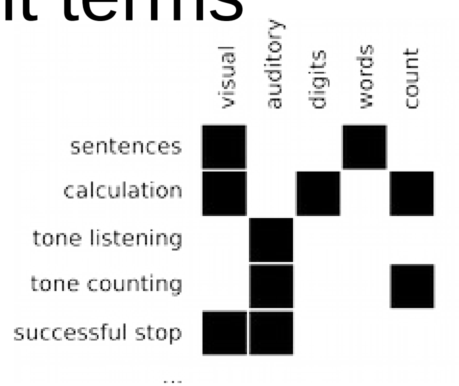
What is
this brain doing?

Which regions are predictive of tasks containing a given term?

- **Multilabel** classification problem
  - more than one class may be associated with each sample
- Predict occurrence of frequent terms



Data: experimental condition images



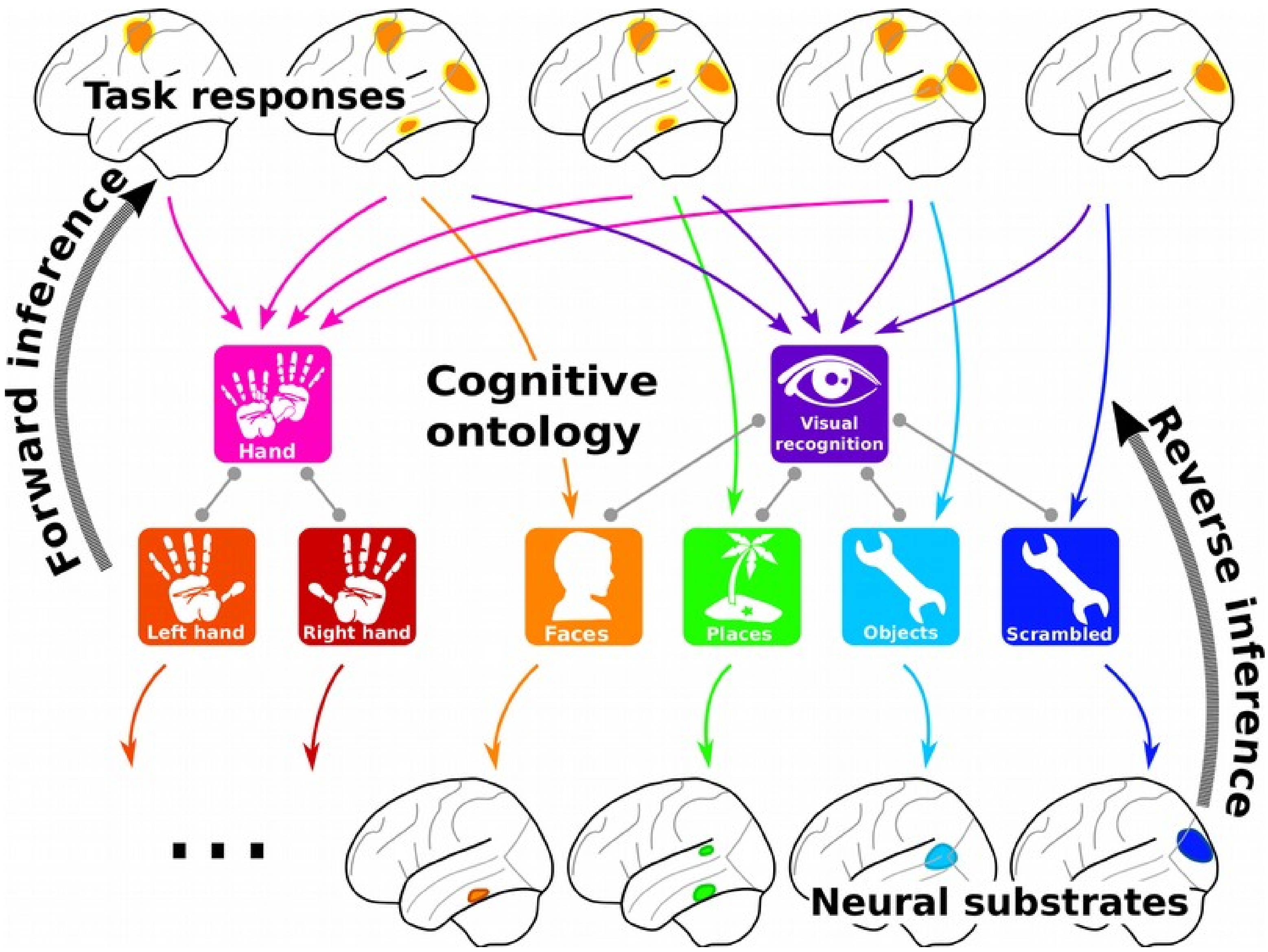
Target

Beyond cognitive tasks: decoding concepts

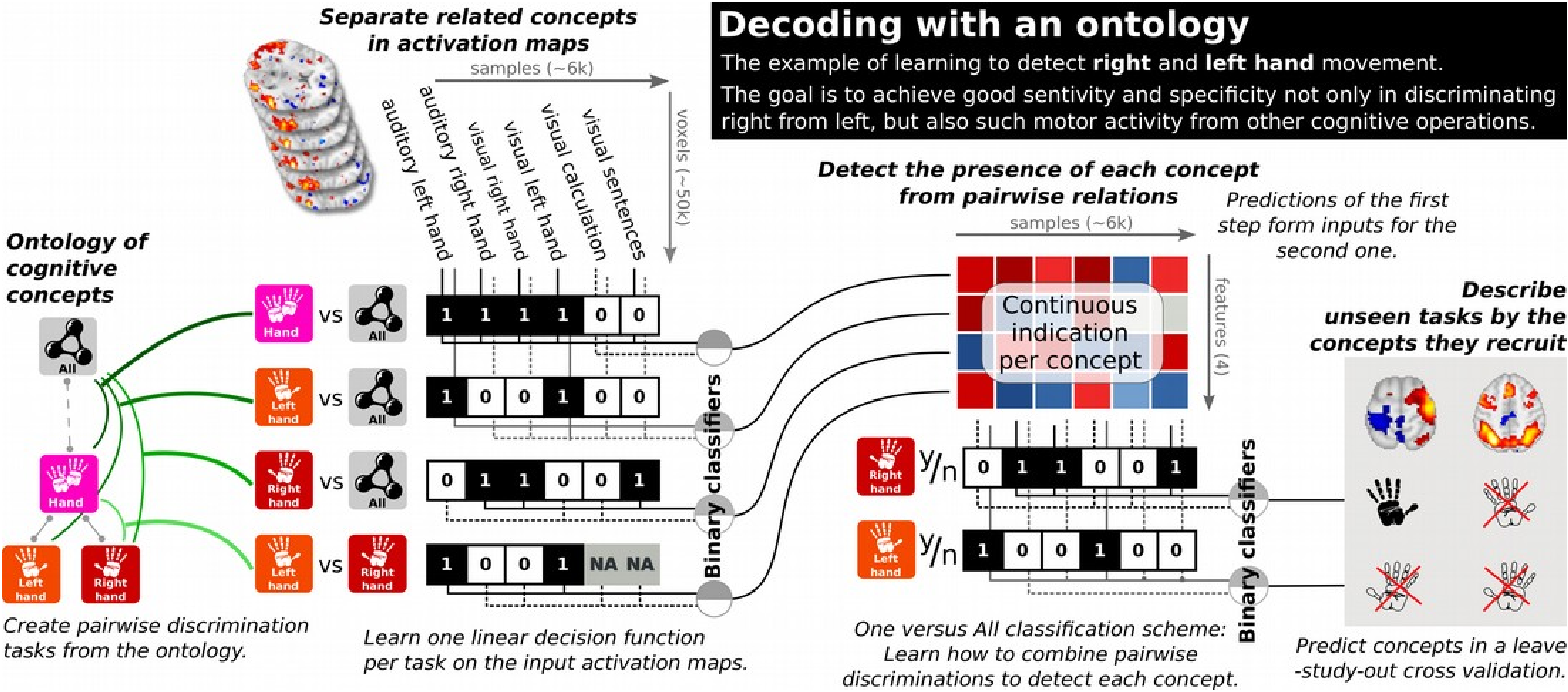
Task Level

Concept Level

Cognitive modules

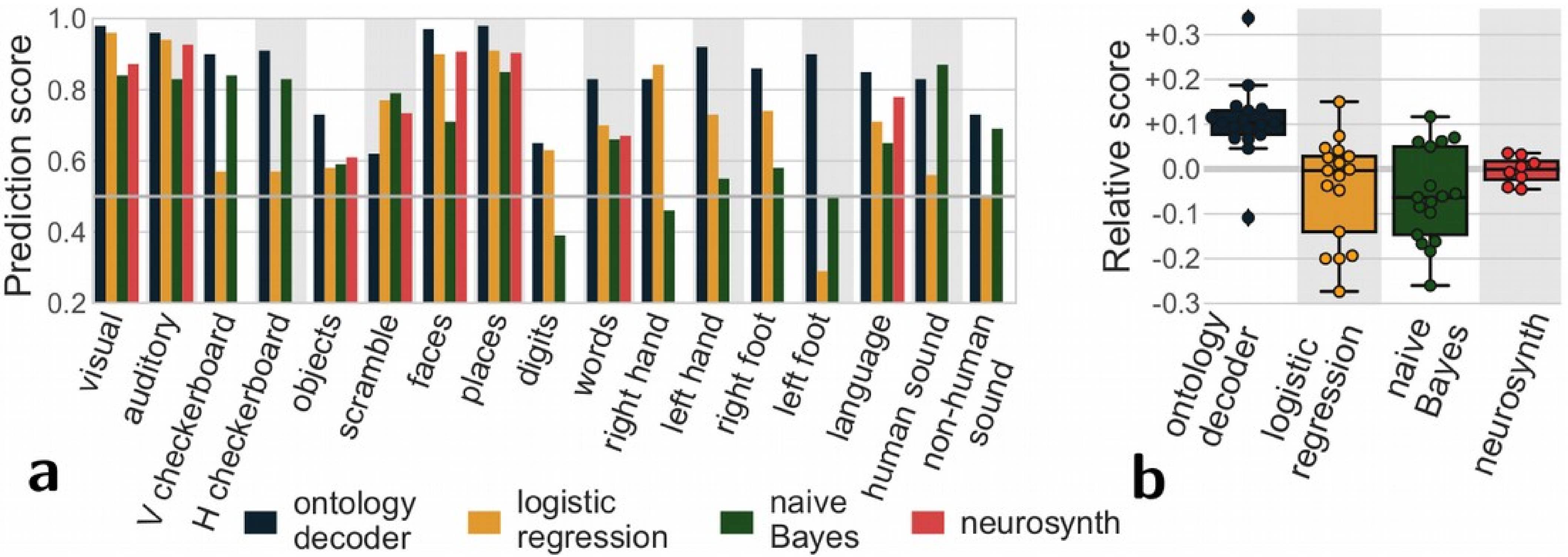


A classifier for mega-analyses



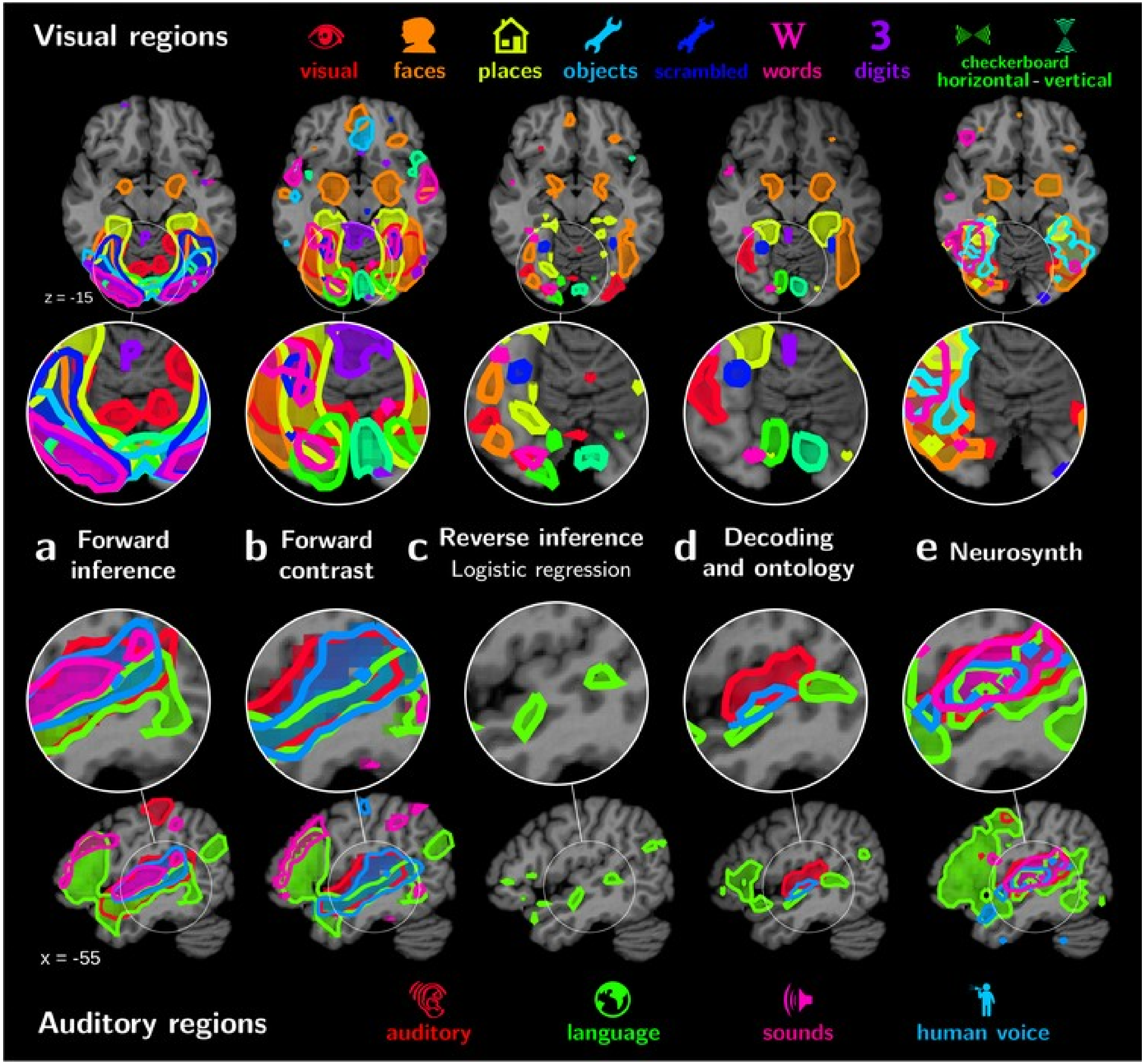
[Schwartz et al. NIPS 2013, Varoquaux et al. PCB 2018]

Classification results

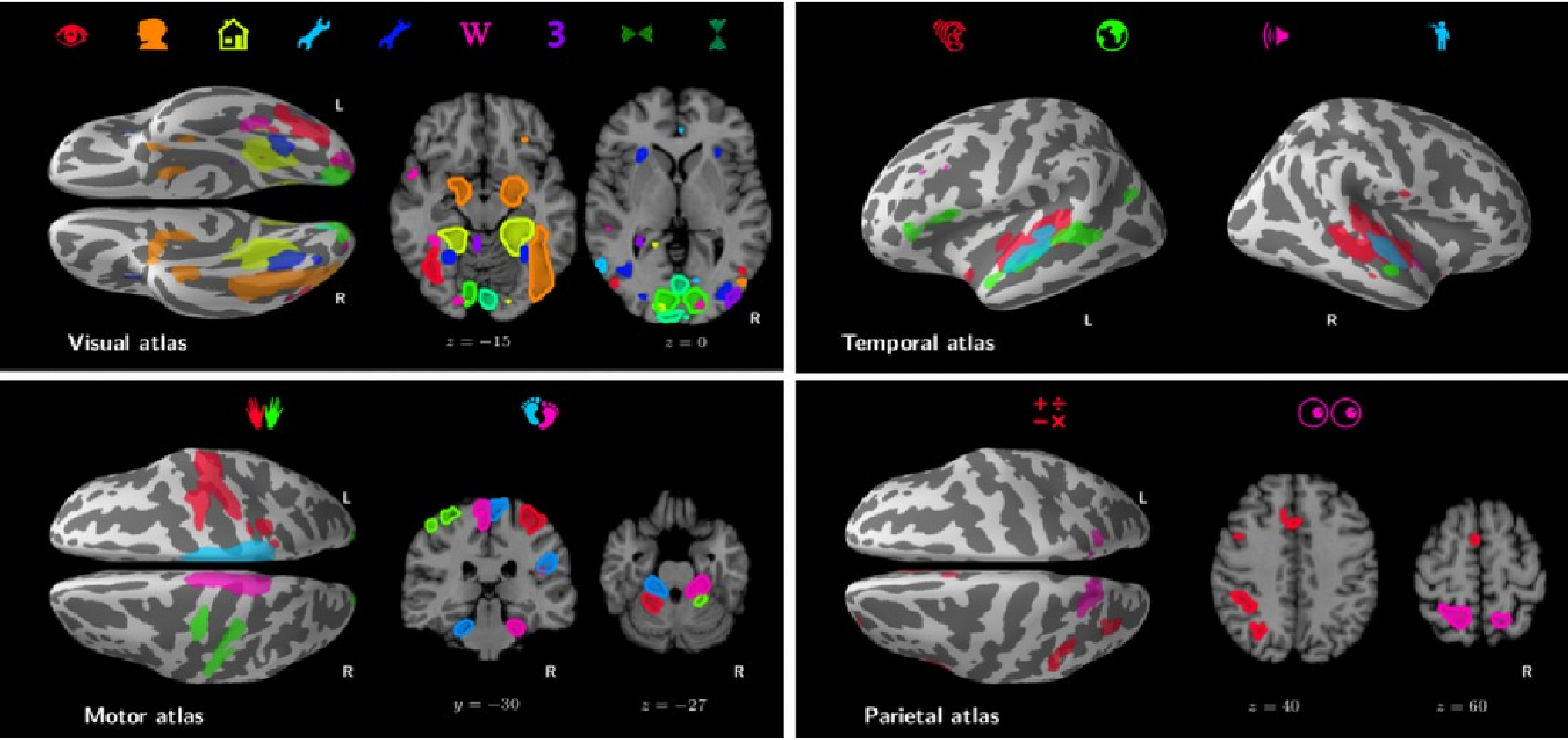


[Schwartz et al. NIPS 2013, Varoquaux et al. PCB 2018]

Decoding maps



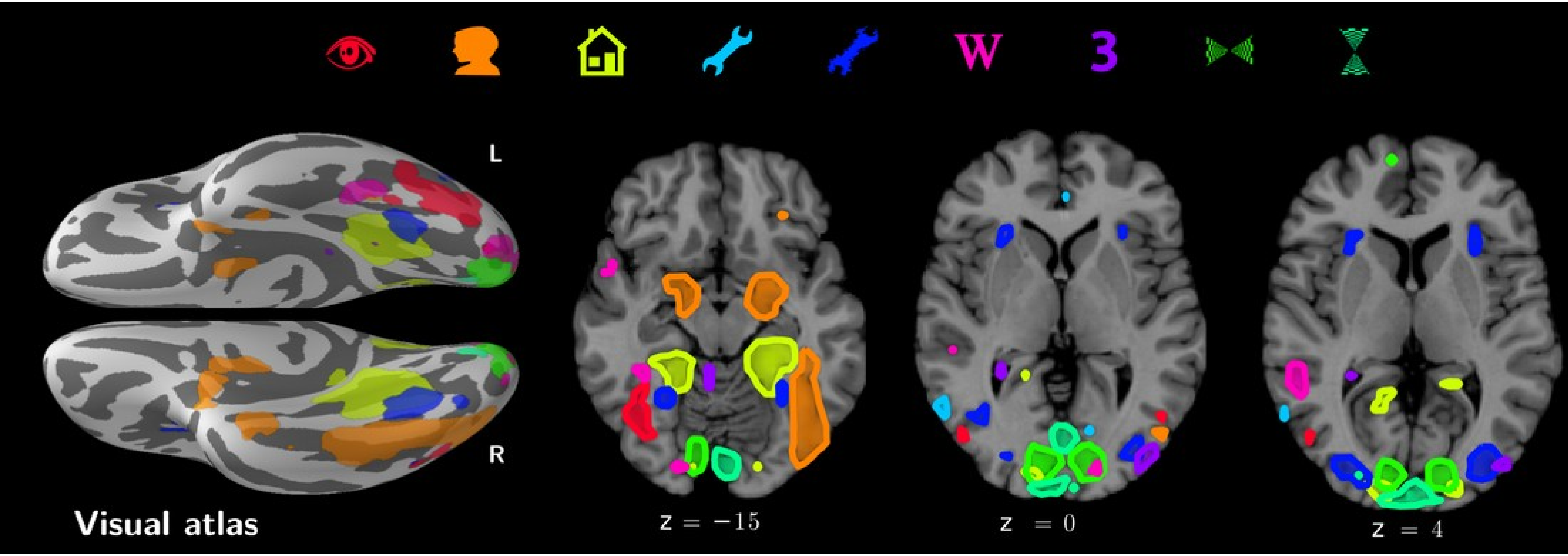
Discriminative patterns



[Schwartz et al. NIPS 2013, Varoquaux et al. PCB 2018.]

Predicting versus identifying

- Unlike BCI, classification performance is not the main goal
- The task you're interested in is unsupervised:
  - Understand the functional specificity of brain regions



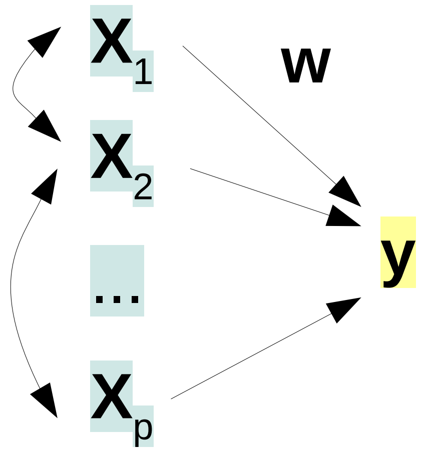
Outline

- Why is decoding important ? A causal persepective
- Intermezzo: Learning representations for brain images with dictionary learning
- Large-scale brain activity decoding
  - coordinated decoding
  - Joint decoding
- Decoding an in inverse problem: what can we learn from it ?
  - Identifiability issues
  - Statistical control

(Non-)identifiability of the model ?

- When solving the inverse problem, you don't recover the true pattern but a poor approximation thereof [Haufe et al. Neuroimage 2013]
- True model: $\mathbf{y} = \mathbf{X}\,\mathbf{w}_0 + e$
- Estimated model: $\hat{\mathbf{w}} = \mathrm{argmin}_{\mathbf{w}}(l(\mathbf{w}) + R(\mathbf{w}))$
- $\hat{\mathbf{w}}$ cannot be equal to $\mathbf{w_0}$, as $\mathbf{X}$ is non-invertible

Brain activity decoding



- behavior = f (brain activity)

$$\mathbf{y} = \mathbf{X}\boldsymbol{w}^* + \sigma_* \varepsilon$$

- error vector: $\varepsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$
- noise magnitude: $\sigma_* > 0$

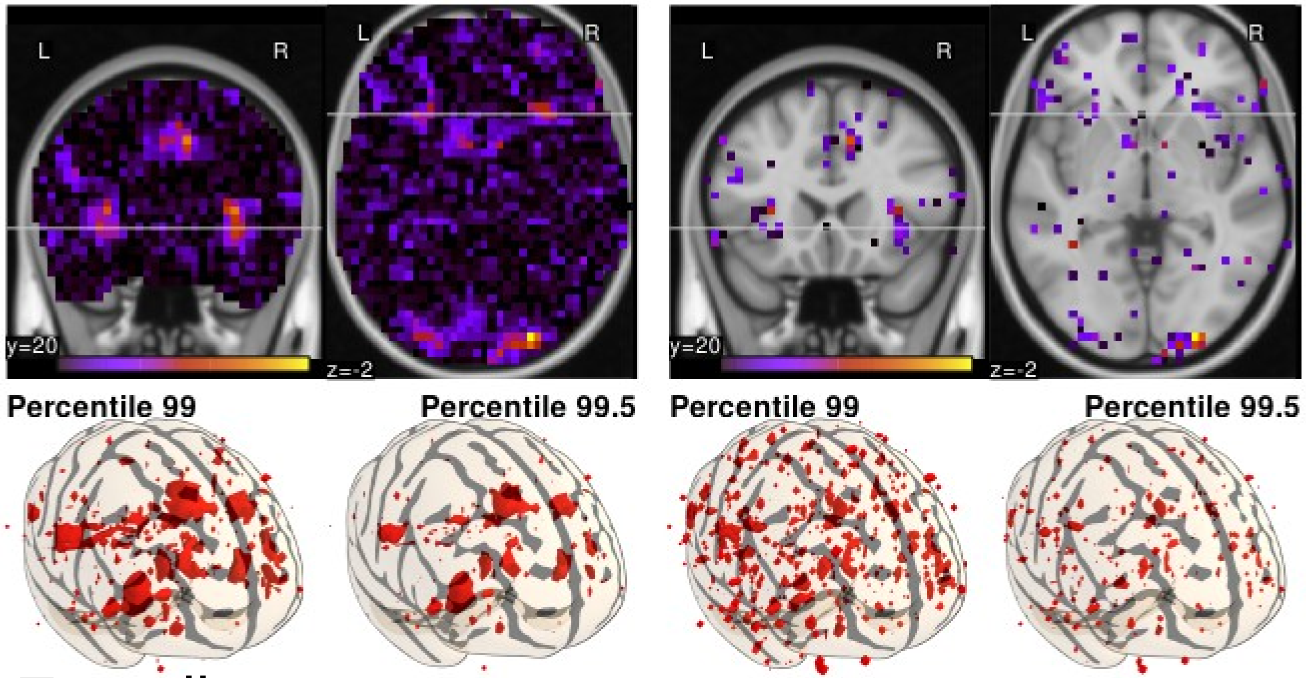
- prediction: find $\hat{\boldsymbol{w}}$ that minimizes $\|\mathbf{X}\hat{\boldsymbol{w}} - \mathbf{X}\boldsymbol{w}^*\|_2$
- estimation: find $\hat{\boldsymbol{w}}$ with control on $|\hat{w}_j - w_j^*|$ for all $j \in [p]$

(Non-)identifiability of the model ?

- Can $\hat{\mathbf{w}}$ have at least the correct support ?
- No: the encoding model violates the conditions for accurate reconstruction [Varoquaux et al. 2012]
- Better support recovery by introducing relevant priors on the decoder [Varoquaux et al. 2012]
  - Sparsity
  - Small variations

(Non-)identifiability of the model

Can nevertheless be improved with adapted techniques



Encoding

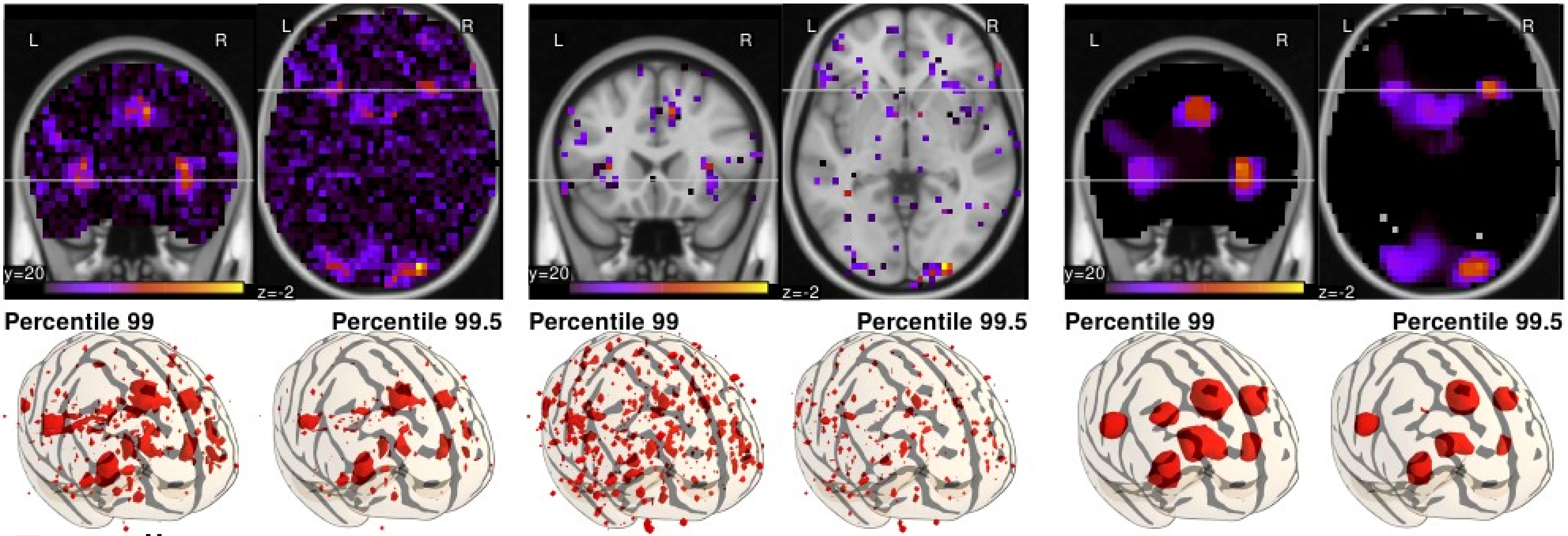
Elastic net decoding

$$(\hat{\mathbf{w}}) = \operatorname{argmin}_{\mathbf{w}} \ell(\mathbf{X}, \mathbf{Y}\mathbf{w}) + \lambda_1 \|\mathbf{w}\|_1 + \lambda_2 \|\mathbf{w}\|_2^2$$

[Gramfort et al PRNI 2013]

(Non-)identifiability of the model

Can nevertheless be improved with adapted techniques



Encoding

Elastic net decoding

Piecewise cst decoding

$$(\hat{\mathbf{w}}) = \text{argmin}_{\mathbf{w}} \ell(\mathbf{X}, \mathbf{Y}\mathbf{w}) + \lambda_1 \|\mathbf{w}\|_1 + \lambda_2 \|\mathbf{w}\|_2^2$$

$$(\hat{\mathbf{w}}) = \text{argmin}_{\mathbf{w}} \ell(\mathbf{X}, \mathbf{Y}\mathbf{w}) + \lambda_1 \|\mathbf{w}\|_1 + \lambda_2 \|\nabla \mathbf{w}\|_1$$

[Gramfort et al PRNI 2013]

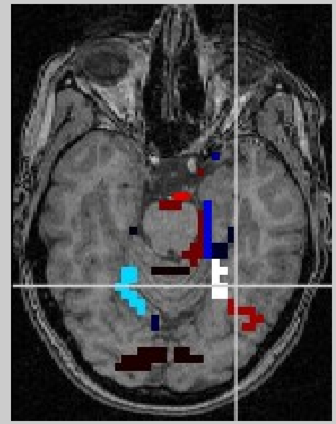
Bagging of sparse clustered models

X

y

Clustering (create contiguous regions)

Solve **Lasso** on cluster-based representation



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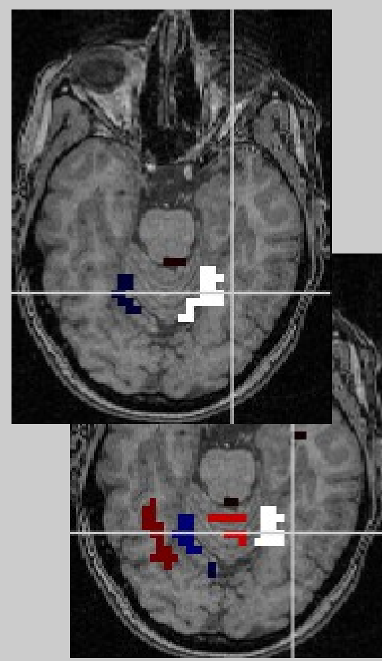
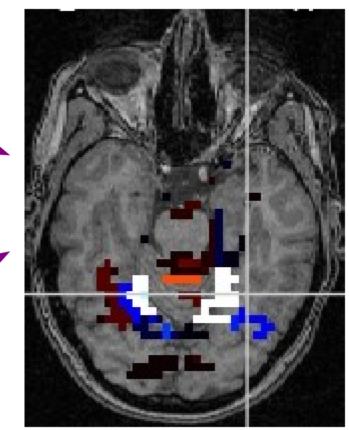


various clusterings

average

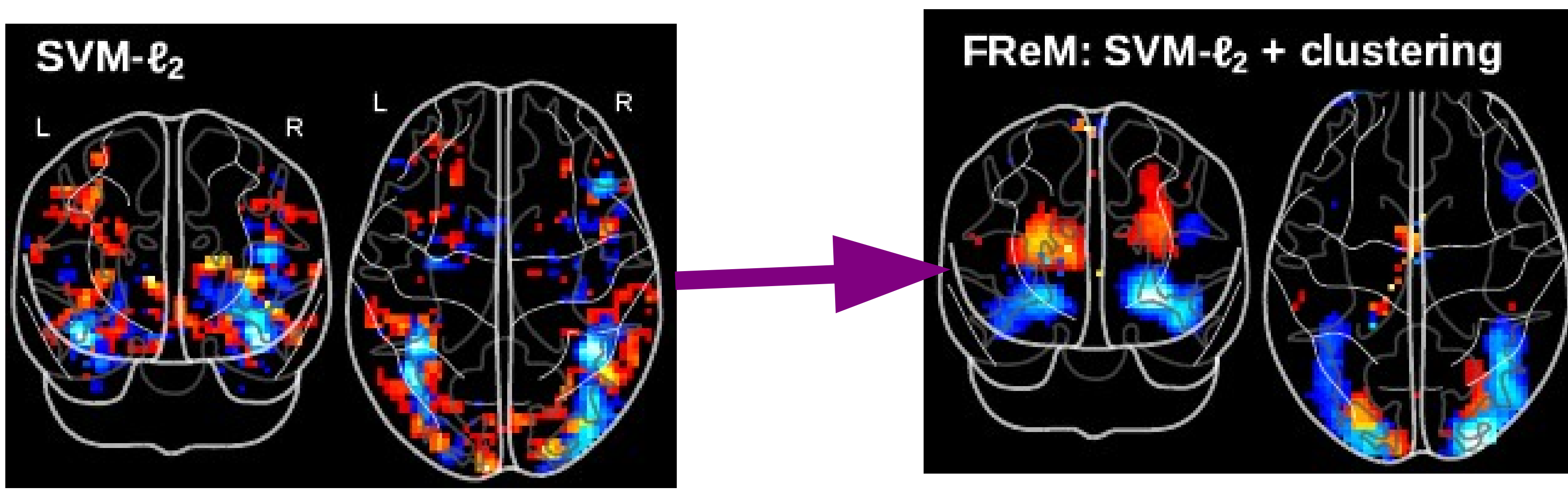


[Varoquaux et al ICML 2012
Hoyos idrobo et al. Nimg 2017]

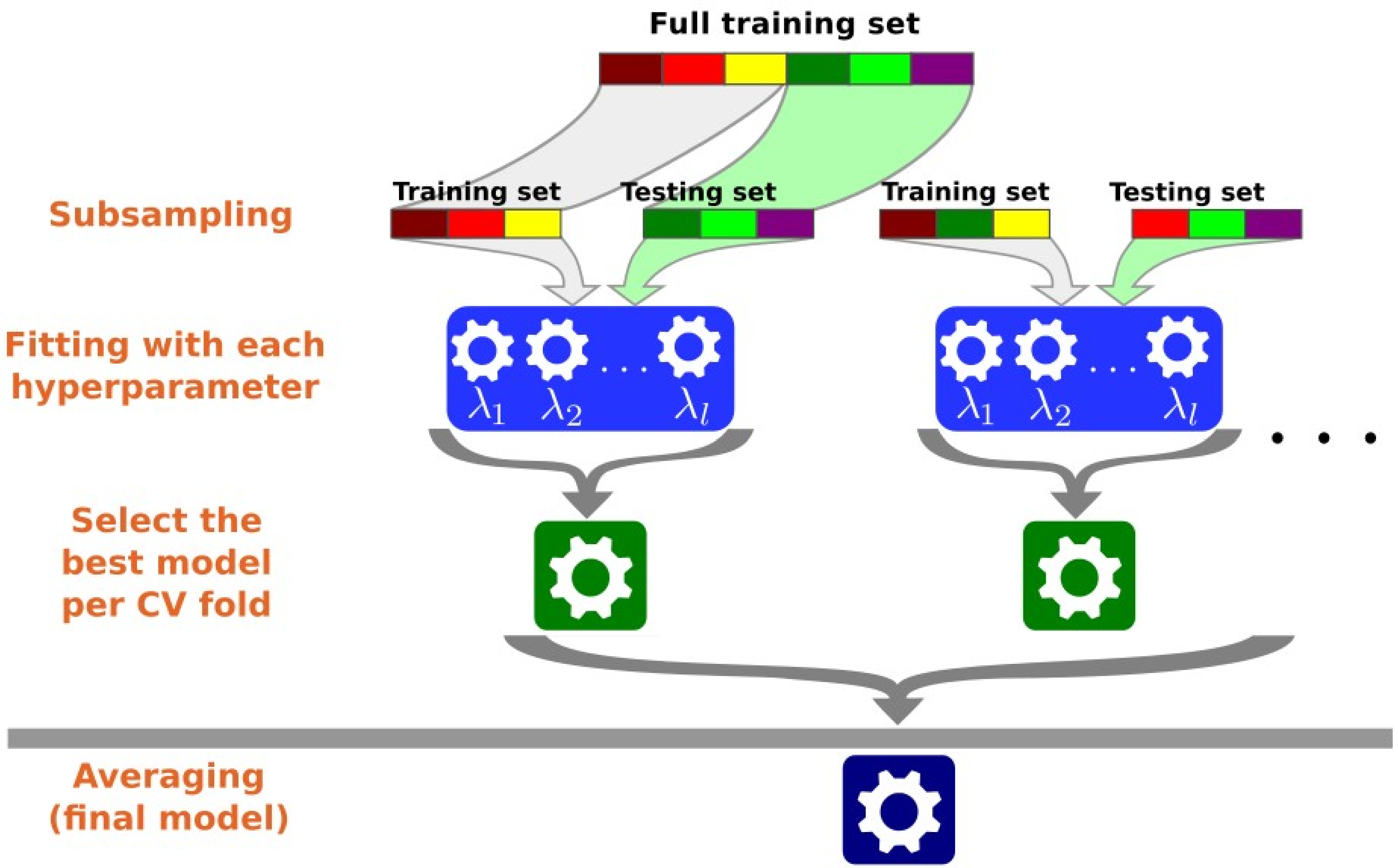
Computationally efficient structure

“fast regularized ensembles of models”

State of the art solution: not very stable, but cheap



Computationally efficient structure

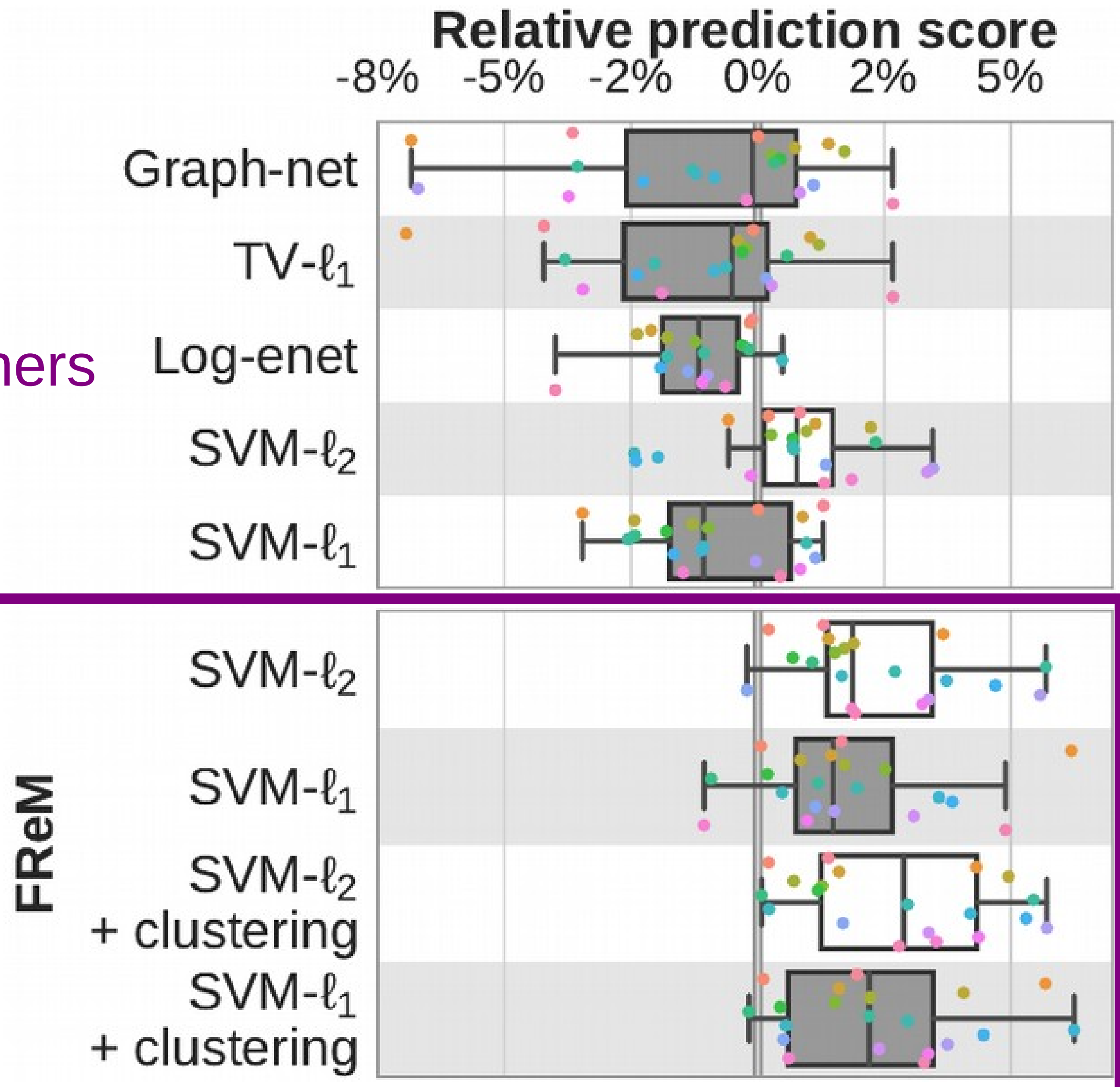


Effect on prediction accuracy

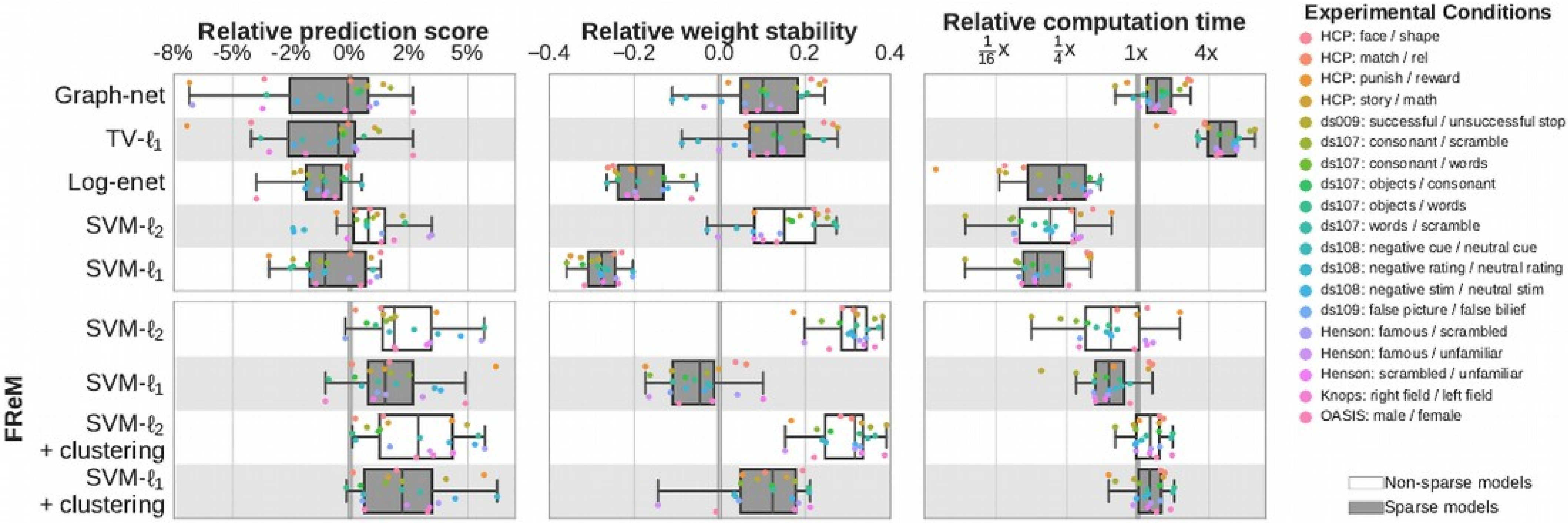
[Hoyos Idrobo et al PRNI 2015, Neuroimage 2017, PAMI 2018]

Convex learners

"fast regularized ensembles of models"

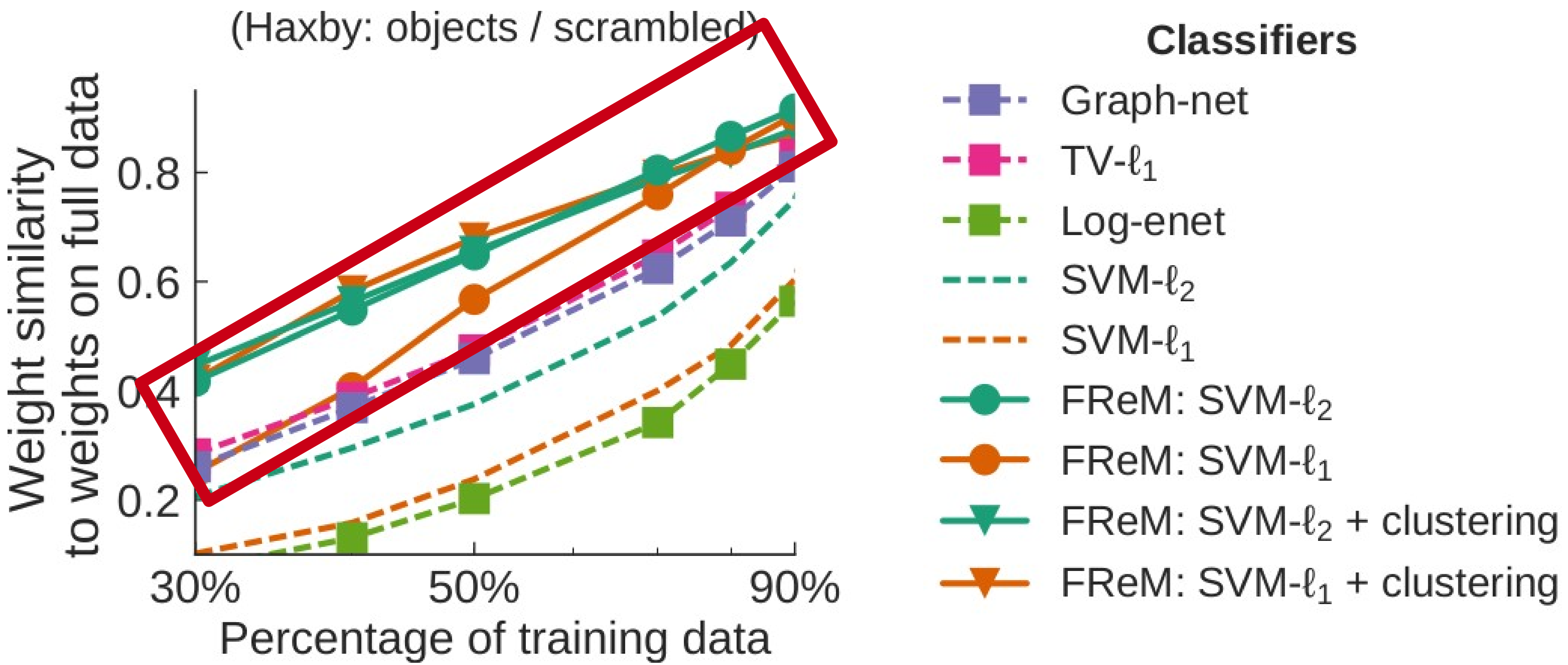


More results



[Hoyos Idrobo et al PRNI 2015, Neuroimage 2017, PAMI 2018]

Learning curve



[Hoyos Idrobo et al PRNI 2015, Neuroimage 2017]

Good recovery is great, but could we have probabilistic guarantees on the solution ?

Statistical inference on w

- Inference: find {j: $\mathbf{w}_j > 0$} with some statistical guarantees

- Standard solutions for high-dimensional linear models (p > n)
  - Corrected ridge [Bühlmann 2013]
  - Desparsified Lasso [Zhang & Zhang 2014, Montanari 2014]
  - Multi-split [Meinshausen 2009], knockoffs [Candès 2015+]
- **Fail for $p \gg n$**

Desparsified Lasso

- **Objective:** construct confidence bounds on the coefficients of $\boldsymbol{w}^*$
- **Principle:** [Zhang & Zhang 2014 Series B Stat Meth]
  - construct an unbiased estimator of $\boldsymbol{w}^*$ (generalization of $\hat{\boldsymbol{w}}^{\text{OLS}}$)
  - compute its covariance matrix
- **Heuristic argument:** in low dimension we can prove that:

$$\hat{w}_j^{\text{OLS}} = \frac{\mathbf{z}_j^\top \mathbf{y}}{\mathbf{z}_j^\top \mathbf{x}_j} \quad ,$$

where $\mathbf{z}_j$ is the residual of the OLS regression of $\mathbf{x}_j$ versus $\mathbf{X}^{(-j)}$:

$$\mathbf{z}_j = \mathbf{x}_j - \mathbf{P}_{\mathbf{X}^{(-j)}} \mathbf{x}_j \quad ,$$

where $\mathbf{P}_{\mathbf{X}^{(-j)}}$ is the projection onto $\text{Span}(\mathbf{X}^{(-j)}) \subset \mathbb{R}^{p-1}$

Desparsified Lasso

- **Desparsified Lasso estimator:** when $n < p$, $\mathbf{z}_j$ is the residual of a Lasso-CV regression of $\mathbf{x}_j$ vs $\mathbf{X}^{(-j)}$ and the debiased estimator is:

$$\hat{w}_j = \frac{\mathbf{z}_j^\top \mathbf{y}}{\mathbf{z}_j^\top \mathbf{x}_j} - \sum_{k \neq j} \frac{\mathbf{z}_j^\top \mathbf{x}_k \hat{w}_k^{(init)}}{\mathbf{z}_j^\top \mathbf{x}_j} \quad ,$$

  where $\hat{\boldsymbol{w}}^{(init)}$ is an initial non linear estimator of $\boldsymbol{w}^*$ (*e.g.*, Lasso)

- **Covariance:** the covariance matrix of this estimator is:

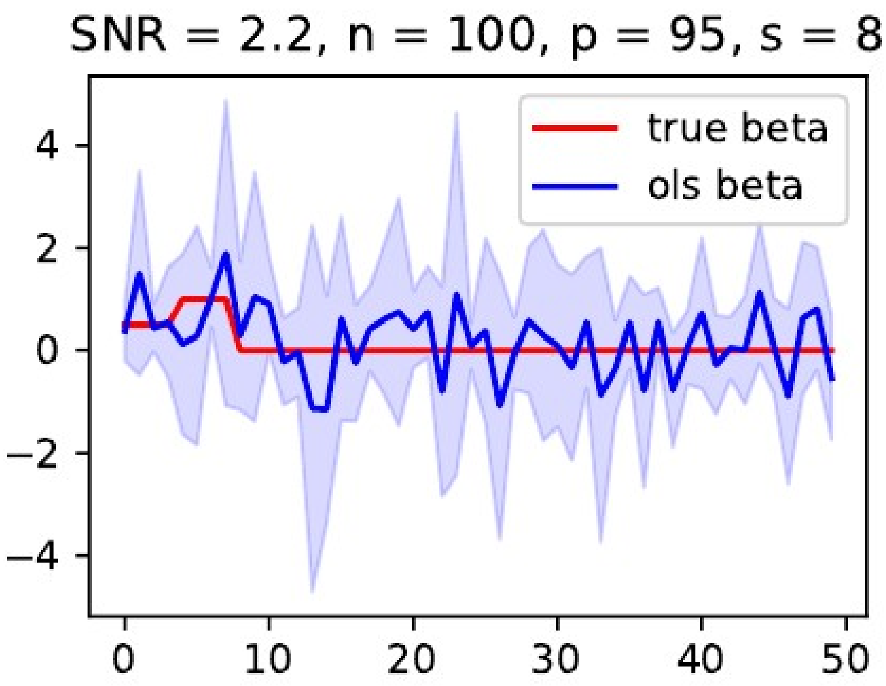
$$\Omega_{jk} = \frac{n \mathbf{z}_j^\top \mathbf{z}_k}{(\mathbf{z}_j^\top \mathbf{x}_j)(\mathbf{z}_k^\top \mathbf{x}_k)}$$

- **Confidence bounds:** under few assumptions (Dezeure et al. [2015]):

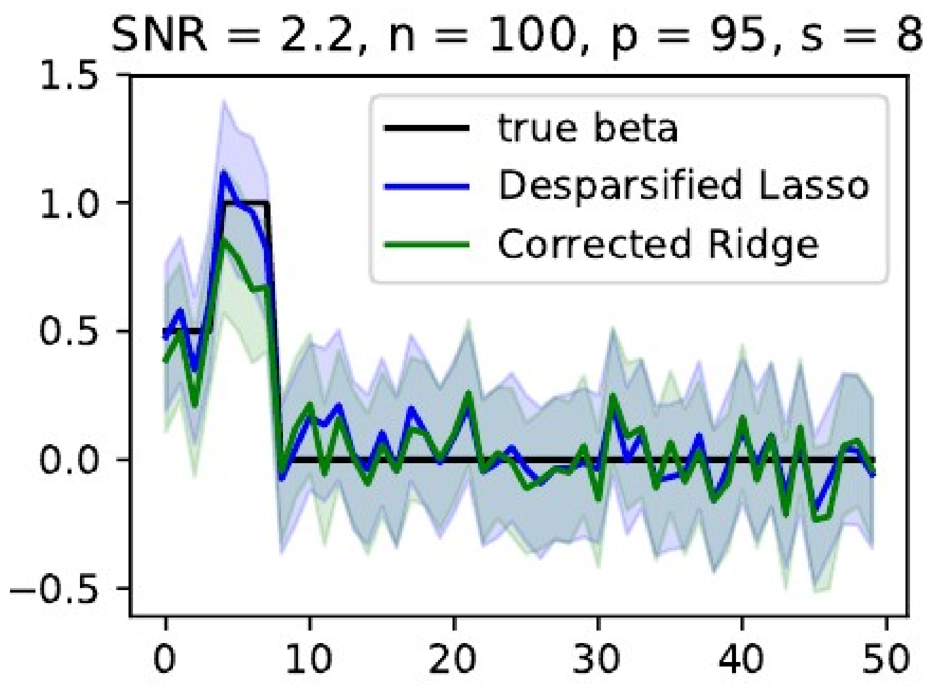
$$\boxed{\sigma_*^{-1}(\Omega_{jj})^{-1/2}(\hat{w}_j - w_j^*) \sim \mathcal{N}(0, 1)}$$

Preliminary assessment

- **Low dimension:** $n = 100$ and $p = 95$
- **OLS versus corrected Ridge and desparsified Lasso:**



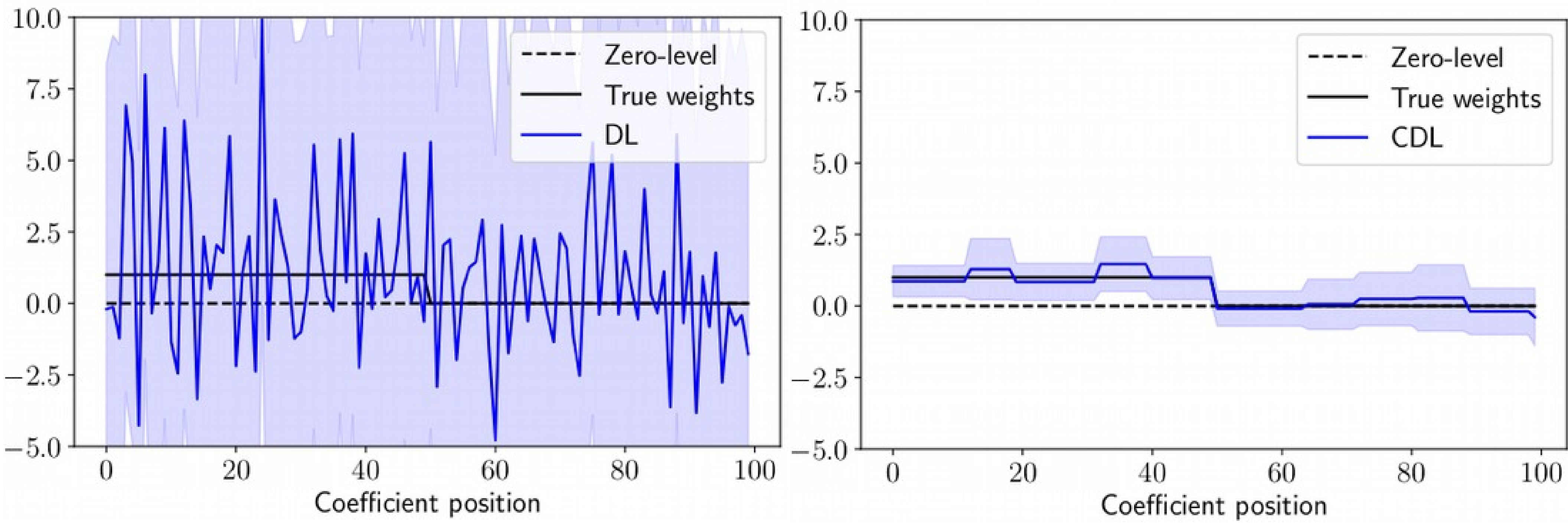
OLS regression when $p \approx n$



Corrected Ridge and **Desparsified Lasso** when $p \approx n$

Large p → need dimension reduction

p=2000, n=100



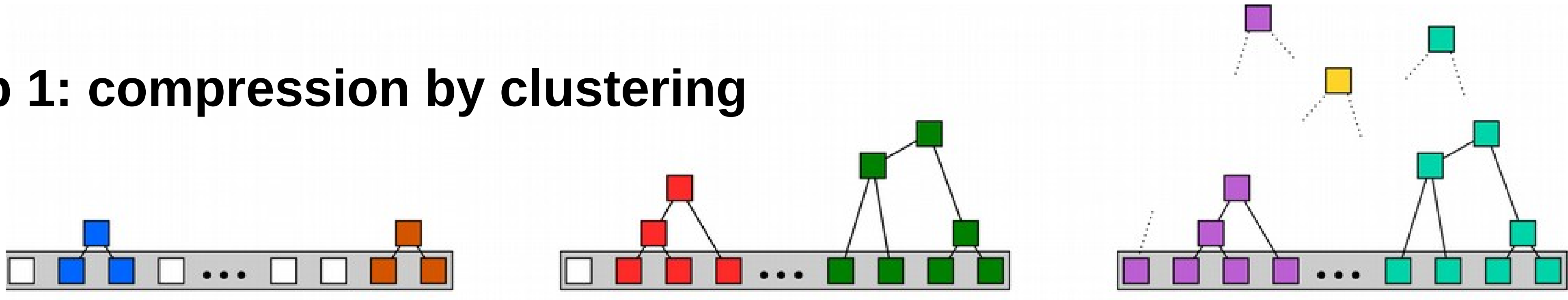
Large p kills statistical power

Clustering features tames the variance

[Chevalier et al. MICCAI 2018]

Adaptation to brain imaging

Step 1: compression by clustering



Step 2: inference on compressed representations

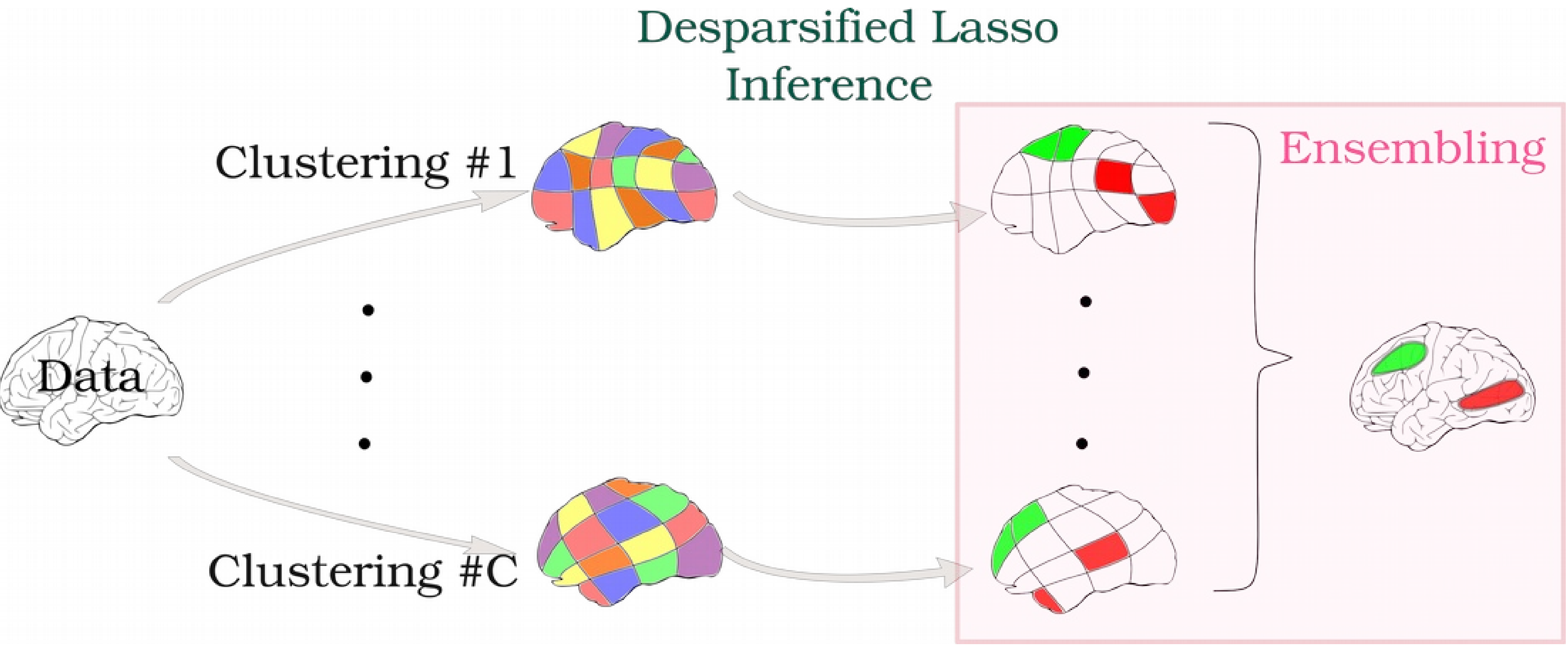
$$\sigma_*^{-1}(\Omega_{jj})^{-1/2}(\hat{w}_j - w_j^*) \sim \mathcal{N}(0,1)$$

***C**lustered*
***D**esparsified*
***L**asso*

Step 3: ensembling iterate with different parcellations
→ **aggregate p-values** (FReM-like approach)

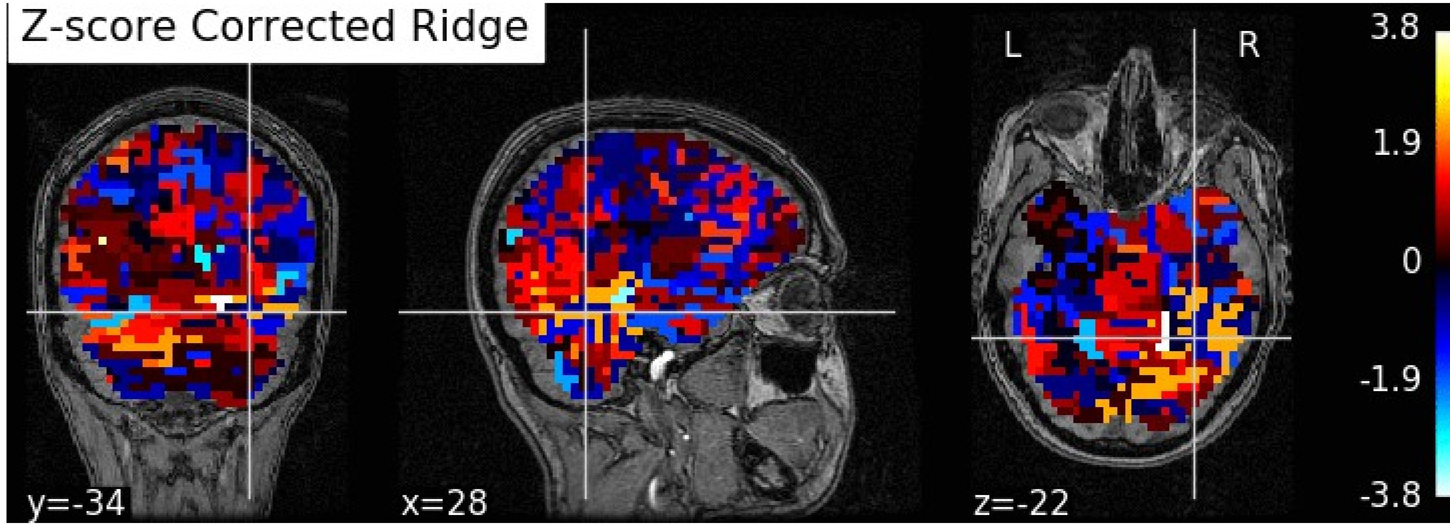
***E**nsemble of*
***C**lustered*
***D**esparsified*
***L**asso*

Adaptation to brain imaging

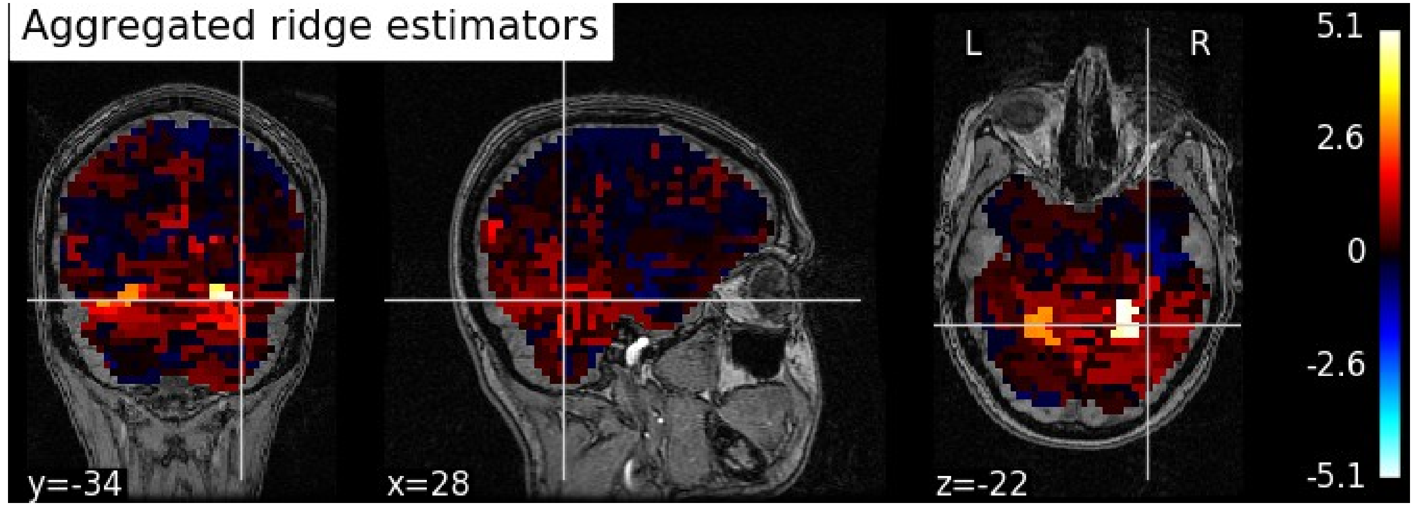


From CDL to ECDL

DL p-values from different clusterings



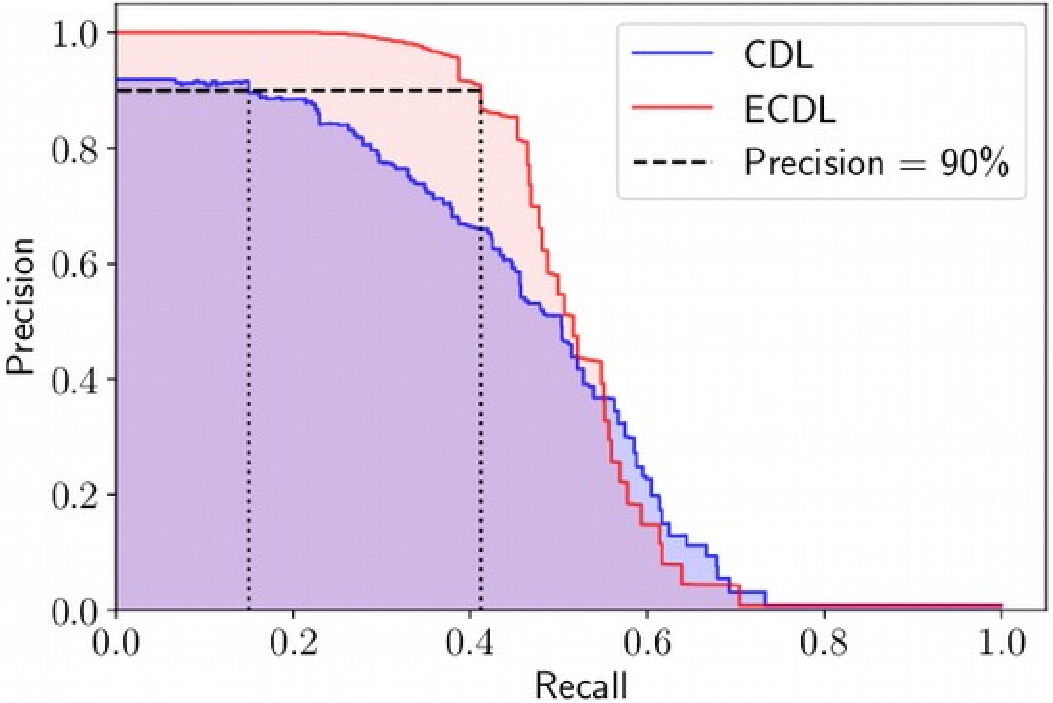
aggregation

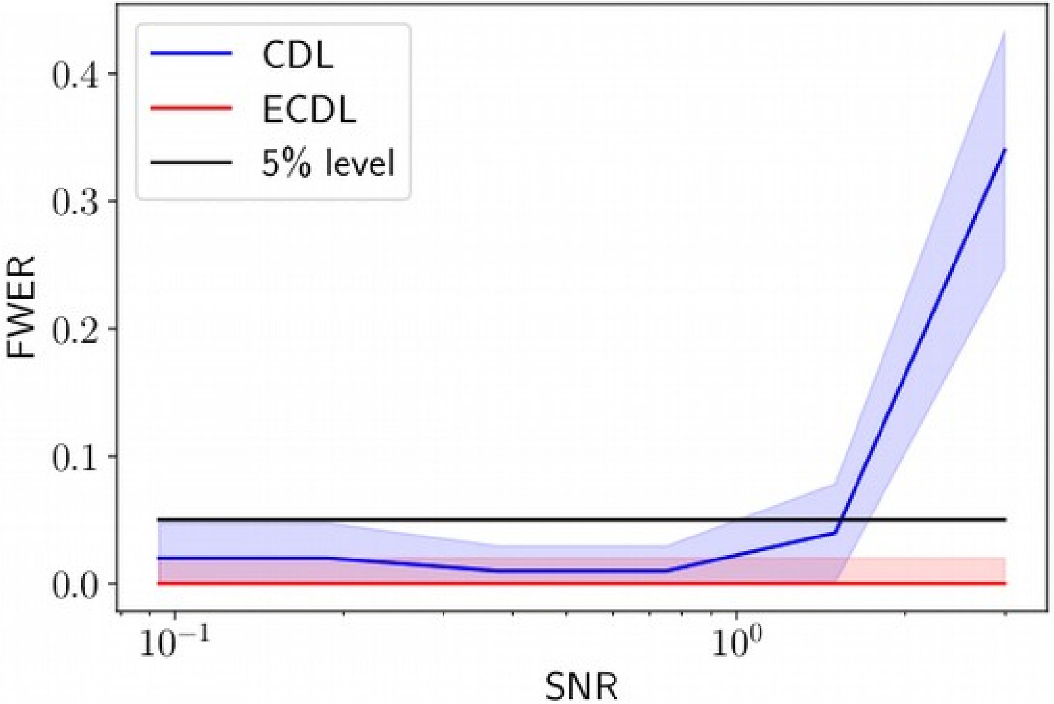


Experiments: PR and FWER control

$$\text{Recall} = \frac{\text{Number of true positive}}{\text{Size of the active set}} \quad \text{Precision} = \frac{\text{Number of true positive}}{\text{Number of discoveries}}$$

$$\text{FWER} = \text{Prob}(\text{Number of false positive} \geq 1)$$



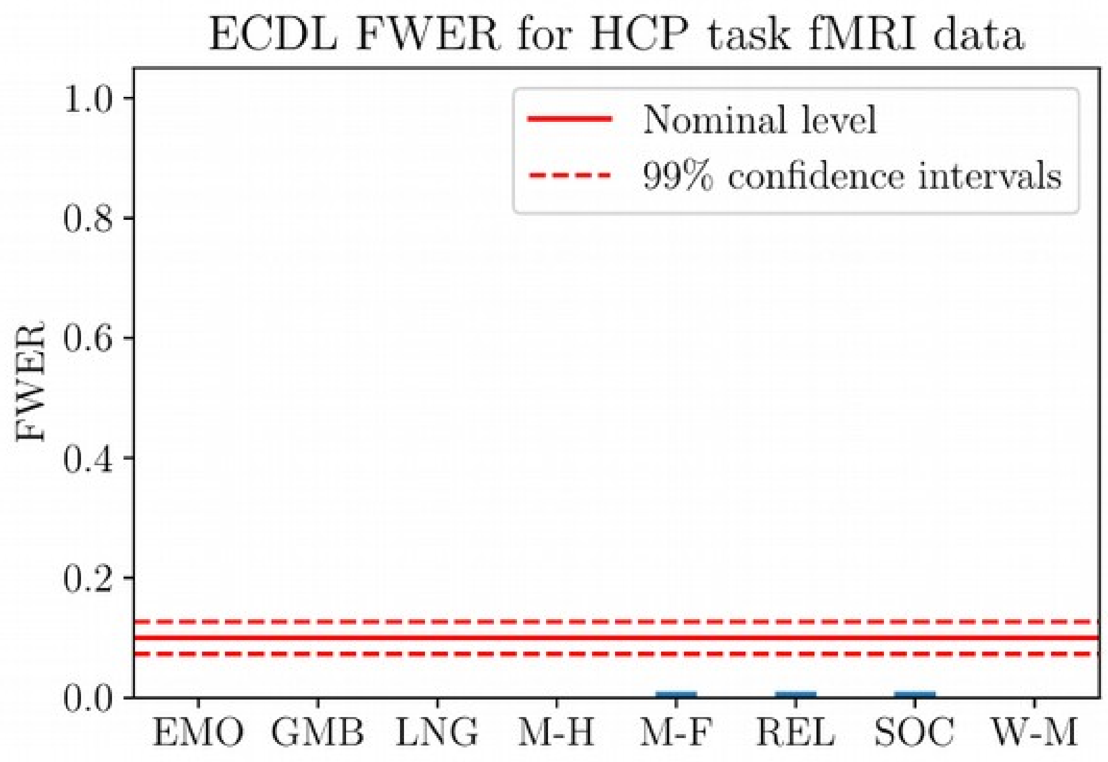


Better PR with ECDL

+ More accurate FWER control

[Chevalier et al. MICCAI 2018]

ECDL: Face validity on real data



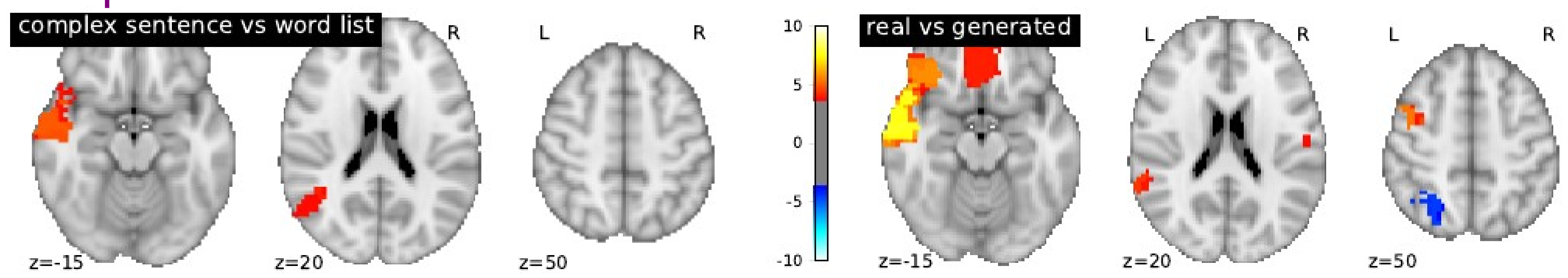
Task paradigm:

EMO = Emotion
GMB = Gambling
LNG = Language
M-H = Motor Hand
M-F = Motor Foot
REL = Relational
SOC = Social
W-M = Working Memory

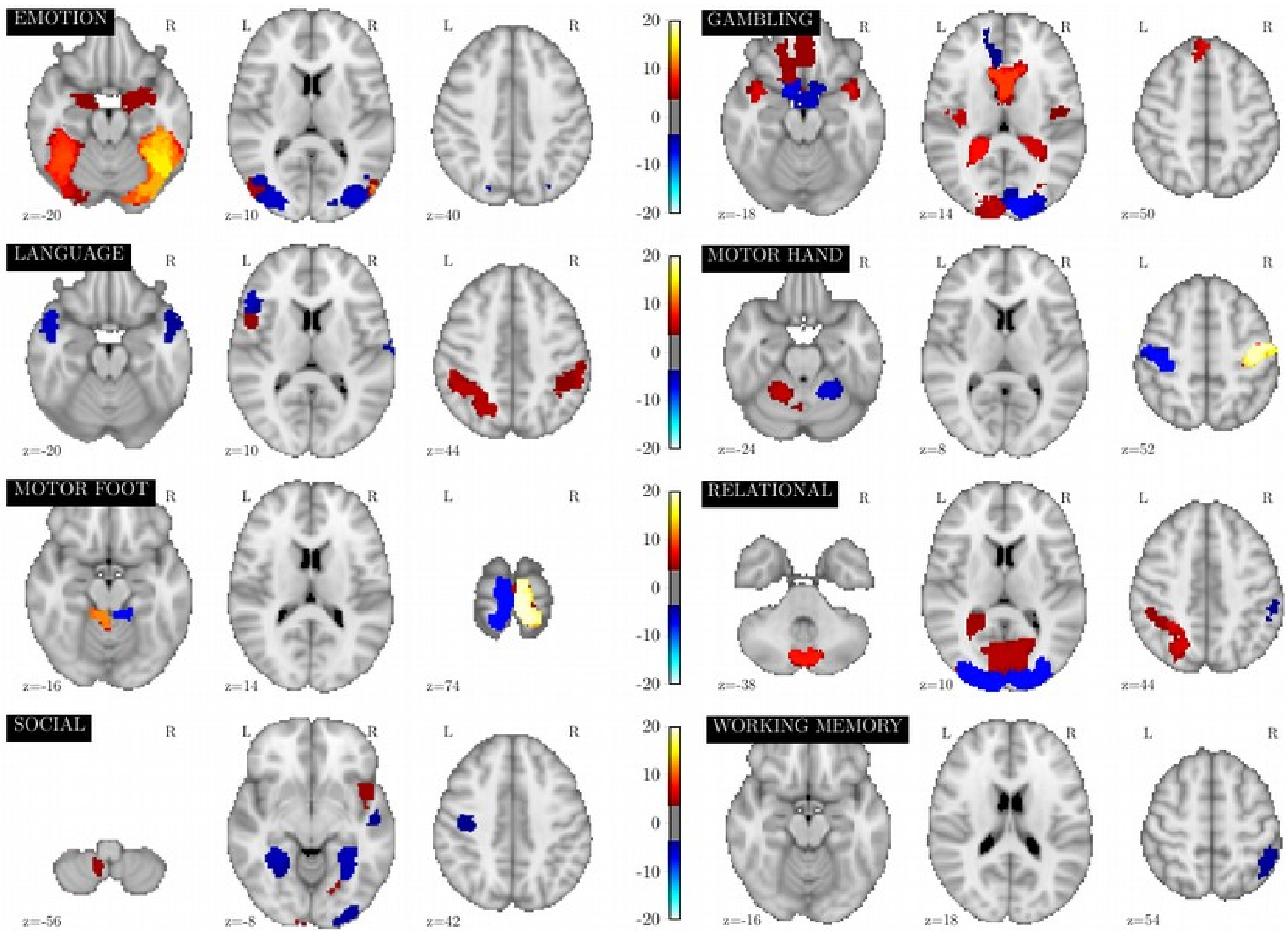
No spurious detection on **null** (permuted) data

[Chevalier et al. In prep]

No spurious detection on unmasked data



ECDL: Face validity on real data



On non-permuted data, the maps are (mostly) what one would expect

Conclusion

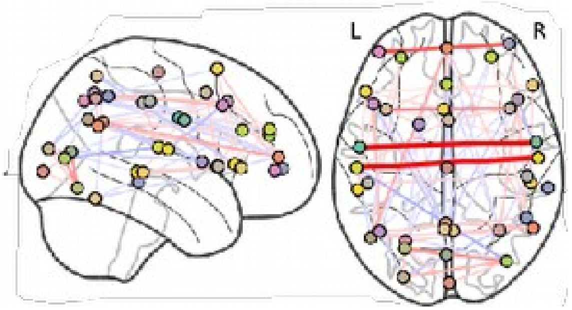
- Joint decoding/encoding for better functional specificity
- Finding commonalities across cognitive studies is hard
- Big data approach:
  - Extract weak signals from huge amounts of data
  - Common representation across datasets (*bottleneck*)

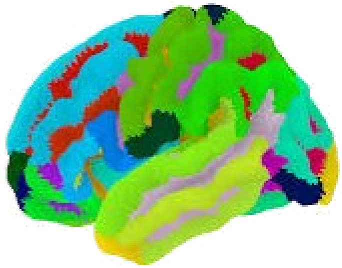
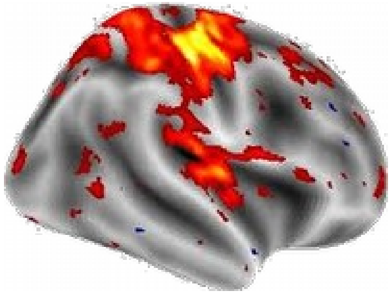
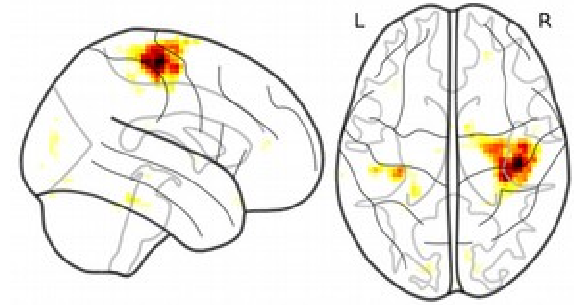
WIP

- Structure underlying cognitive concepts

From good ideas to good practices: software

- Machine learning in Python
- Machine learning for neuroimaging http://nilearn.github.io
- BSD, Python, OSS
  - Classification of (neuroimaging) data
  - Network analysis



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