Pattern Recognition for NeuroImaging (PR4NI)

# Interpreting predictive models in terms of anatomically labelled regions

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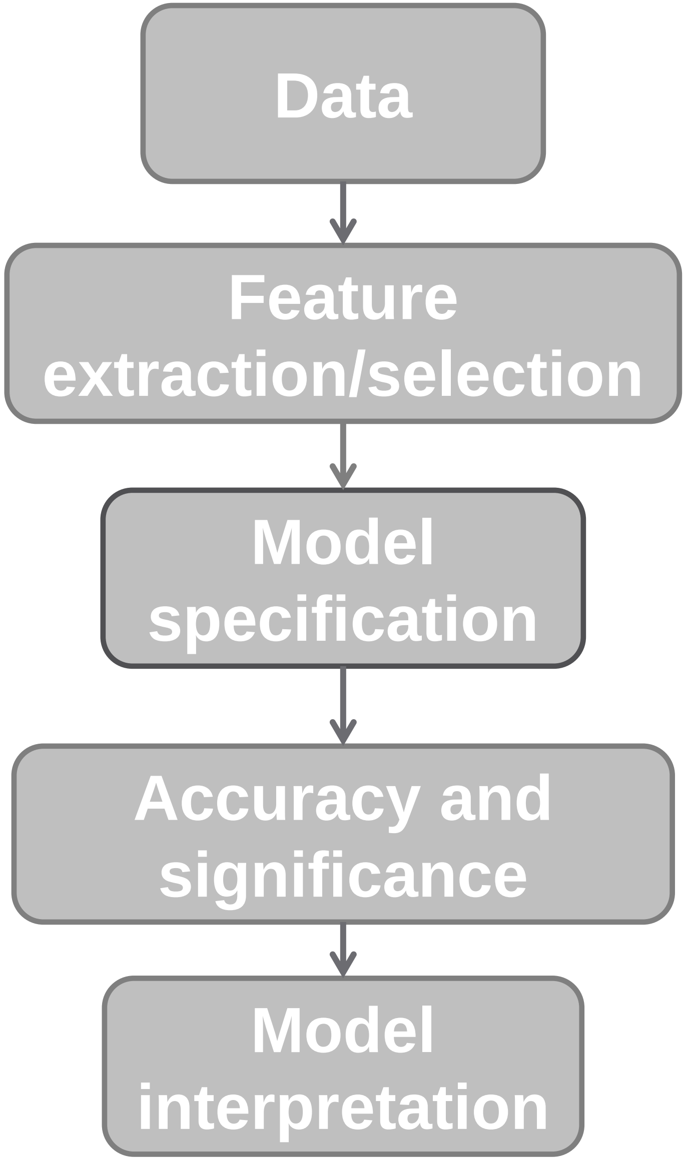
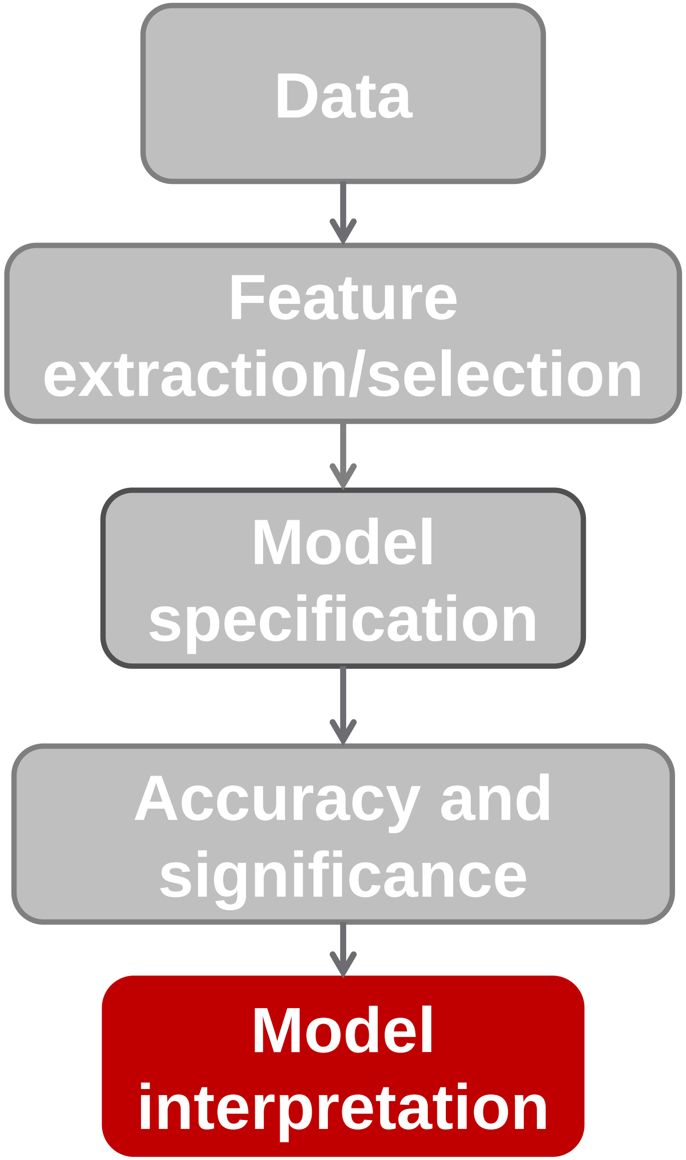

Data
Feature extraction/selection
Model specification
Accuracy and significance
Model interpretation




Where in the brain is the information of interest?

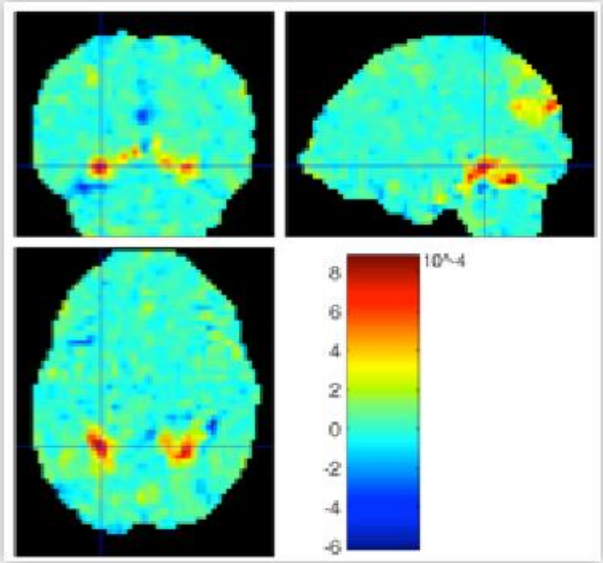
i.e. Which brain areas contribute most to the model's prediction?

Computing “weight maps”:

- From linear (kernel) methods
- Attributing one weight per feature

- For an SVM model:

$$\mathbf{w} = \sum_{i=1}^{n} y_i \alpha_i^* \ \mathbf{x_i}$$

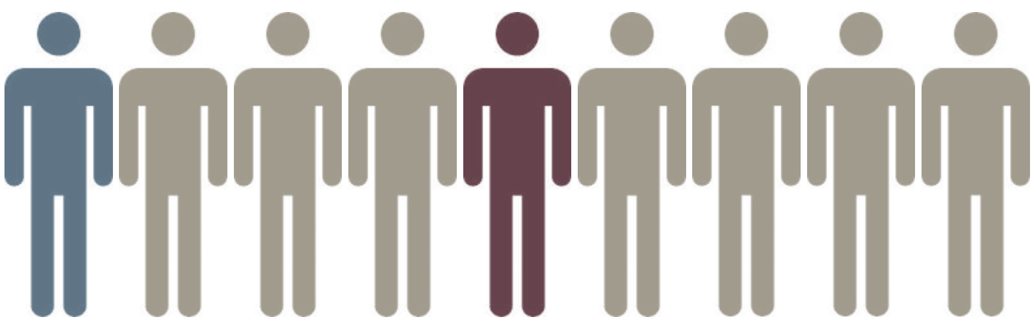


Thresholding weight maps:

*Can we choose to look only at the largest contributions?*

- Linear combination
- As in an election
- Each vote counts

$$f(\mathbf{x}_i) = \langle \mathbf{w}, \mathbf{x_i} \rangle + b$$



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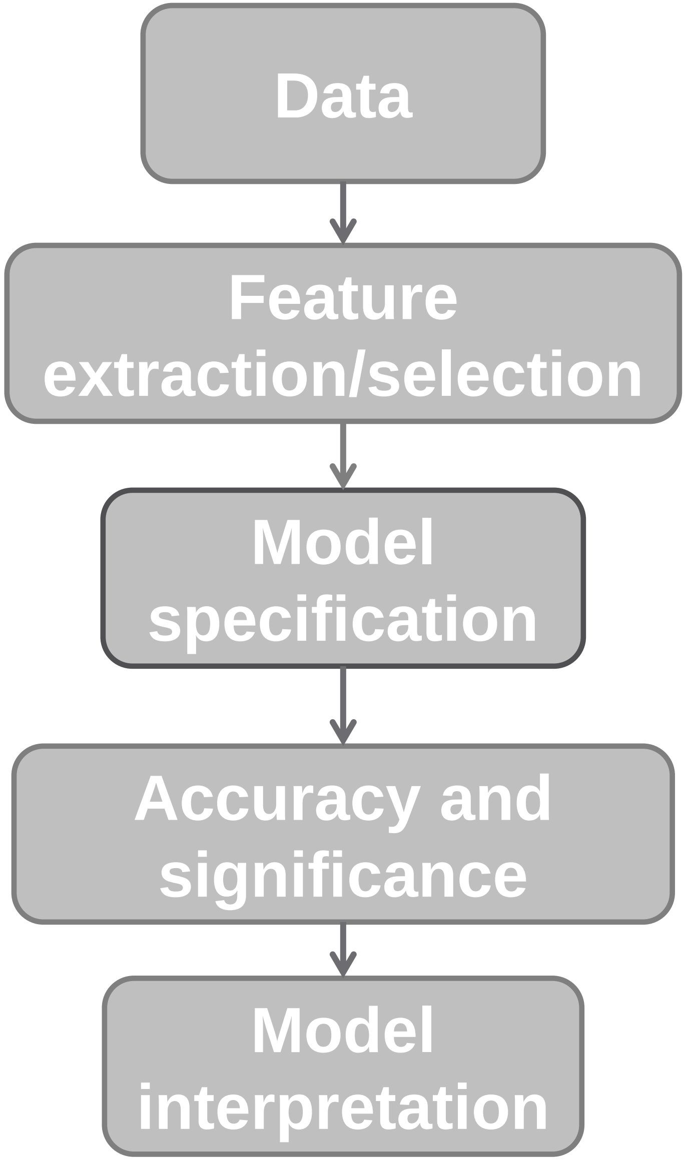
Different strategies:

1. A priori knowledge: ROI selection
2. Searchlight
3. Feature selection
4. Sparse algorithms
5. Multiple Kernel Learning (MKL)
6. A posteriori knowledge: weight summarization




Different strategies:

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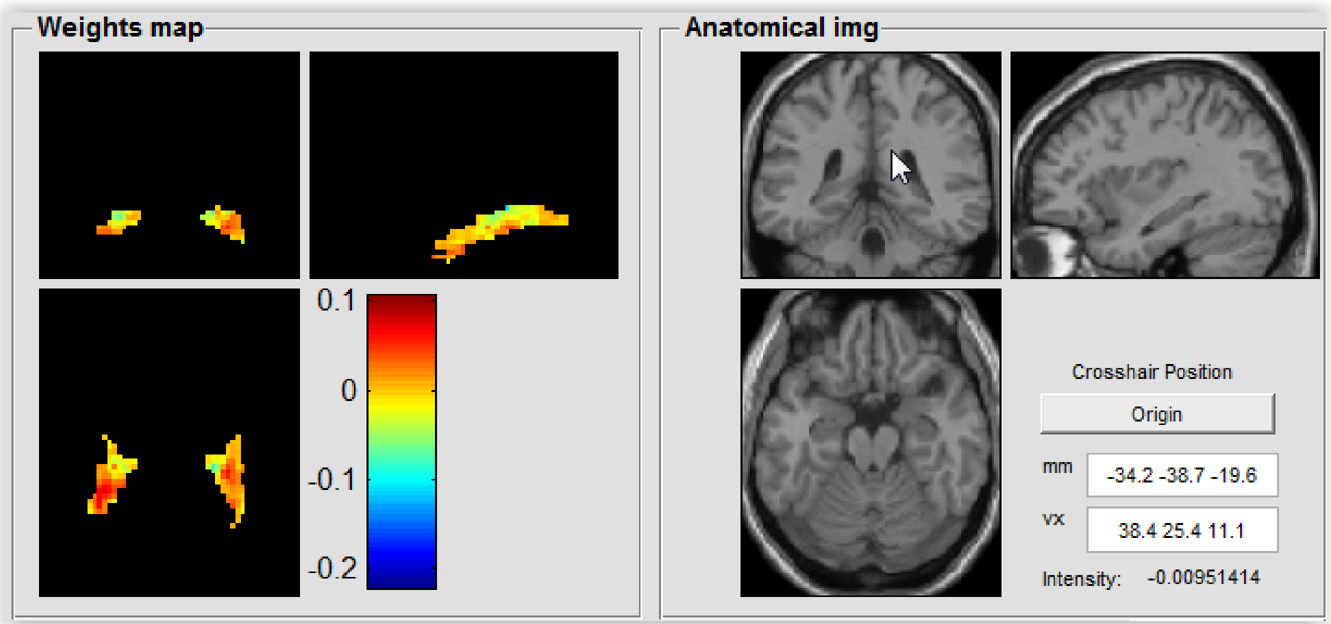
1. A priori knowledge: ROI selection

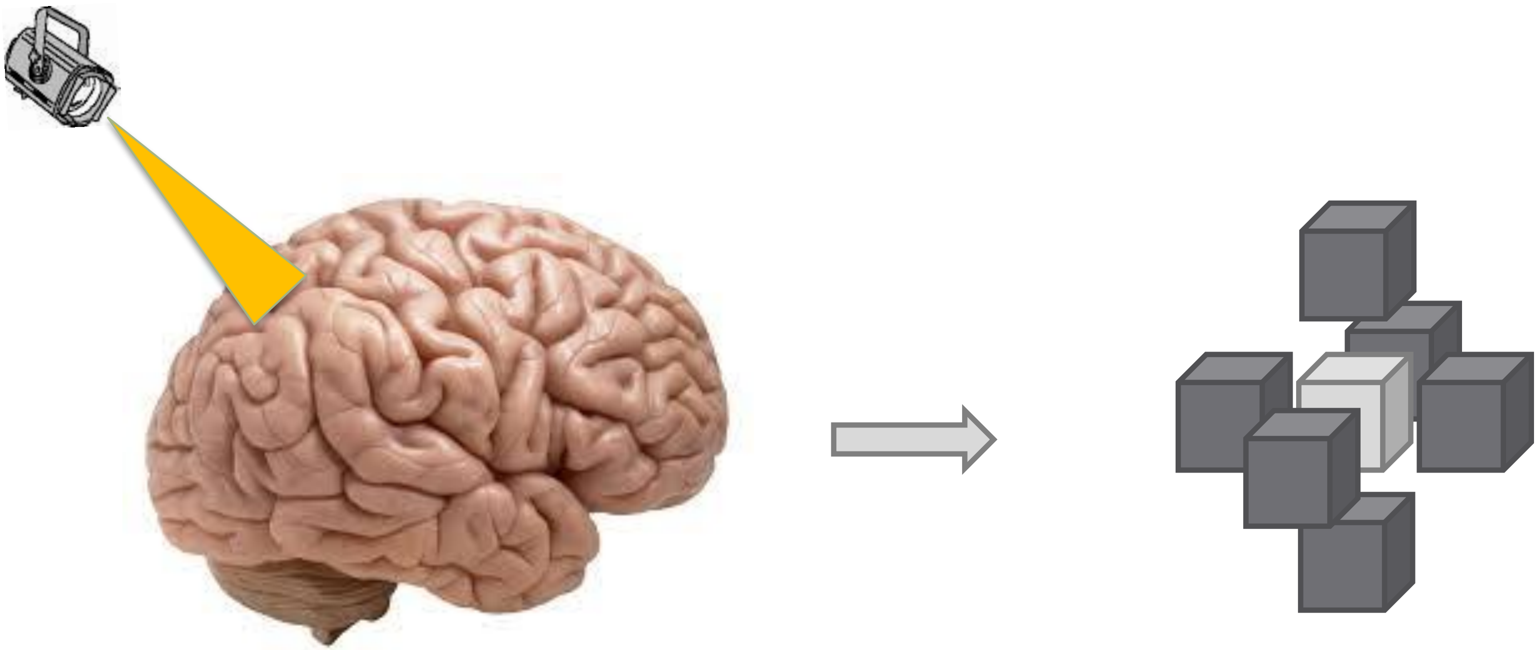
e.g. Choosing voxels/features based on literature or on previous univariate results (independent dataset).



1. A priori knowledge: ROI selection

| + | - |
|---|---|
| Good accuracy? | Need an anatomical hypothesis |
| Anatomically/ functionally relevant | Cannot threshold obtained map |
| | Arbitrary choice of region number and size |
| | Multiple models = multiple comparisons |

## 2. Searchlight (Kriegeskorte et al., 2006)



## 2. Searchlight (Kriegeskorte et al., 2006)

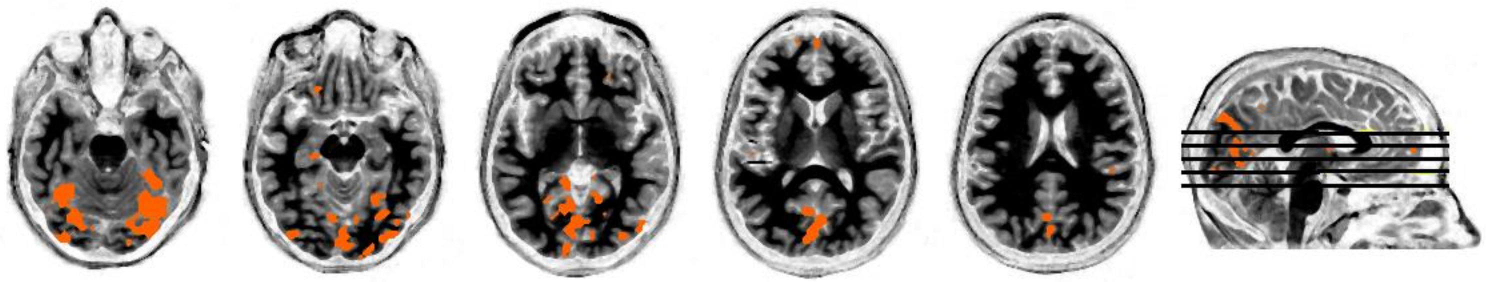
| + | - |
|---|---|
| Threshold for each neighborhood | Not anatomically/functionally relevant (spheres) |
| | Locally multivariate |
| | Arbitrary choice of neighborhood size |
| | Multiple models = multiple comparisons |
| | Time-consuming |

## 3. Feature selection

Rank the features according to a specific criterion and select a subset.

Example:

- Univariate t-test
- Recursive Feature Elimination (RFE, De Martino, 2008) based on SVM weights



## 3. Feature selection

| + | - |
|---|---|
| Data-driven | Not anatomically/functionally relevant (voxel sparse) |
| | Time-consuming: nested CV |
| | Depends on selected technique: flaws in feature selection are reflected in model. → user choice must be informed. |
| | Different strategies = different patterns with same accuracy. |

4. Sparse algorithms

Algorithms with regularization constraints such that the weight of some features is perfectly null.

Examples:

- LASSO (Tibshirani, 1996)
- Elastic-net (Zou and Hastie, 2005)

## 4. Sparse algorithms

| + | - |
|---|---|
| Data-driven | Not anatomically/functionally relevant (voxel sparse) |
| Embedded in model | Stability of selected voxels (Baldassarre, et al., 2012): different regularization terms = different patterns for same accuracy. |

## 4. Sparse algorithms

| + | - |
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| Data-driven | Not anatomically/functionally relevant |
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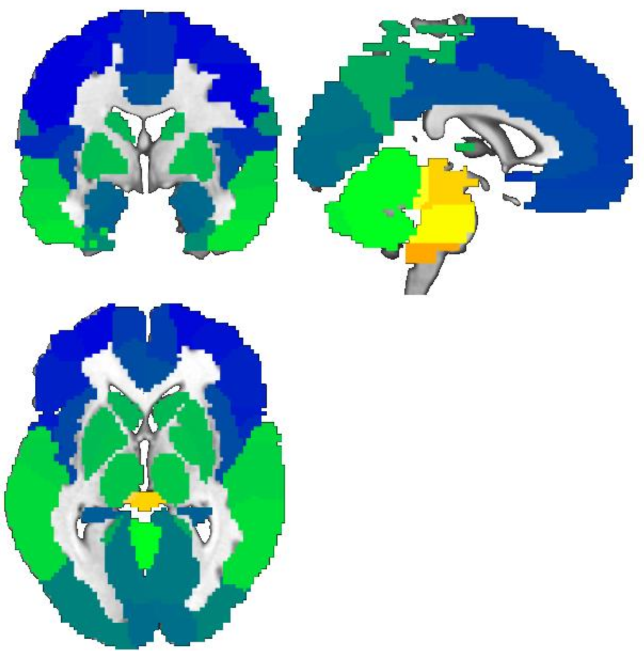
Note: stability selection (Rondina et al., 2014).

## 5. Multiple Kernel Learning (MKL)

Build one kernel per anatomically defined region as input of a (sparse) MKL algorithm (Filippone, 2012).



$$K(\boldsymbol{x},\boldsymbol{x}') = \sum_{m=1}^{M} d_m K_m(\boldsymbol{x},\boldsymbol{x}')$$

with $d_m \geq 0, \ \sum_{m=1}^{M} d_m = 1$

## 5. Multiple Kernel Learning (MKL)

Decision function of an MKL problem:

$$f(\mathbf{x}_i) = \sum_m \langle \mathbf{w}_m, \mathbf{x}_\mathbf{i} \rangle + b$$

Considered algorithm (Rakotomamonjy et al., 2008):

$$\min \frac{1}{2} \sum_m \frac{1}{d_m} \|\mathbf{w}_m\|^2 + C \sum_i \xi_i$$

$$s.t. \quad y_i \left( \sum_m \langle \mathbf{w}_m, \mathbf{x}_\mathbf{i} \rangle + b \right) \geq 1 - \xi_i \qquad \forall i$$

$$\xi_i \geq 0 \qquad \forall i, \sum_m d_m = 1, \qquad d_m \geq 0 \quad \forall m$$

5. Multiple Kernel Learning (MKL)

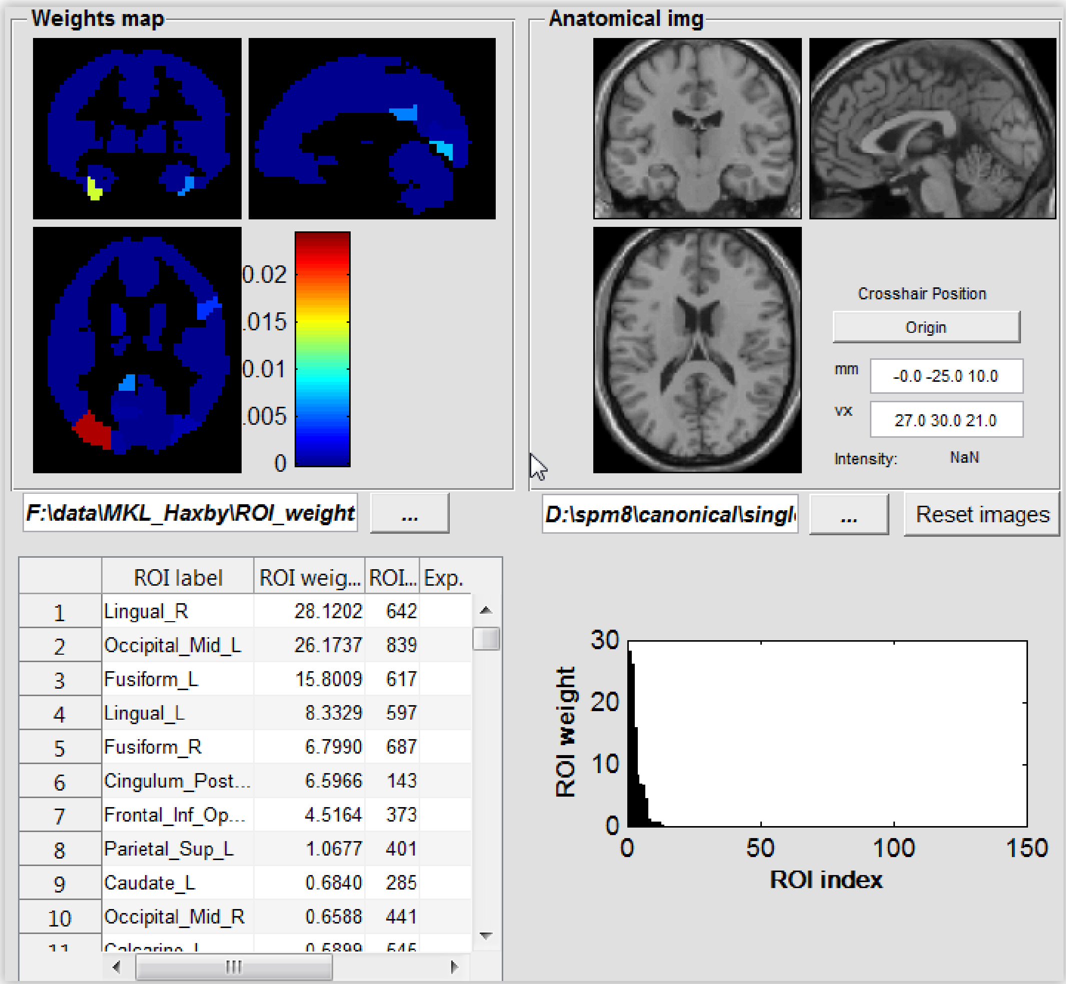
Weight map of an MKL model:

$$\mathbf{w}_{\boldsymbol{m}} = d_m \sum_{i=1}^{n} y_i \alpha_i \ \mathbf{x}_{\mathbf{i}}$$

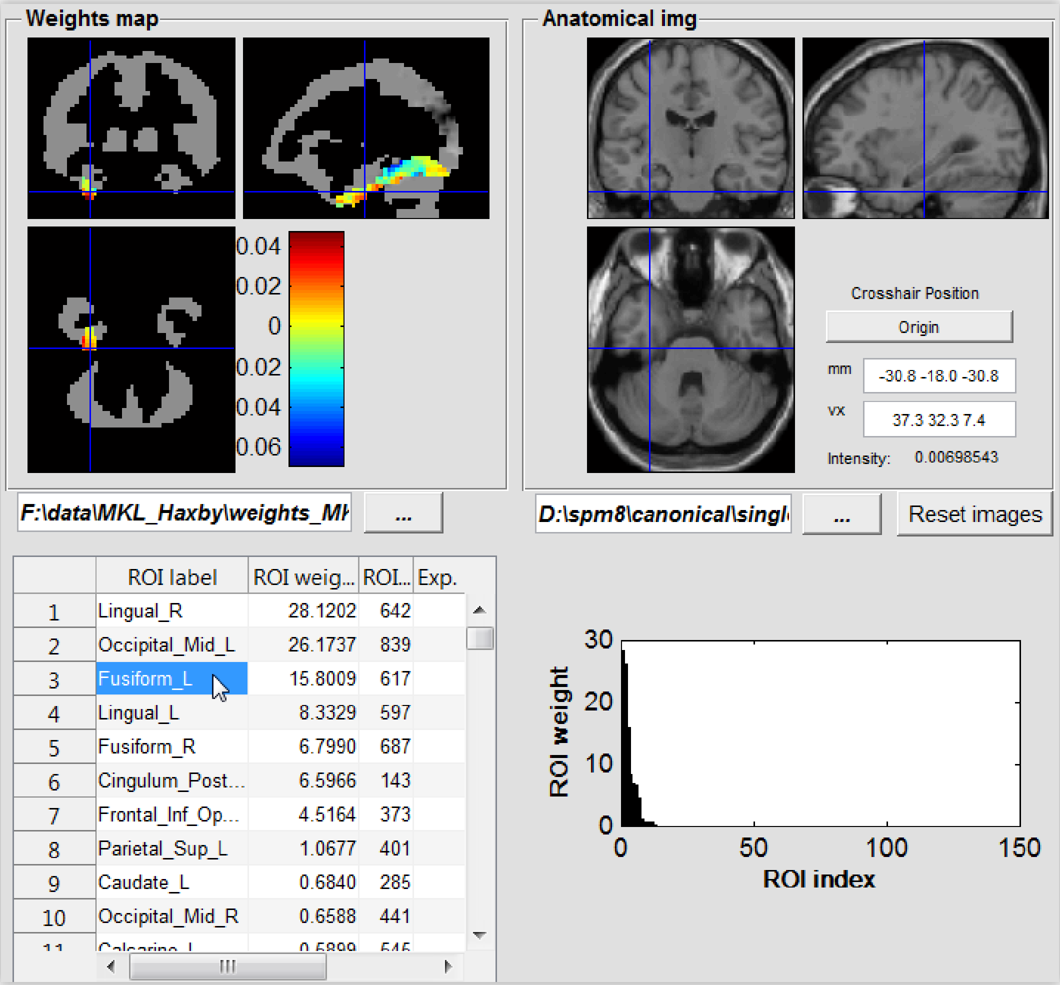
But also $d_m$

→ Can be considered as a hierarchical approach

# 5. Multiple Kernel Learning (MKL)



# 5. Multiple Kernel Learning (MKL)



## 5. Multiple Kernel Learning (MKL)

| + | - |
|---|---|
| Anatomically/ functionally relevant | Stability of the selected regions |
| Used the full pattern to build the model | Depends on atlas |
| Thresholded and sorted list of regions according to $d_m$ | |
| Hierarchical view of the model parameters | |

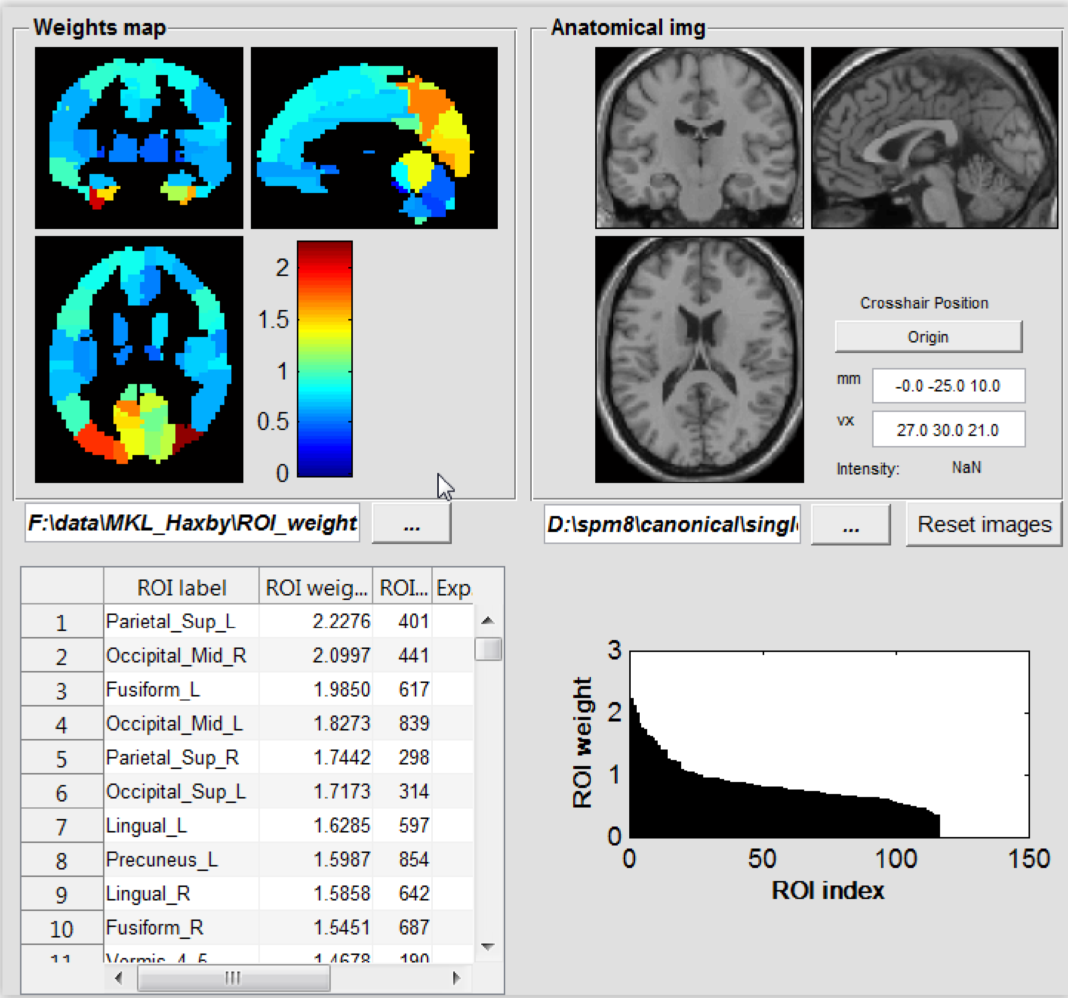
6. A posteriori knowledge: weight summarization (Schrouff et al., 2013)

Build weight maps then summarize weights according to anatomically defined regions (e.g. based on an atlas).

Mathematically:

$$NW_{ROI} = \frac{\sum_{v \in ROI} |W_v|}{\# v \in ROI}$$

# 6. A posteriori knowledge: weight summarization



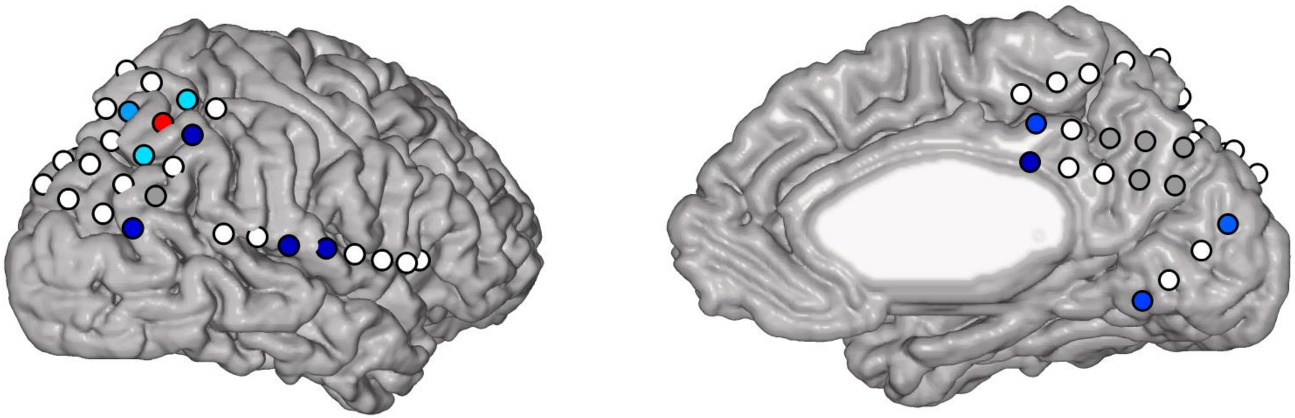

AAL atlas (Tzourio-Mazoyer, 2002).

## 6. A posteriori knowledge: weight summarization

| + | - |
|---|---|
| Anatomically/ functionally relevant | No thresholding of the sorted list of regions |
| Used the full pattern to build the model | Depends on atlas |
| Sorted list of regions according to their proportion of $NW_{ROI}$ | |

How about electrophysiological recordings?

- All strategies explained previously apply
- For MKL, can be applied on each dimension (i.e. channels, time point, frequency band) or combination (e.g. channel + frequency band)



## Conclusions:

- Interpreting machine learning based models can be complex.
- Different strategies exist, but always a trade-off between different parameters:
  - Thresholded list of voxels/regions contributing
  - Anatomical/functional relevance
  - Multivariate power
  - Stability of the pattern
  - Computational time

⟹ Your (informed) choice!

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# References:


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