

# Multivariate pattern analysis in brain imaging

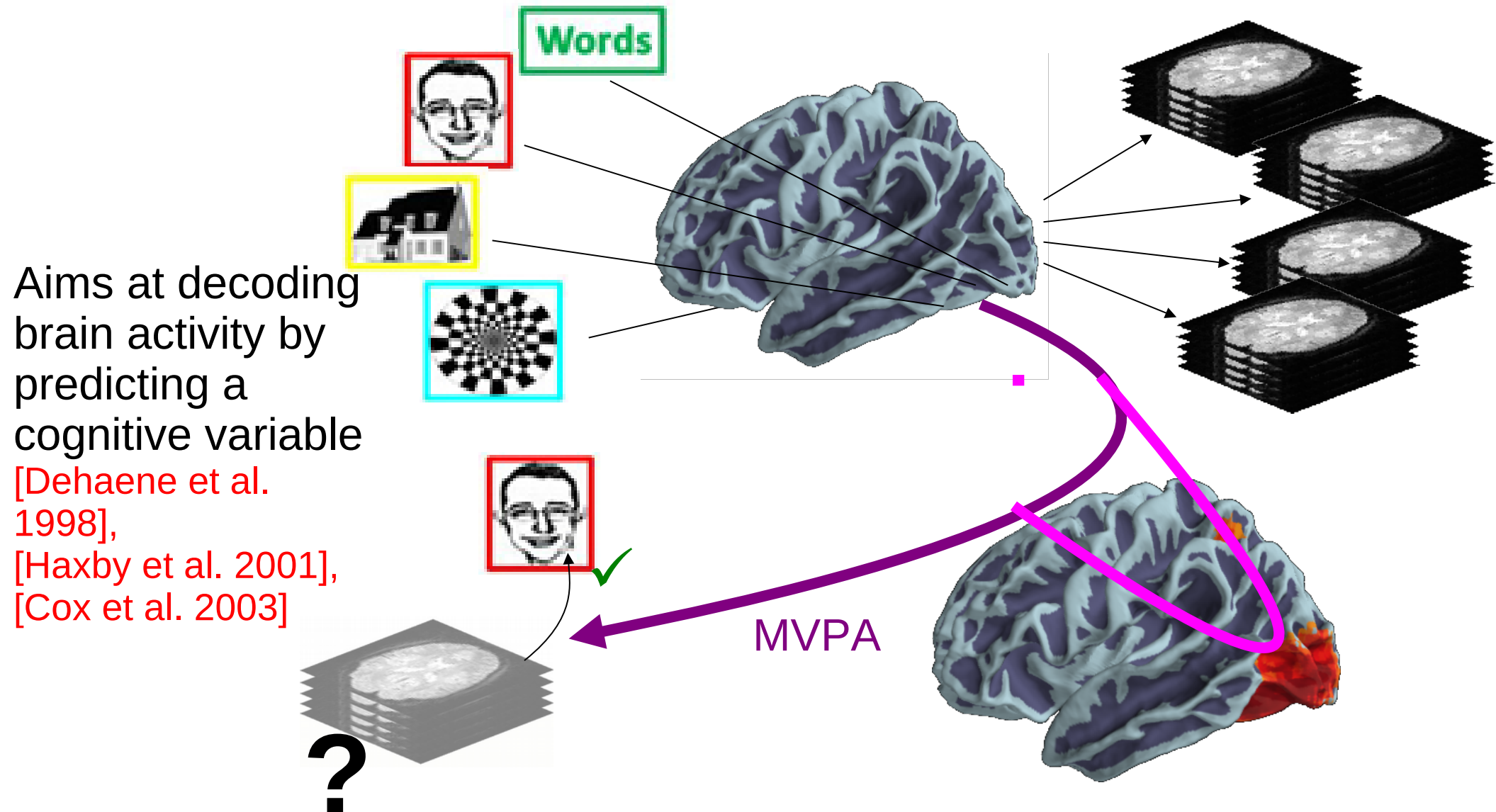
Bertrand Thirion

[bertrand.thirion@inria.fr](mailto:bertrand.thirion@inria.fr)



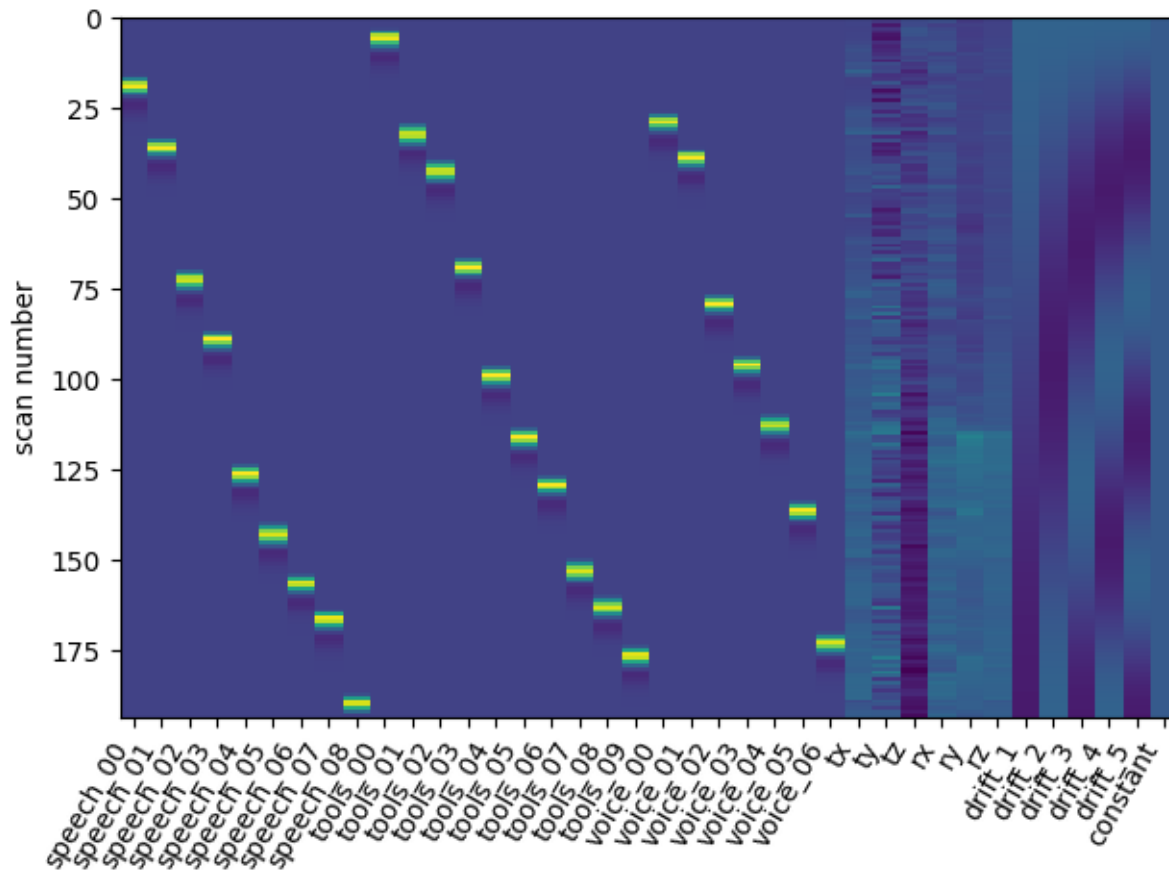
# Basic concepts

# Multivariate pattern analysis



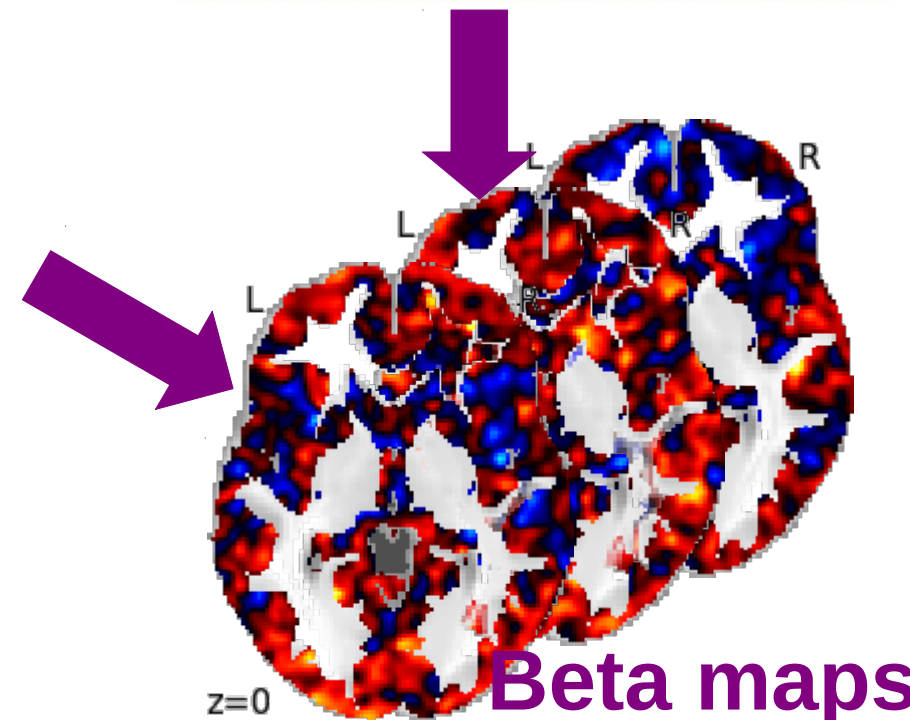
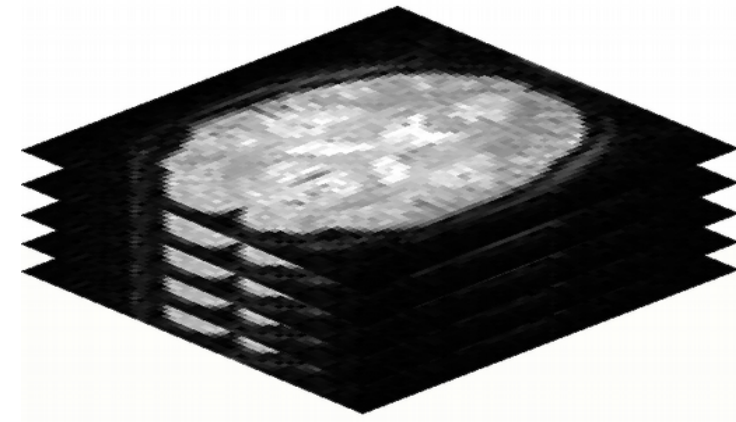
# A pipeline view

Experimental events  
→ trial-wise design matrix



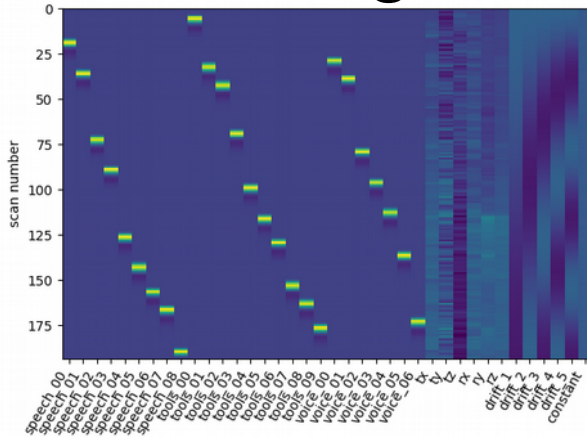
Each event belongs to a class

FMRI data

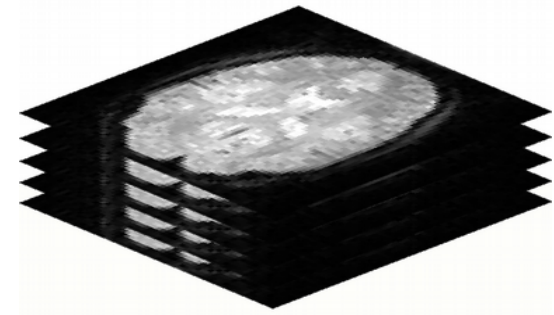


# A pipeline view

# trial-wise design matrix



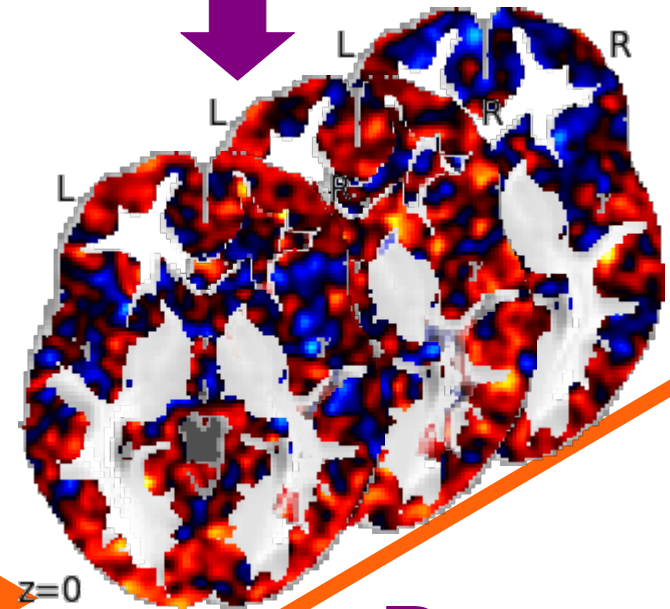
# FMRI data



```

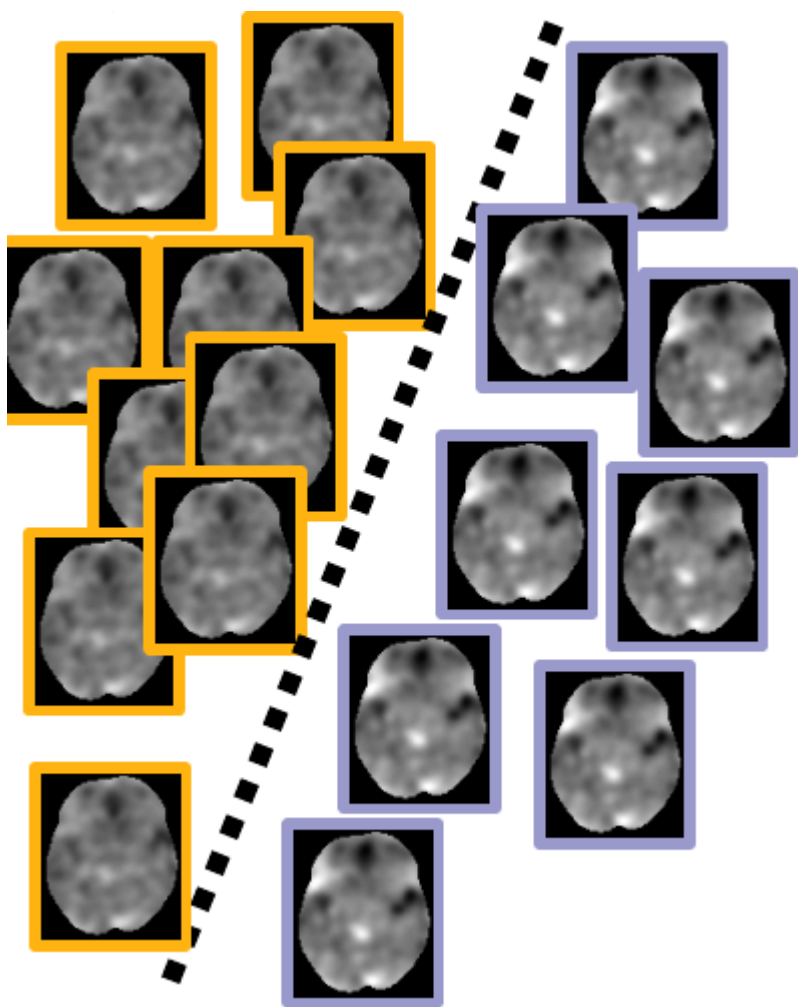
graph TD
    A[Events class] --> B[music]
    A --> C[speech]
    A --> D[music]
    B --> E[...]
    B --> F[...]
    B --> G[...]
  
```

# Decoding model



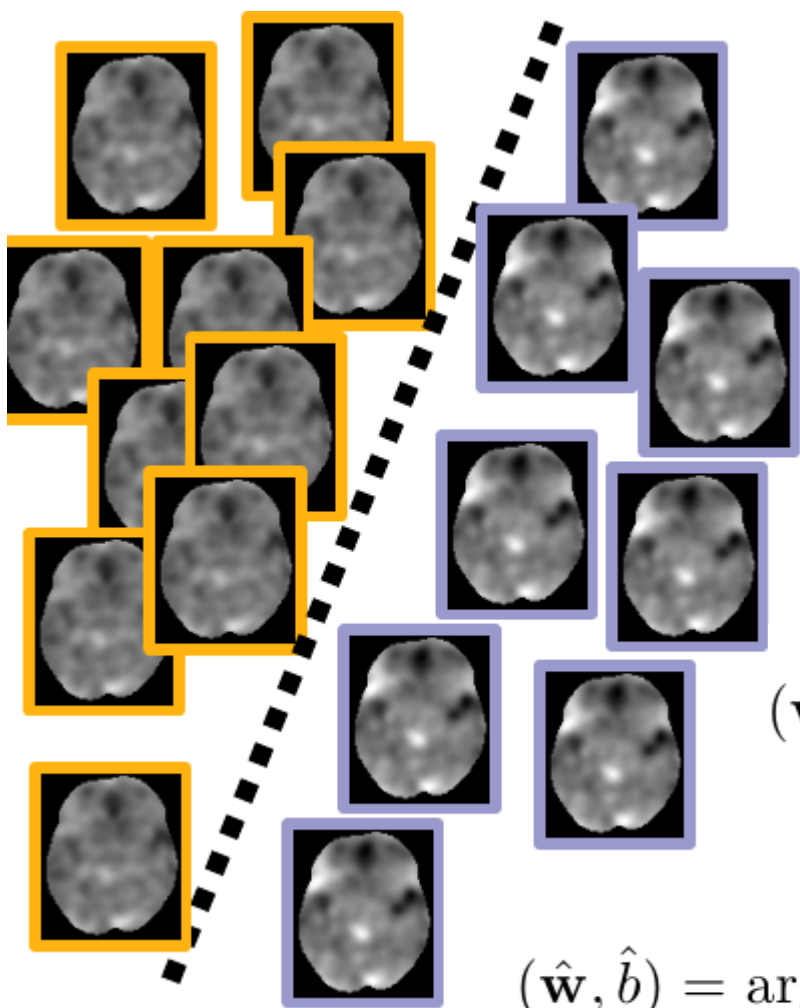
# Beta maps

# Image-based classification



- Given  $x$  in  $\mathbb{R}^p$ , (\*MRI volume with  $p$  voxels), predict a label  $y$  in  $\{-1, 1\}$   
i.e. ■ or ■  
or better the class probability  
 $\text{Proba}(y = 1|x)$

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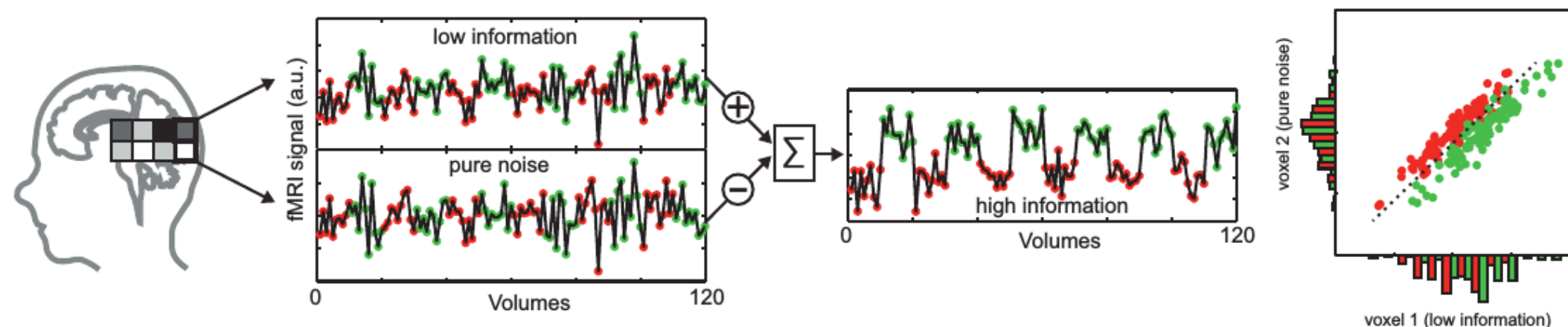
- Use of logistic regression: learn the weight  $\mathbf{w}$  and bias  $b$  such that

$$(\hat{\mathbf{w}}, \hat{b}) = \underset{\mathbf{w}, b}{\operatorname{argmin}} \sum_{i=1}^n \log (1 + \exp (-y_i(\mathbf{x}_i^T \mathbf{w} + b)))$$

- With regularization

$$(\hat{\mathbf{w}}, \hat{b}) = \underset{\mathbf{w}, b}{\operatorname{argmin}} \sum_{i=1}^n \log (1 + \exp (-y_i(\mathbf{x}_i^T \mathbf{w} + b))) + \lambda \|\mathbf{w}\|_2^2$$

# The dream case for MVPA



- Individual voxels corrupted by a noise source → weakly significant
- Their difference is strongly task related: accurate classification

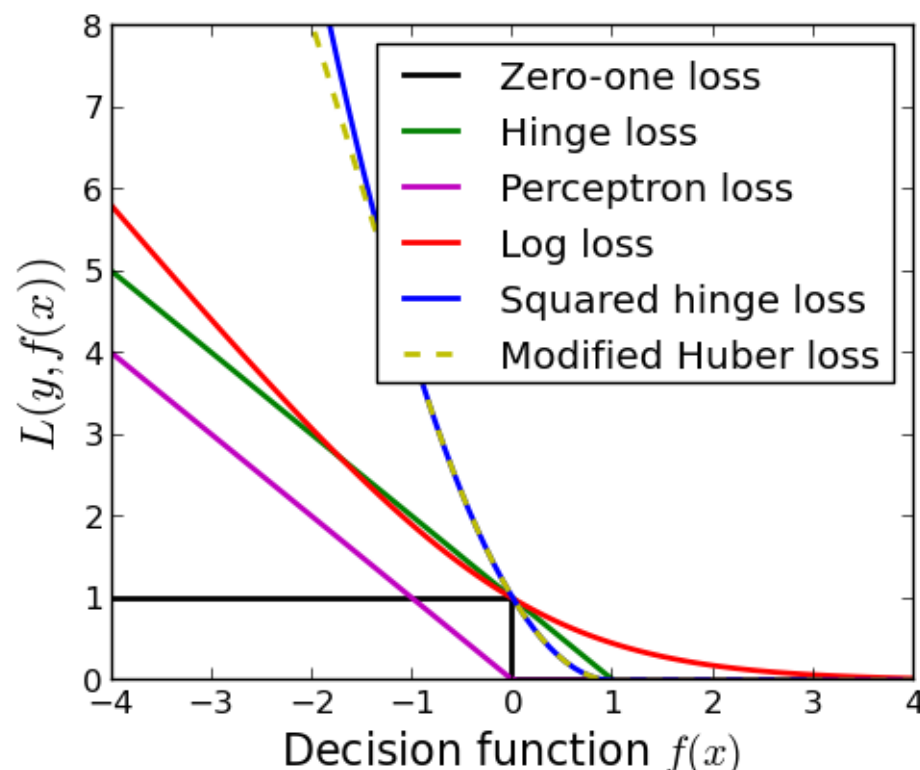
[Haufe et al. nimg 2013, Haynes neuron 2015]



# Training a predictive model

- Learning pattern  $w$  from training set  $(y, X)$
- Choice of the **loss**
  - Regression: Least-squares, Hinge, Huber
  - Classification: Hinge, logistic
- Choice of the **regularizer**
  - Predictive setting: a norm on  $w$
  - Bayesian setting: prior distribution on  $w$

$$\hat{w} = \operatorname{argmin}_{w \in \mathbb{R}^p} \sum_{i=1}^n \ell(y_i, X_i w) + \lambda J(w)$$



# Training a predictive model

- Learning pattern  $w$  from training set  $(v, X)$

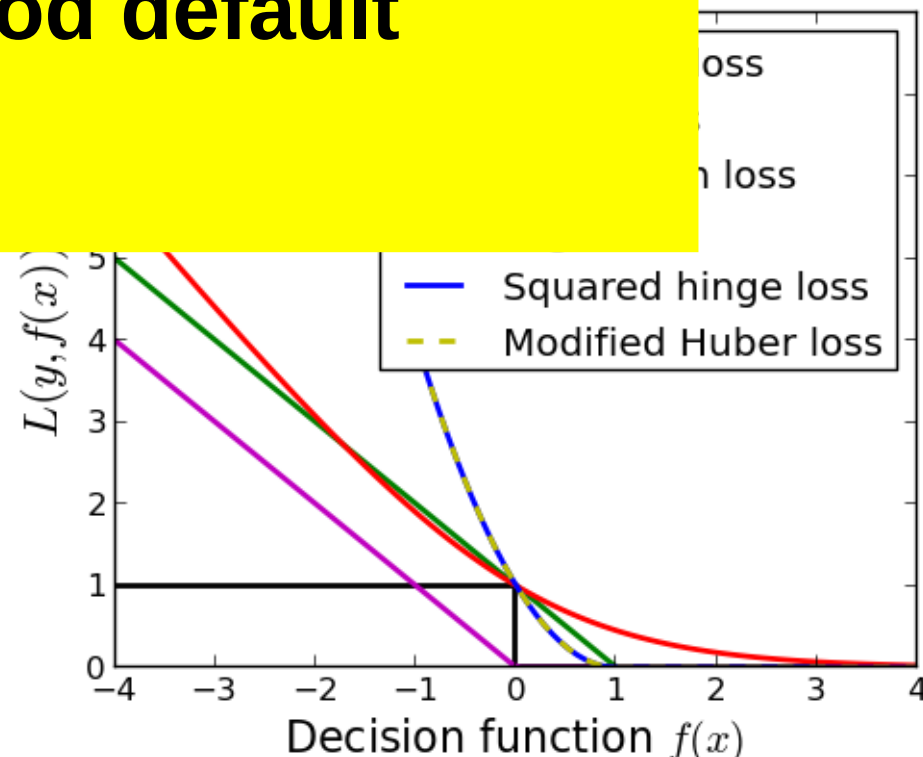
- Choice of

- Regression  
Hinge
- Classification

- Choice of the regularizer

- Predictive setting: a norm on  $w$
- Bayesian setting: prior distribution on  $w$

**SVM classification/regression  
( $C=1$ ) is a good default**



# Evaluation of the decoding

## Measure prediction accuracy

[https://scikit-learn.org/stable/modules/model\\_evaluation.html](https://scikit-learn.org/stable/modules/model_evaluation.html)

Regression →  
Explained variance  $\zeta$  :

$$\zeta(\mathbf{y}^t, \hat{\mathbf{y}}) = \frac{\text{var}(\mathbf{y}^t) - \text{var}(\mathbf{y}^t - \hat{\mathbf{y}})}{\text{var}(\mathbf{y}^t)}$$

Classification score:

$$\kappa(\mathbf{y}^t, \hat{\mathbf{y}}^t) = \frac{\sum_{i=1}^{n^t} \delta(y_i^t, \hat{y}_i^t)}{n^t}$$

→ amount of information about  $y$  in the brain data

# Cross validation

```
X = np.random.randn(*fmri_masked.shape) # replace with null data
prediction = svc.fit(X, conditions).predict(X)
print((prediction == conditions).sum() / float(len(conditions)))
```

1.0

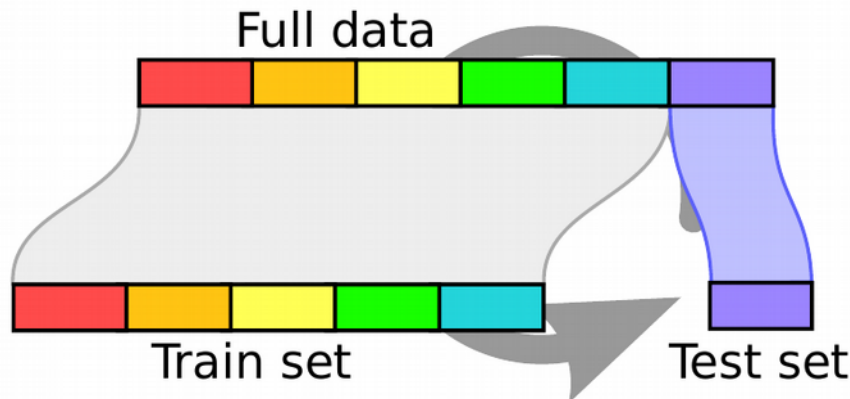
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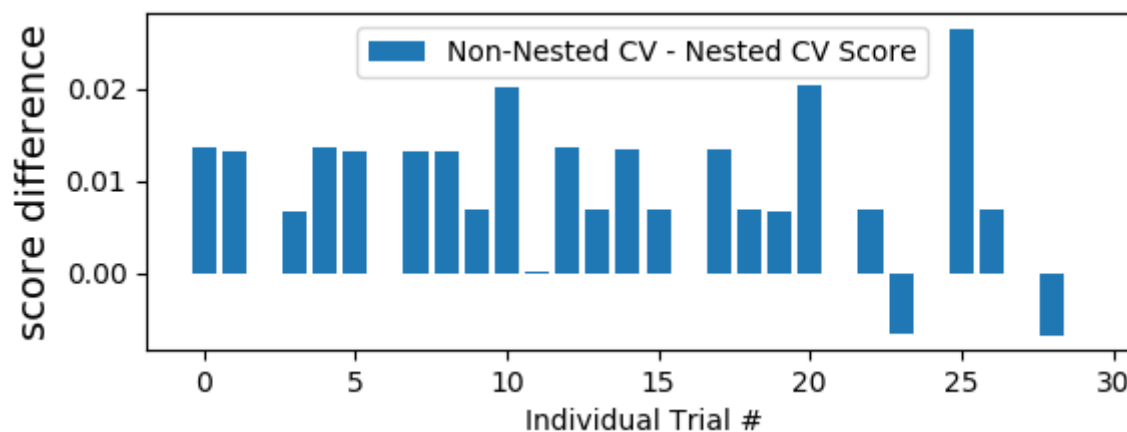
**With cross-validation,  
accuracy is unbiased**

```
cv_score = cross_val_score(svc,
                           X,
                           conditions,
                           cv=cv, # cross-validation scheme
                           groups=session_label, # data splitting scheme
                           )
print(np.mean(cv_score)) # chance is 50%
```

0.4212962962962962

# Parameters to tune

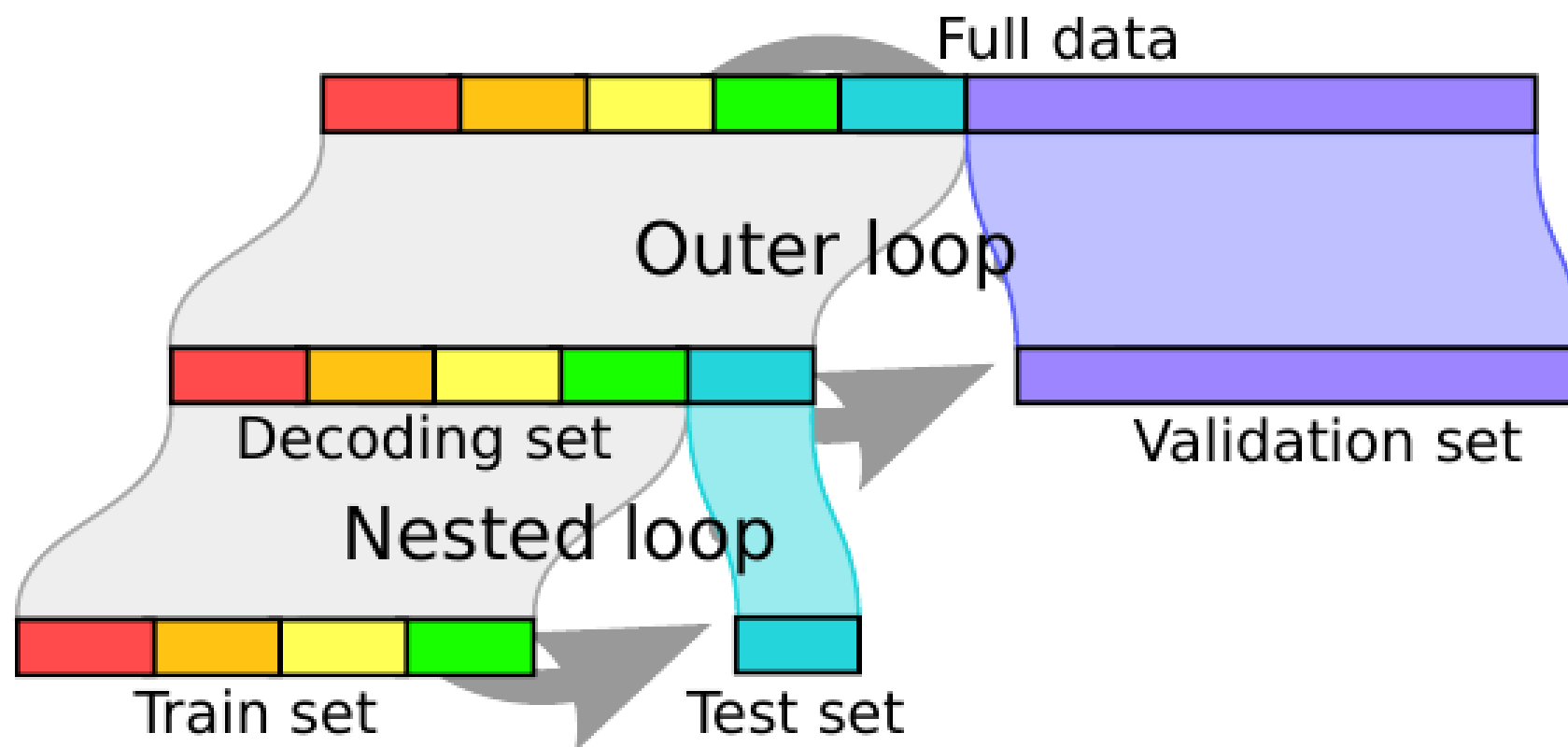
- Parameter/model selection → based on accuracy
- CAVEAT: do not do it with the scoring loop



[https://scikit-learn.org/stable/auto\\_examples/model\\_selection/plot\\_nested\\_cross\\_validation\\_iris.html](https://scikit-learn.org/stable/auto_examples/model_selection/plot_nested_cross_validation_iris.html)

- Need nested loop **“nested cross validation”**

# Nested cross-validation



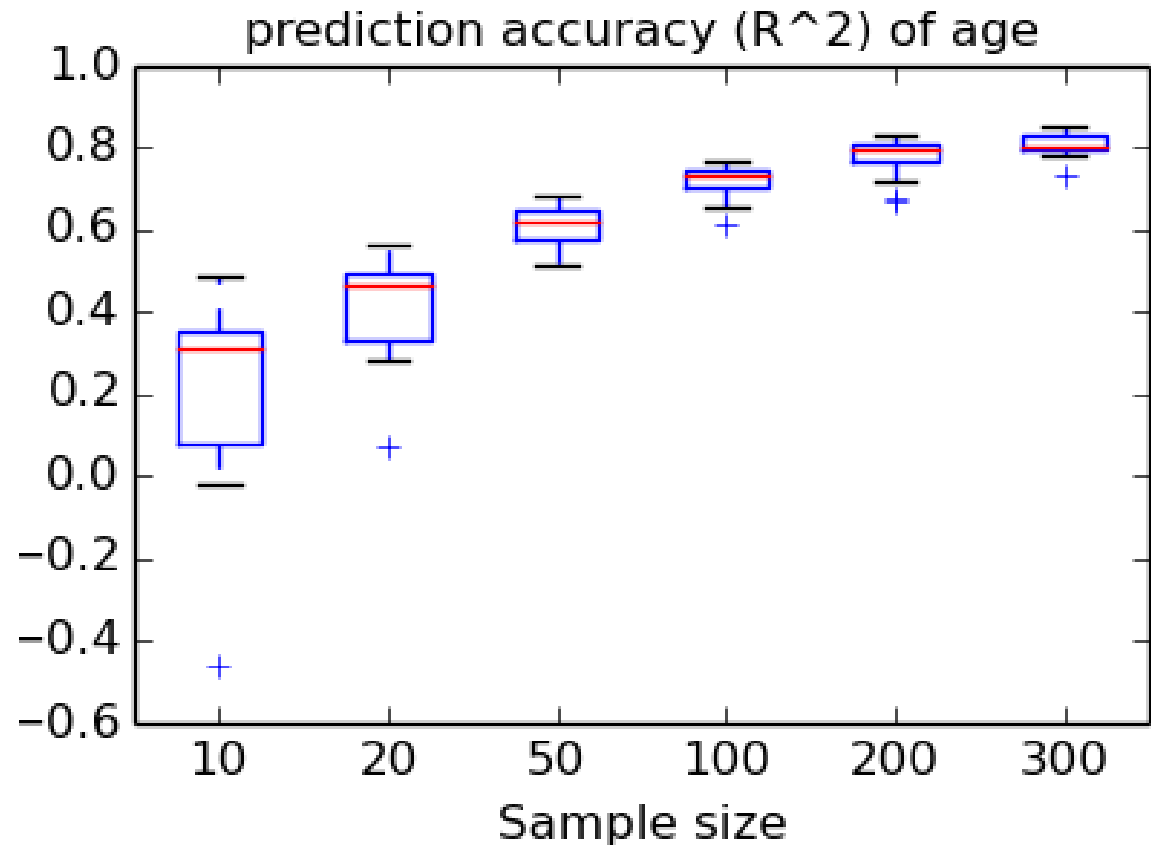
- One loop to tune inner parameters
- One loop to get the accuracy

# Common pitfalls



# Learning curve: how prediction improves with n

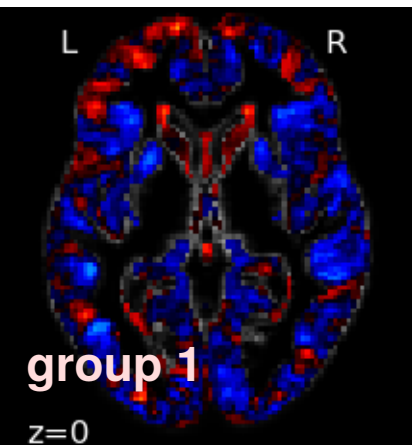
- Predict the age of a subject given gray matter density maps (OASIS dataset,  $n=403$ )



# Weight maps for age prediction / OASIS

The weight map depends on the batch of subject considered (bootstrap):

One question, different datasets, different answers



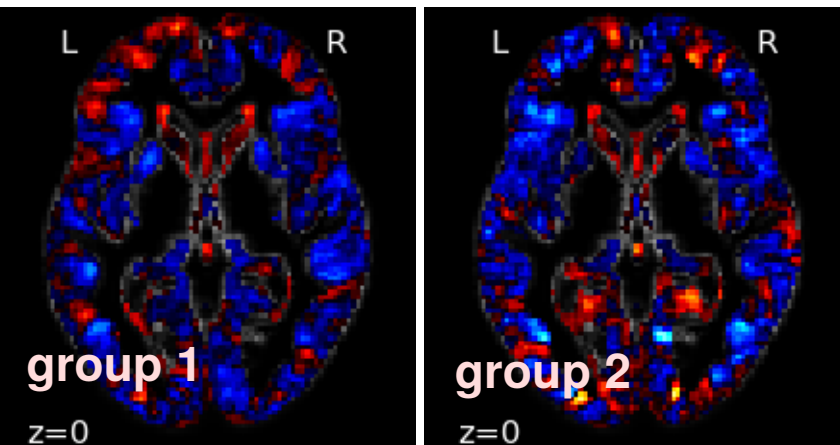
group 6

Variability actually worse than for univariate analysis !

# Weight maps for age prediction / OASIS

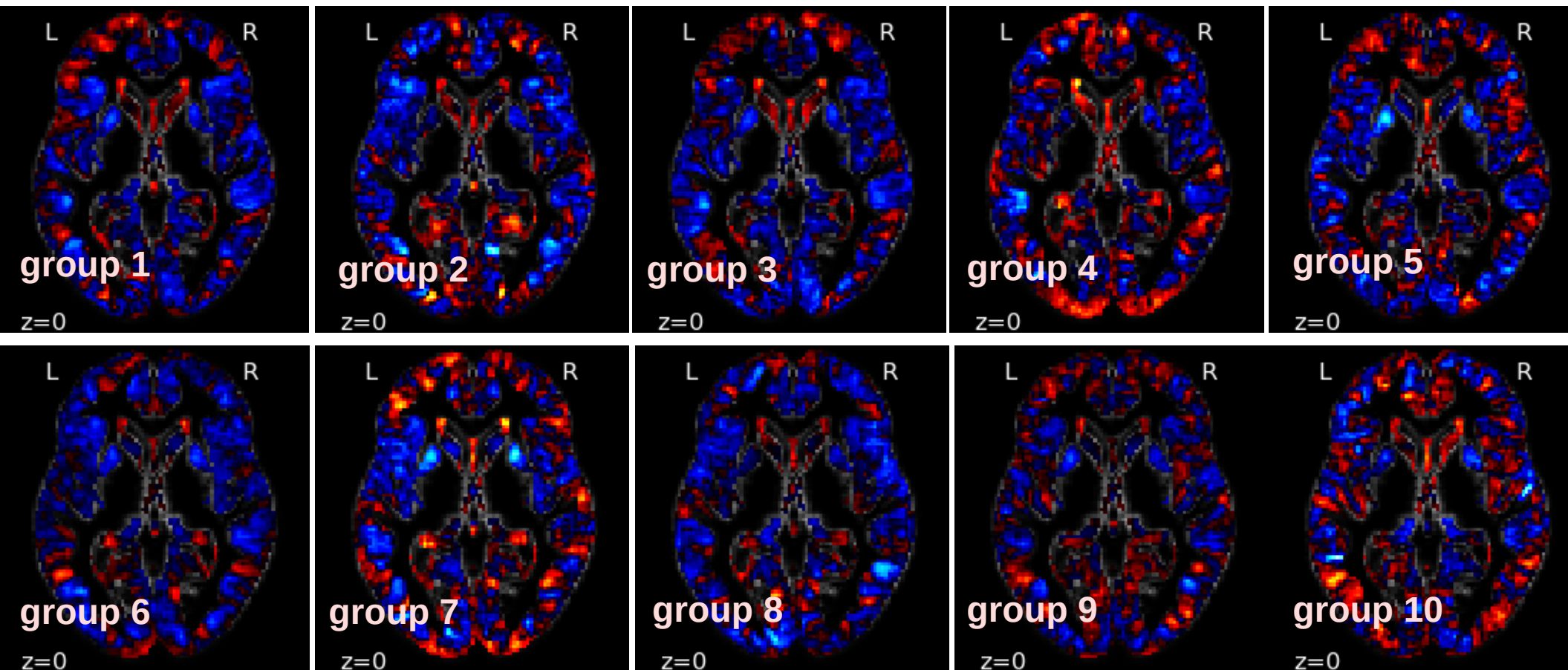
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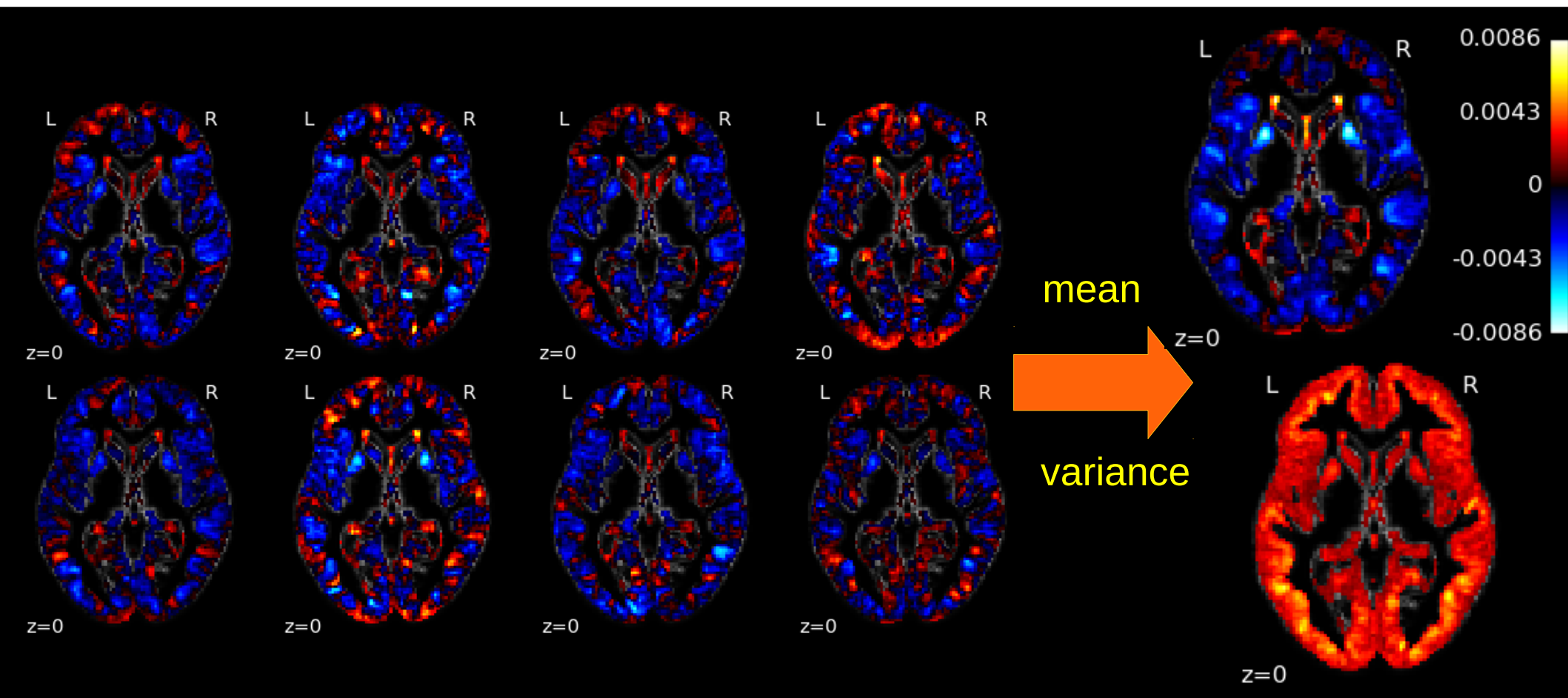
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Variability actually worse than for univariate analysis !

# Weight maps for age prediction / OASIS

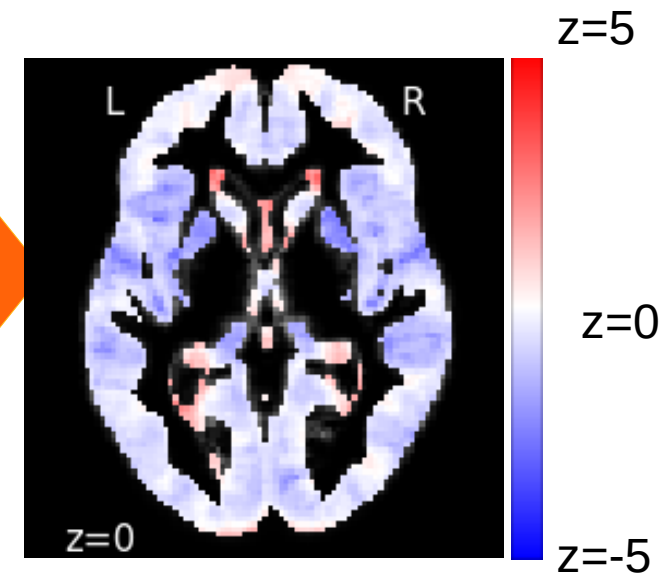
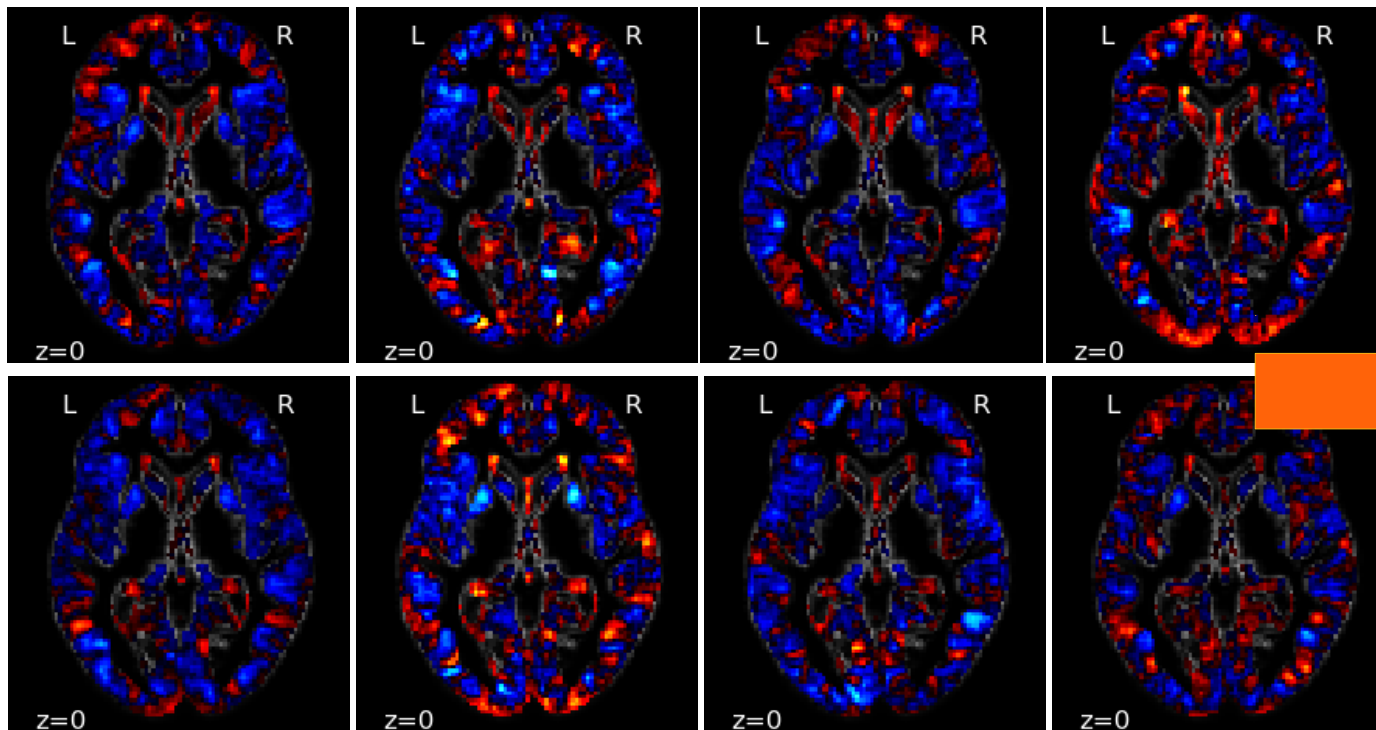
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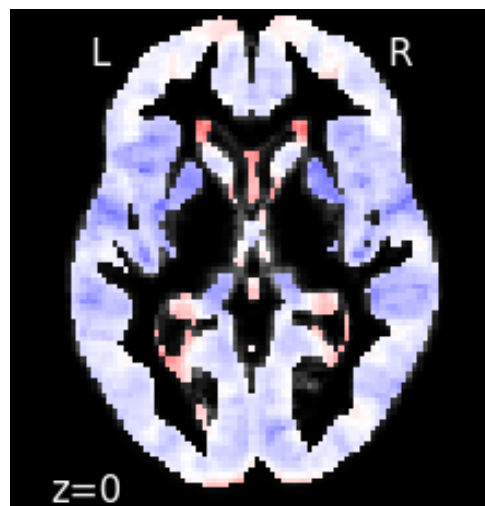
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Summarized into a z image:  
(effect size) / (effect std)

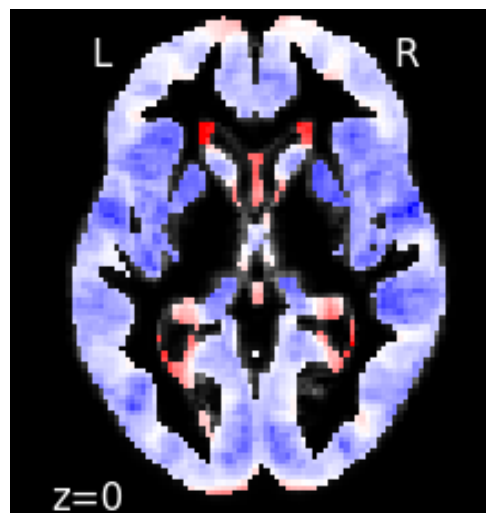


# Weight maps for age prediction / OASIS

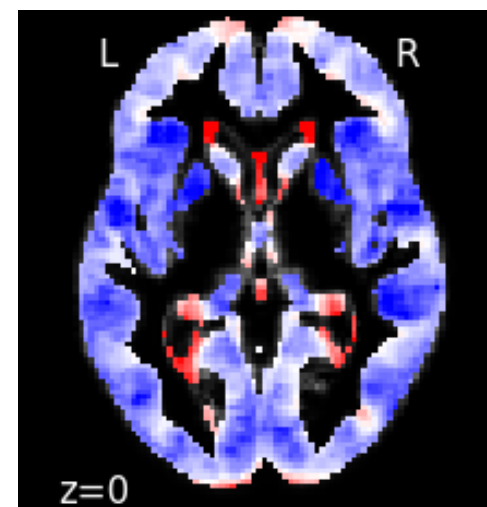
n=10



n=20



n=50



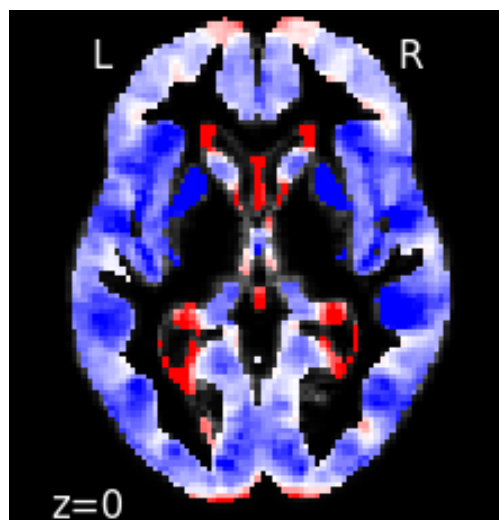
z=5

(effect size  
estimated by  
bootstrap)

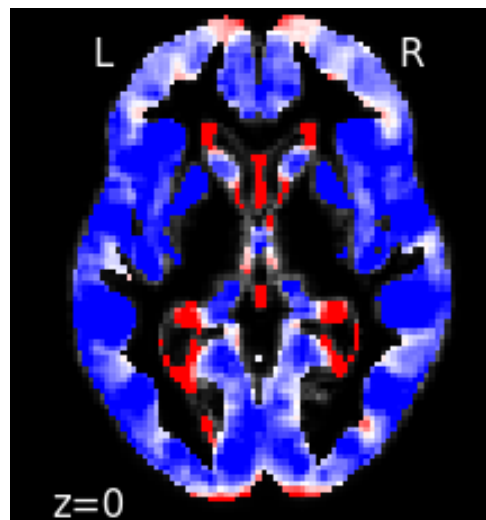
z=0

z=-5

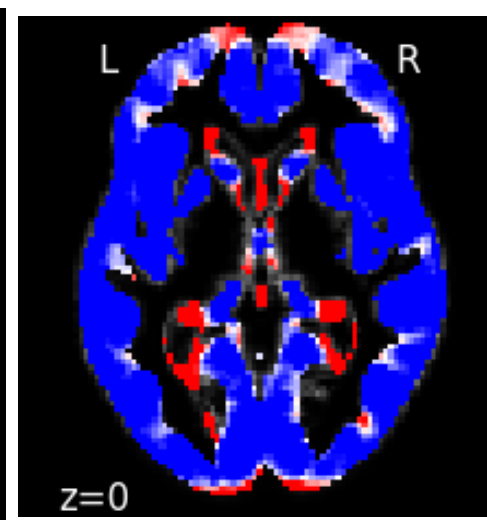
n=100



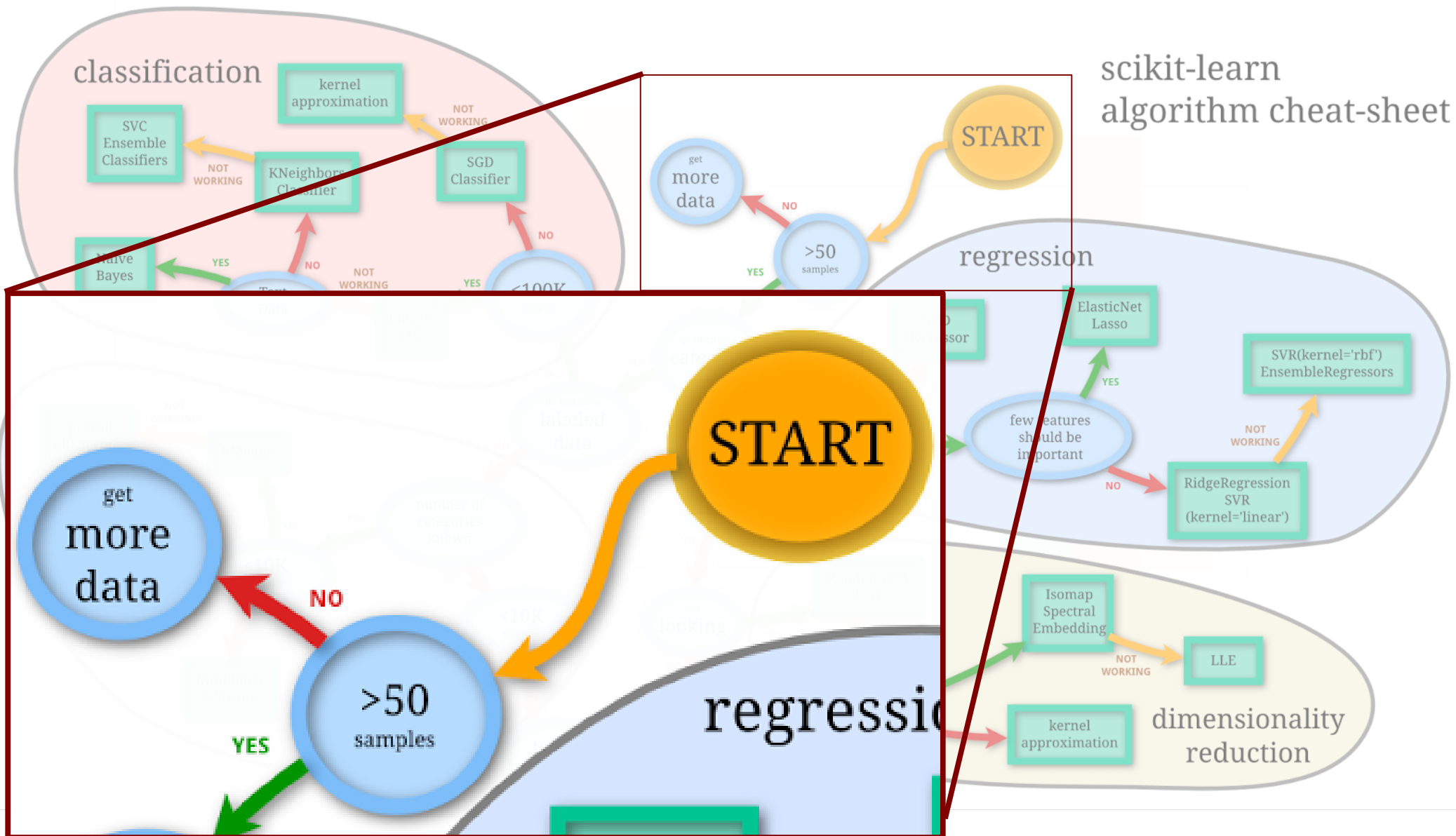
n=200



n=300



## 12

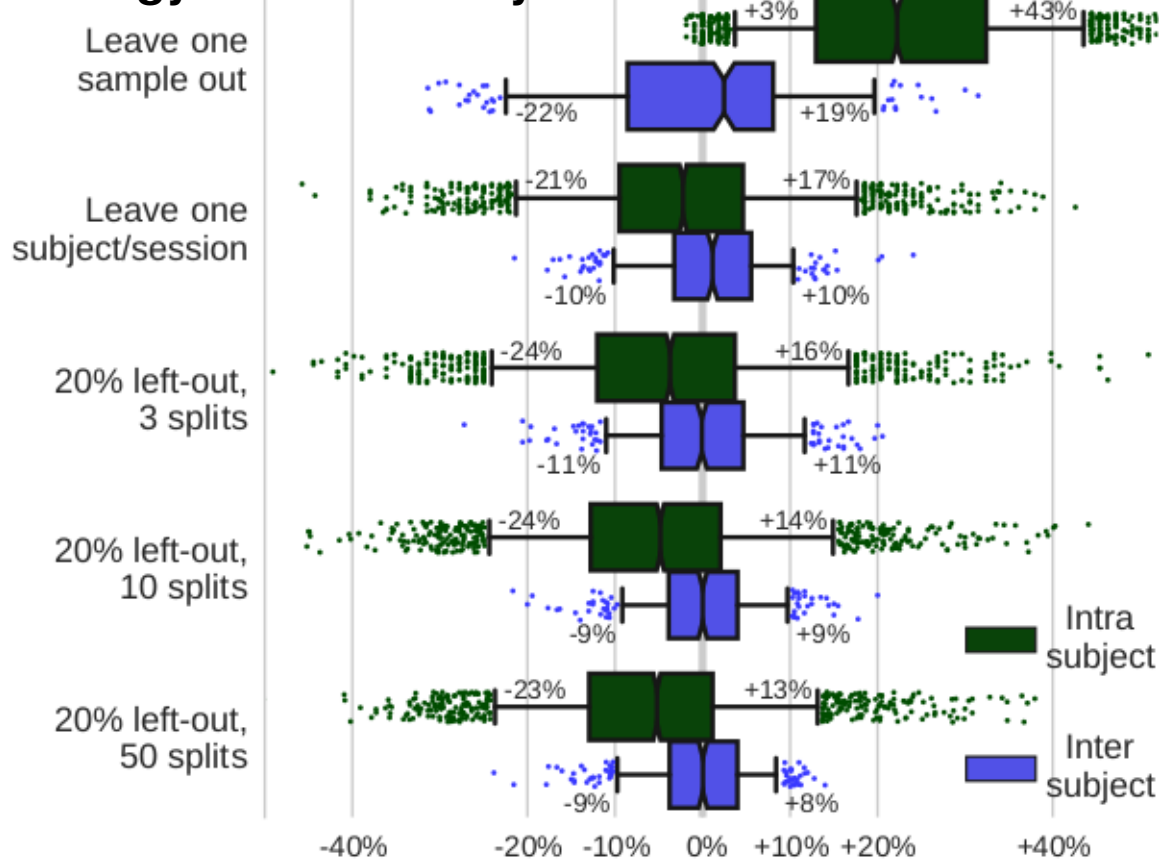




# Sample size & cross-validation

## Cross-validation strategy

Difference in accuracy measured by cross-validation and on validation set



Large-scale experiment:  
4 classifiers, 7 datasets, 1 anatomical dataset, 1 MEG dataset

cross-validation < validation set

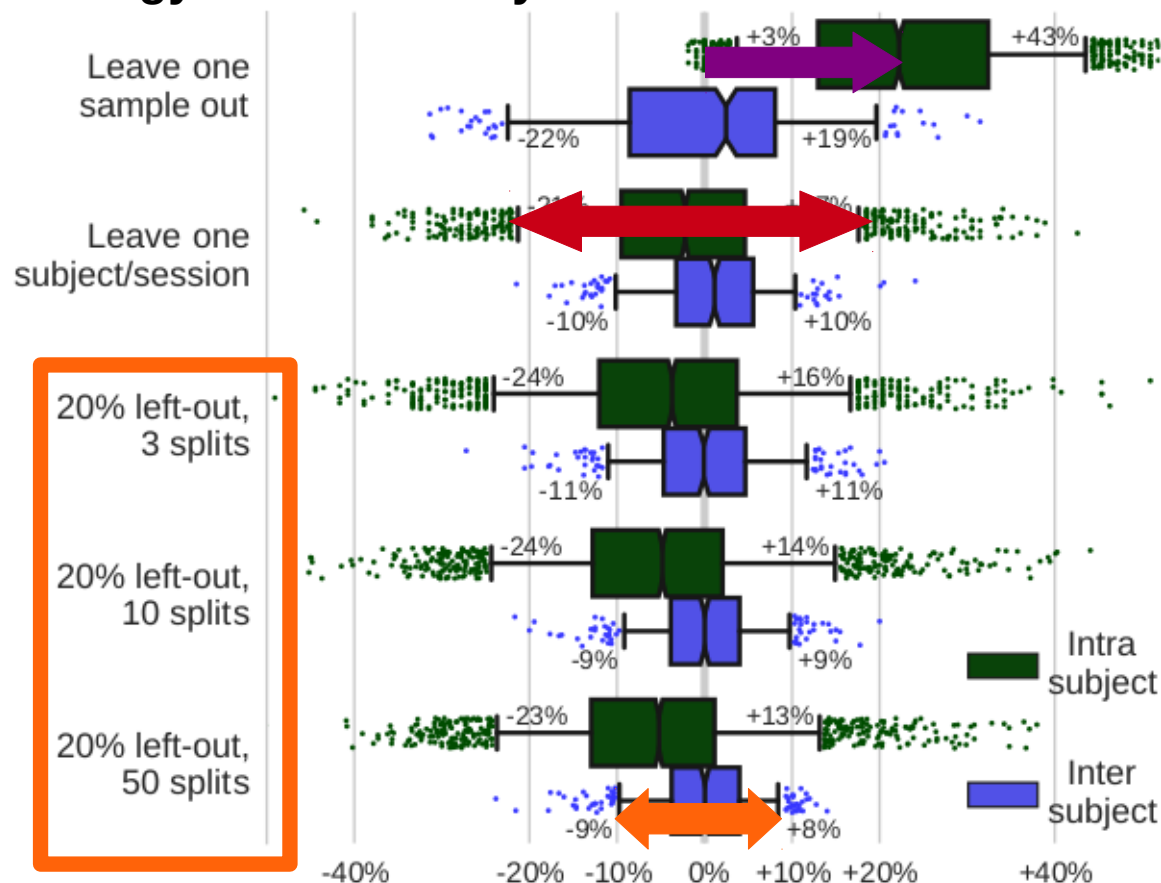
cross-validation > validation set

[Varoquaux et al. NIMG 2016]

# Sample size & cross-validation

## Cross-validation strategy

Difference in accuracy measured by cross-validation and on validation set



- optimistic bias in LOO for non-independent samples
- higher variance in LOO
- variance large overall  
→ use shuffle-split with many splits

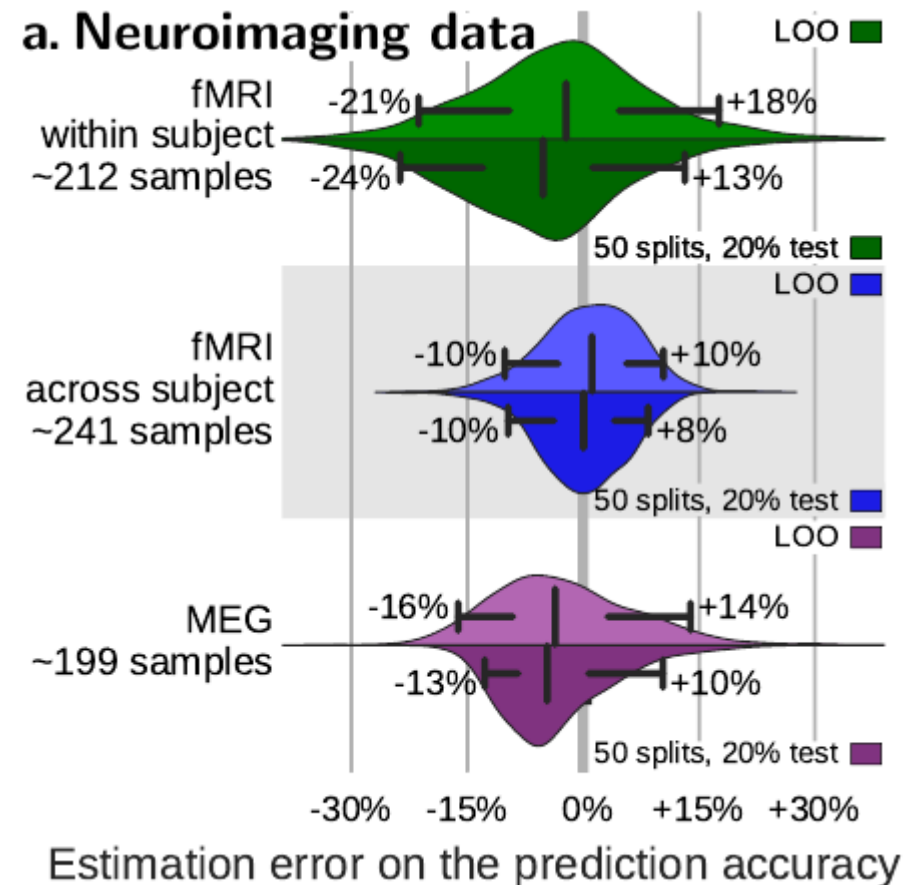
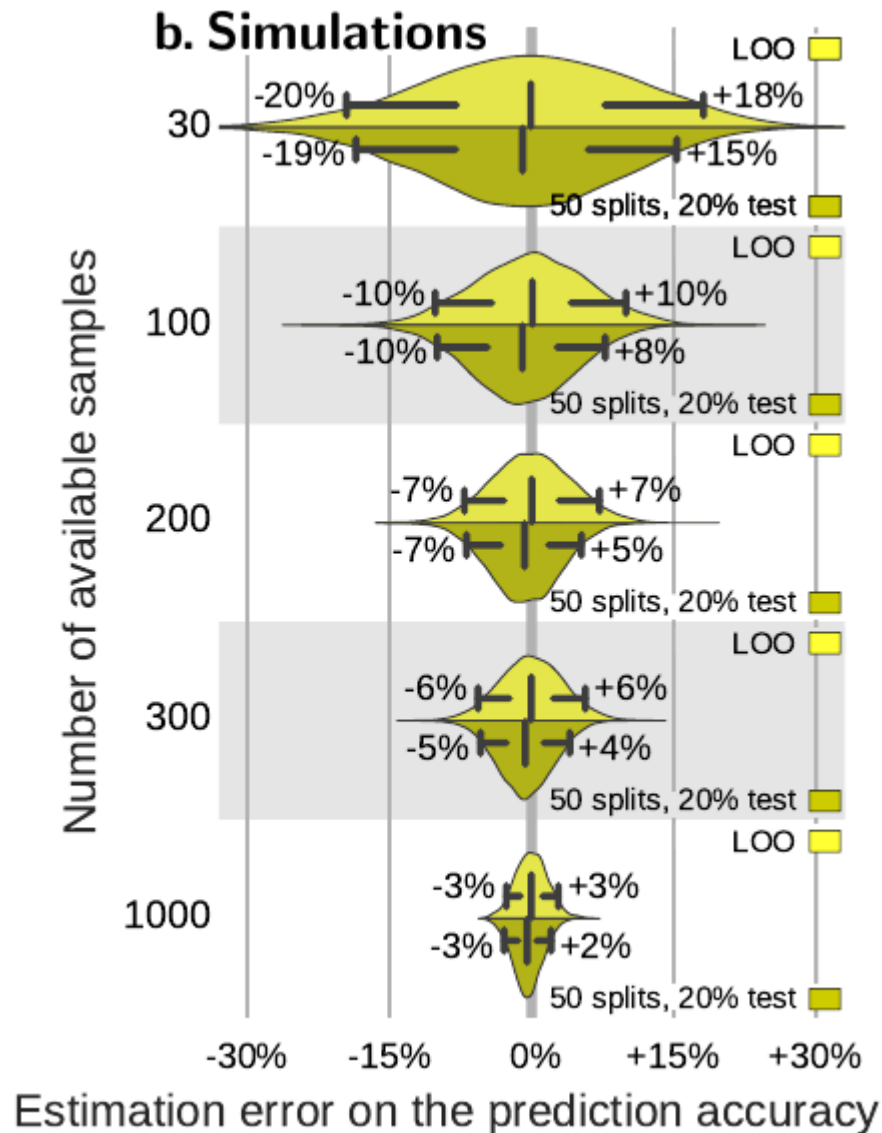
cross-validation < validation set

cross-validation > validation set

[Varoquaux et al. NIMG 2016]

# Sample size and cross-validation

Rule of the thumb: uncertainty in prediction decreases with  $1/\sqrt{n}$



[G. Varoquaux nimg 2017]

# Why don't we use deep neural networks ?

- They are expensive, hard to tune, hard to interpret and do not bring performance gains in most neuroimaging settings

<https://www.biorxiv.org/content/10.1101/473603v1>

# Do it yourself !

<http://nilearn.github.io/>

