Alternatives to support vector machines in neuroimaging

ensembles of decision trees for classification and information mapping with predictive models

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Decision trees deserve more attention

Scopus june 2013:

(mapping OR "brain decoding" OR "brain reading" OR classification OR MVPA OR "multi-voxel pattern analysis") AND (neuroimaging OR "brain imaging" OR fMRI OR MRI or "magnetic resonance imaging")

+ ("support vector machine" OR "SVM") = 657 docs
(1282 if adding EEG OR electroencephalography OR MEG OR magnetoencephalography)

+ ("random forest" OR "decision tree") = 71 docs
(199 if adding EEG OR electroencephalography OR MEG OR magnetoencephalography)

Roughly speaking, more used at MICCAI (segmentation, geometry extraction, image reconstruction, skull stripping...) than at HBM

Tutorial agenda

Lecture

Basics

Growing trees

Ensembling

The random forest

Other forests

Tuning your forests

Information mapping

Correlated features

Practical

Datasets

Matlab/
PRoNTo

Python/Scikit

Information mapping relates model input to output

In supervised learning for classification, we seek a function mapping voxels to class labels

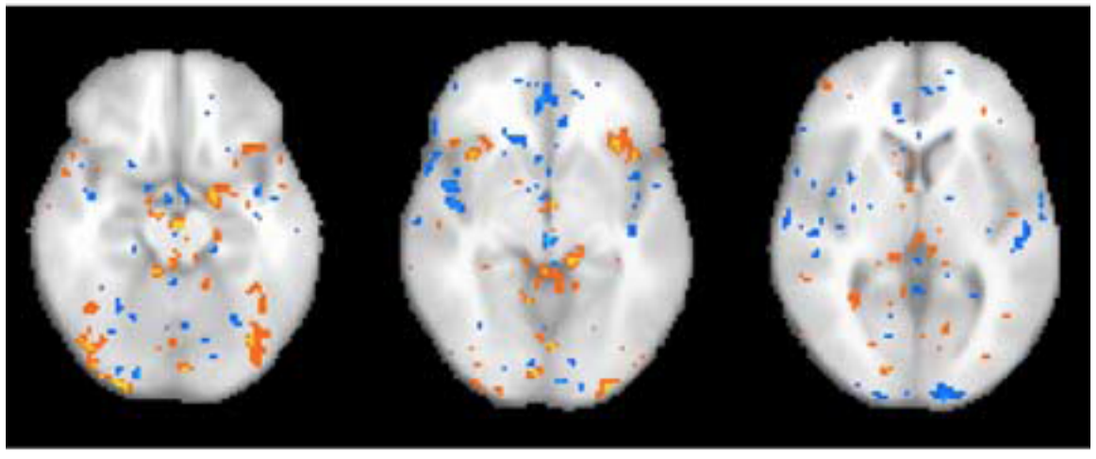
$$f(\mathbf{x}) : \mathbb{R}^D \rightarrow y$$

$$y = \{0, 1\},\ \mathbf{x} \in \mathbb{R}^D \quad \mathcal{S} = \{(\mathbf{x}_n, y_n)\},\ n = 1, \ldots, N$$

As neuroimagers, if some voxels in **x** contain information about y, the function should reflect it, and we are interested in *mapping* it

$$f(\mathbf{x}) = \mathrm{sgn}(\mathbf{w}^{\mathrm{T}}\mathbf{x} + b)$$

tells us about **relative** discriminative importance



[Mourao-Miranda et al., NeuroImage, 2005]

Mutual information measures uncertainty reduction

We can also *explicitly* measure the amount of information **x** and y share using *mutual information*.

$$I(Y;X) \equiv H(Y) - H(Y|X)$$

$$H(Y) \equiv \sum_{y} P(y) log \frac{1}{P(y)}$$

high if classes are balanced (high uncertainty about class membership)

$$H(Y|X) \equiv \sum_{y,x} P(y,x) log \frac{1}{P(y|x)}$$

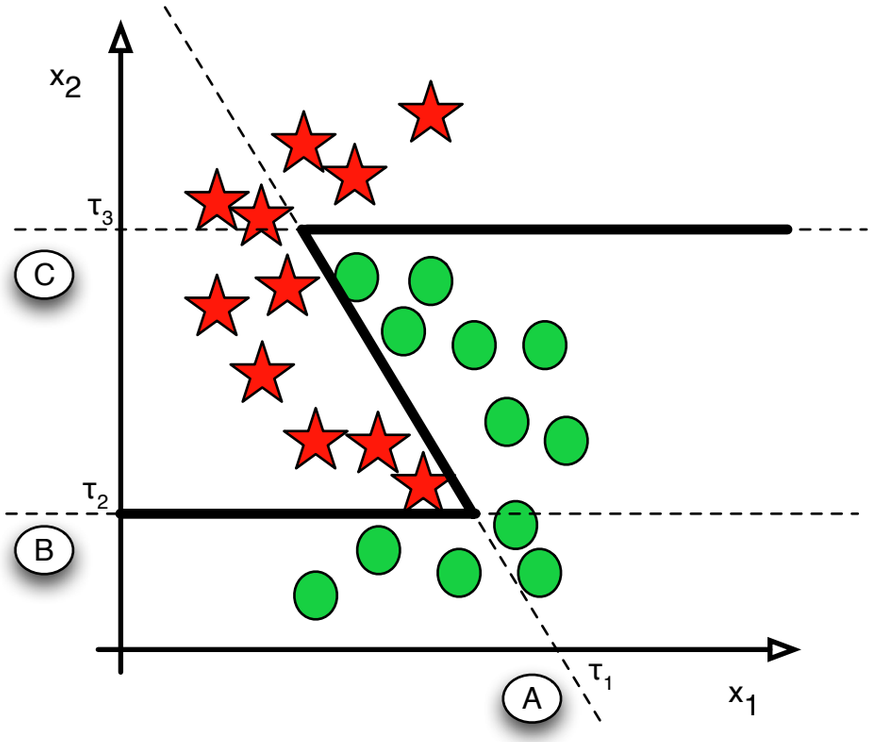
average uncertainty remaining about class label if we know the voxel intensity

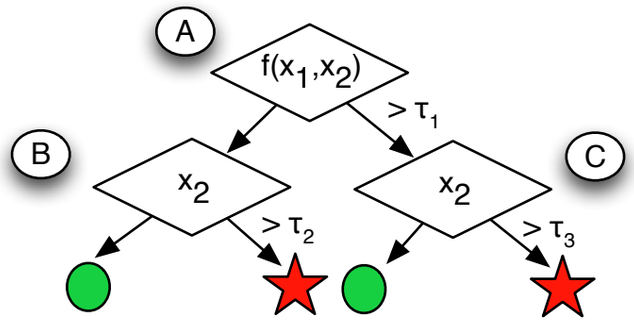
$$I(Y;X) \equiv \sum_{y,x} P(y,x) log \frac{P(y,x)}{P(y)P(x)}$$

average **reduction in uncertainty** about class label if we know voxel intensity

Growing trees recursively reduces entropy

Decision trees seek to partition voxel space by intensity values to decrease uncertainty about class label





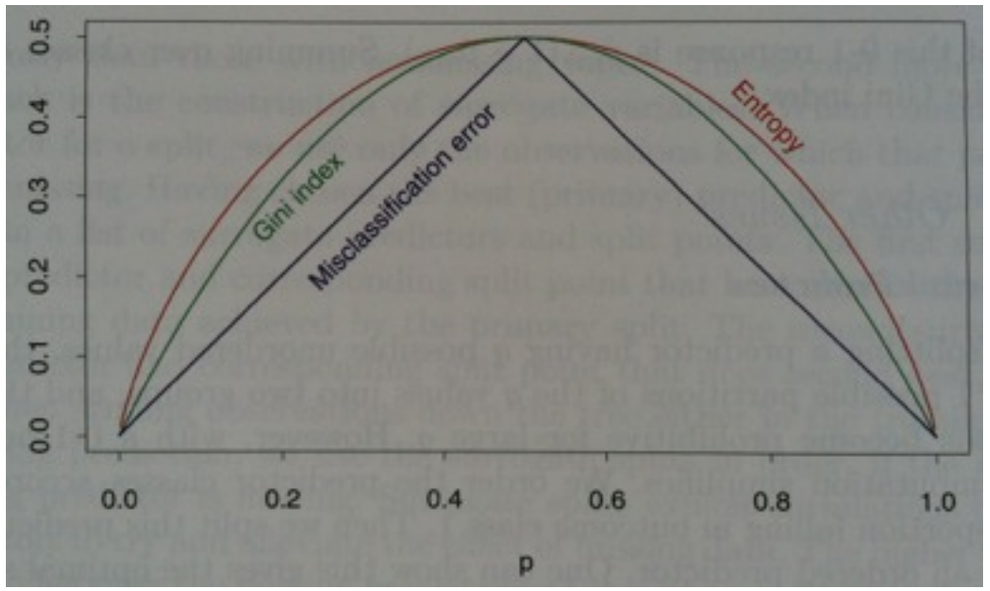
This *leaves* a few questions... How to measure goodness of splits? How to choose voxels and where to cut ? When to stop growing?

```
>rpart::rpart
>>stats::classregtree
>>>sklearn::tree
```

Split goodness can be measured

Entropy impurity: $H(\mathcal{S}) \equiv \sum_y P(y) log \frac{1}{P(y)}$

Gini impurity: $G(\mathcal{S}) \equiv \sum_{y_i \neq y_j} P(y_i) P(y_j)$

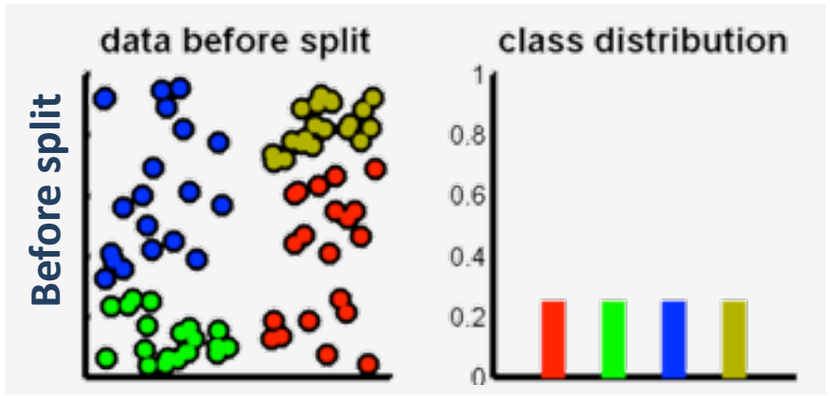


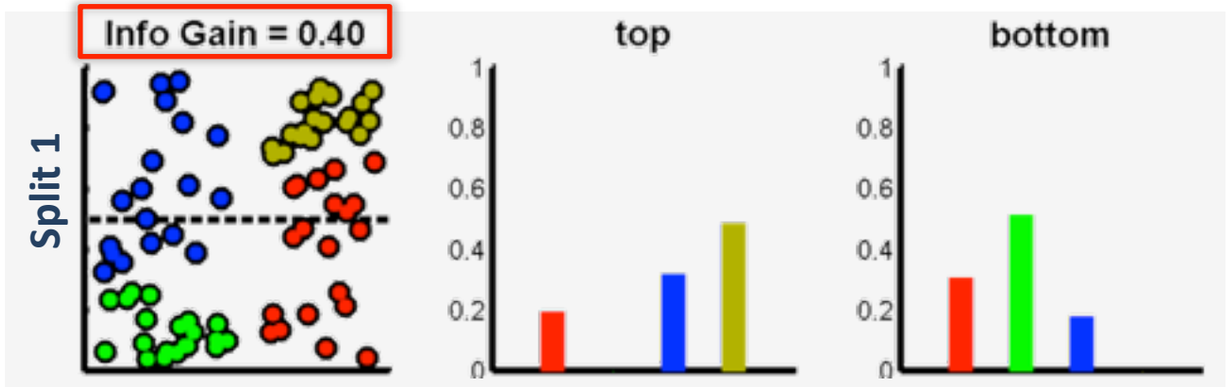
[Hastie et al., 2001]

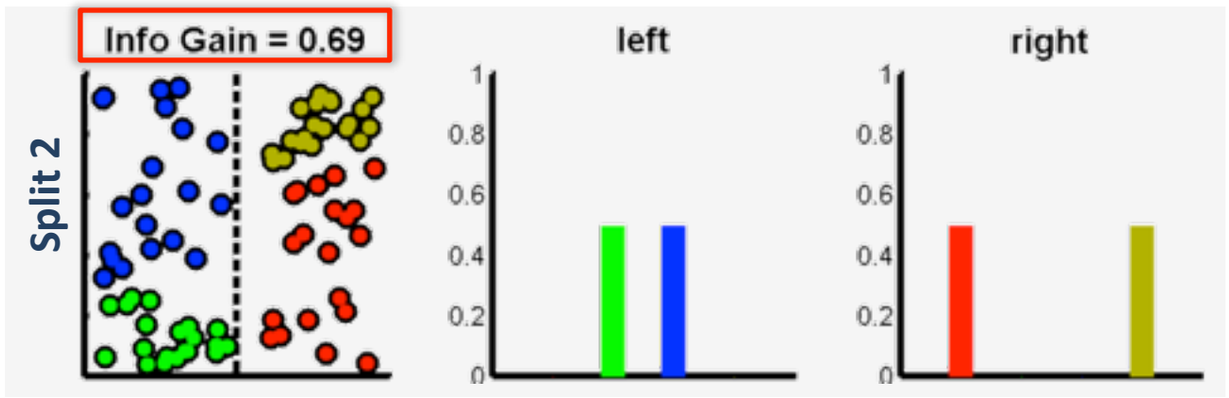
Information Gain (decrease in impurity):

$$\Delta I(\mathcal{S}; x, \tau) \equiv H(\mathcal{S}) - \sum_{i=L,R} \frac{|\mathcal{S}^i|}{|\mathcal{S}|} H(\mathcal{S}^i)$$

Information gain helps choose the best split







[Criminisi & Shotton, 2013]

Stopping and pruning matter

We can stop growing the tree

When the info gain is small

When the number of points in a leaf is small (relative or absolute) - dense regions of voxel space will be split more

When (nested) CV error does not improve any more

... but stopping criteria are hard to set

We can grow fully and then prune

Merge leaves where miminal impurity increase ensues

We can leave unpruned

These choices generally matter more than split goodness criterion (see CART vs C4.5)

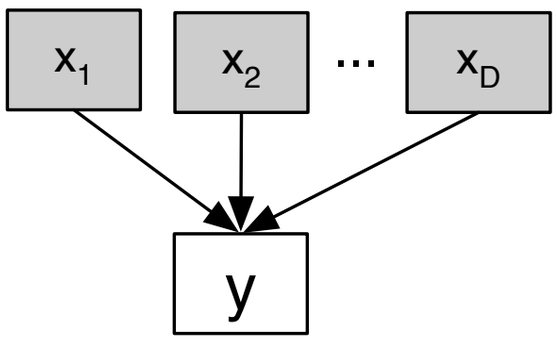
Trees relate to other models

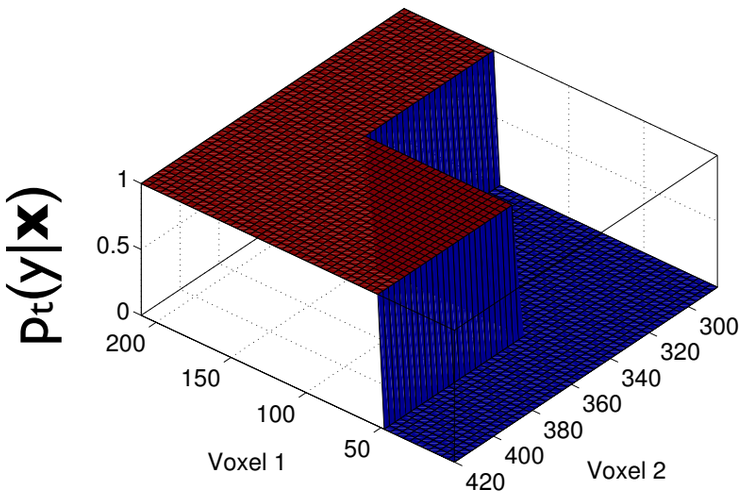
We can view trees as *kernels*: build a feature space mapping with indicator functions

$$\Phi(\mathbf{x}) = (\mathbf{1}_1(\mathbf{x}) \ldots \mathbf{1}_B(\mathbf{x}))^T$$

Then $k_b(\mathbf{x}, \mathbf{x}') = \Phi(\mathbf{x})^T \Phi(\mathbf{x}')$ is a positive kernel (only = 1 if x and x' in same leaf). Can also do 'soft' version

We can also view trees as encoding conditional probability distributions, e.g. represented by *Bayesian Networks*:



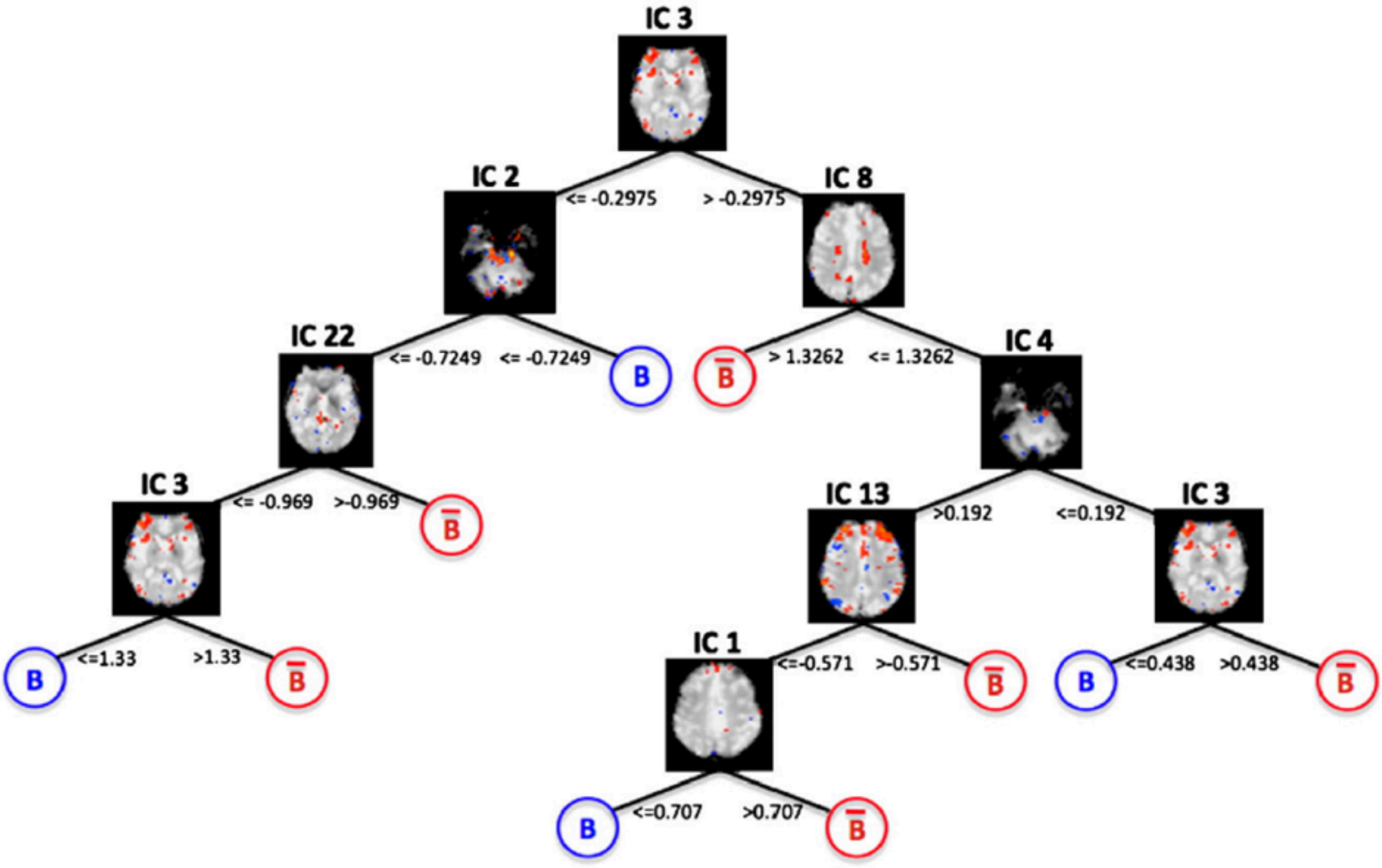


$$P(x_1, \ldots, x_D, y) = P(x_1) \cdot \ldots \cdot P(x_D) P(y|x_1, \ldots, x_D)$$

Kernel view: [Geurts et al., 2006]

BN view: [Richiardi, 2007], others

Trees are rule-based classifiers



[Douglas et al. 2011]

Many trees are more complex

Multivariate trees query >1 voxels per node

Splits don't have to be axis-parallel (can be oblique)

Model trees use MV regression in leaves

Functional Trees can use several voxels either at nodes or leaves

At each node, use ΔI to split on either a voxel x, or a logistic regression estimate of class probability P(y)

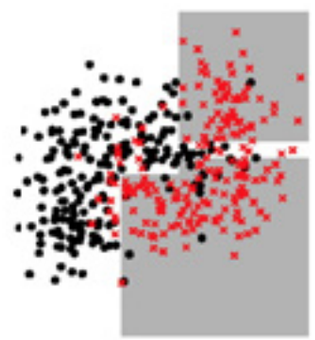
Multivariate nodes (FT-inner) reduce bias

Multivariate leaves (FT-leaves) reduces variance

Functional trees: [Gama, 2004]

Single trees vs SVMs

	SVM	Tree
Interpretability	+	+
Irrelevant voxels	+-	+
Input scaling	-	+
Speed	+ (linear)	+
Generalisation error	++	-
Information mapping	+-	-



[Kuncheva&Rodriguez 2010]

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Lecture	**Practical**
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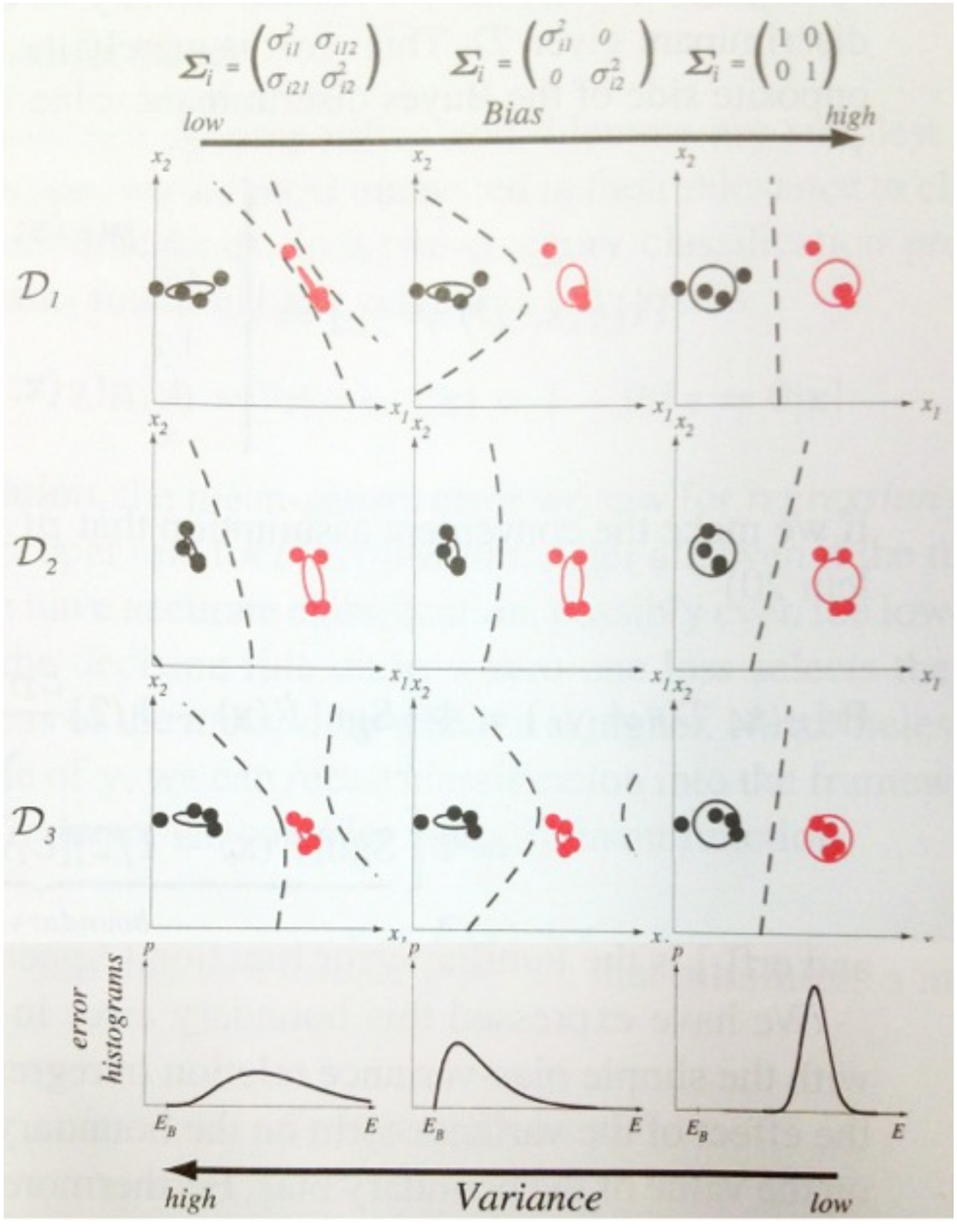
Single trees tend to have high variance

The **bias-variance tradeoff** applies as usual:

We can decrease prediction error arbitrarily on a given dataset, thus yielding low **bias**.

However, this systematically comes at a price in **variance**: the parameters of f can change a lot if the training set varies.

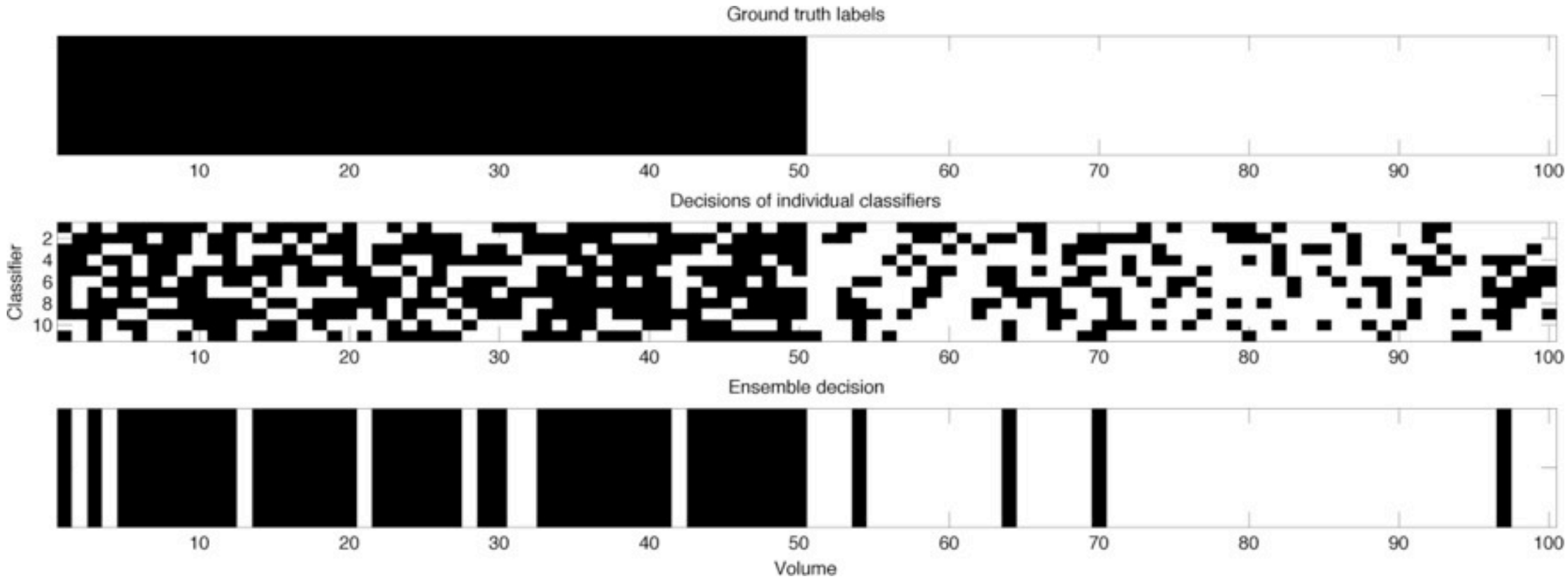
Single trees are not 'stable' - they tend to reduce bias by increasing variance



[Duda et al, 2001]

Ensembling exploits diversity

Train set of classifiers, combine predictions, get reduced ensemble variance and/or bias



Tree diversity has multiple sources

Training set **variability/resampling**, random **projection**, choice of **cut point** (, pruning strategy...)

Bagging classifiers generates diversity

Bagging = **B**oostrap **agg**regat**ing**

1. Resample with replacement B times from training dataset $\mathcal{S}$, yielding $\{\mathcal{S}_b\},\ b = 1, \ldots, B$

2. Train B *base classifiers* $\{f_b\}$

3. Get B predictions $\hat{\mathcal{F}} = \{\hat{f}_1(\mathbf{x}), \ldots, \hat{f}_B(\mathbf{x})\}$

4. Combine by majority vote $\hat{f}(\mathbf{x}) = Mo(\hat{\mathcal{F}})$

If the base classifiers have high variance, accuracy tends to improve with bagging since this generates diversity

Good news for trees!

[Breiman, 1996]


```
>::sample
>>stats::ClassificationBaggedEnsemble
>>>sklearn::ensemble
```

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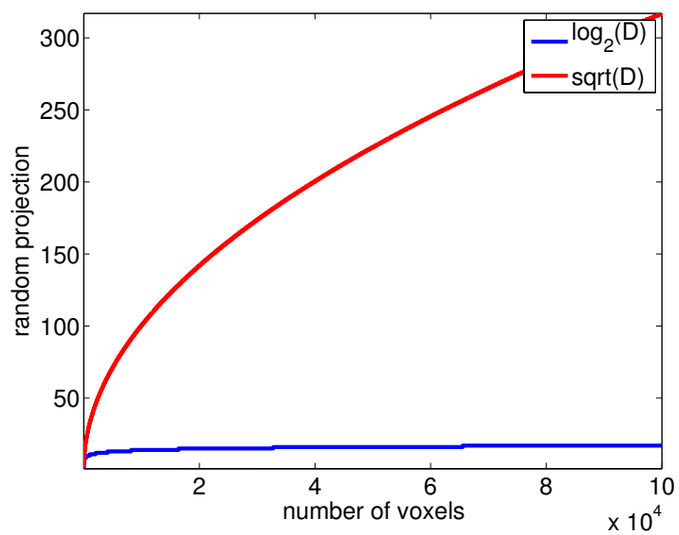
The random forest bags trees

RF combines several diversity-producing methods

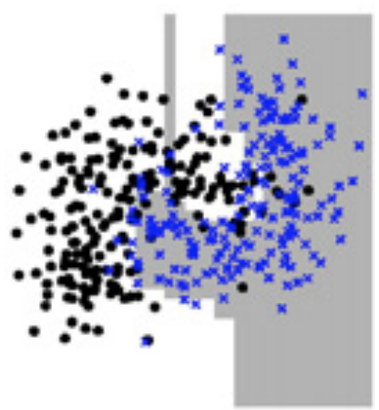
1. Generate B bootstrap replicates

2. At each node, randomly select a few voxels. Typically $K = \lfloor log_2 D + 1 \rfloor$ or $\lfloor \sqrt{D} \rfloor$. Since K << D, randomisation is high.

3. No pruning



With a 'large enough' number of trees, RFs typically performs well with no tuning on many datasets



[Kuncheva&Rodriguez 2010]

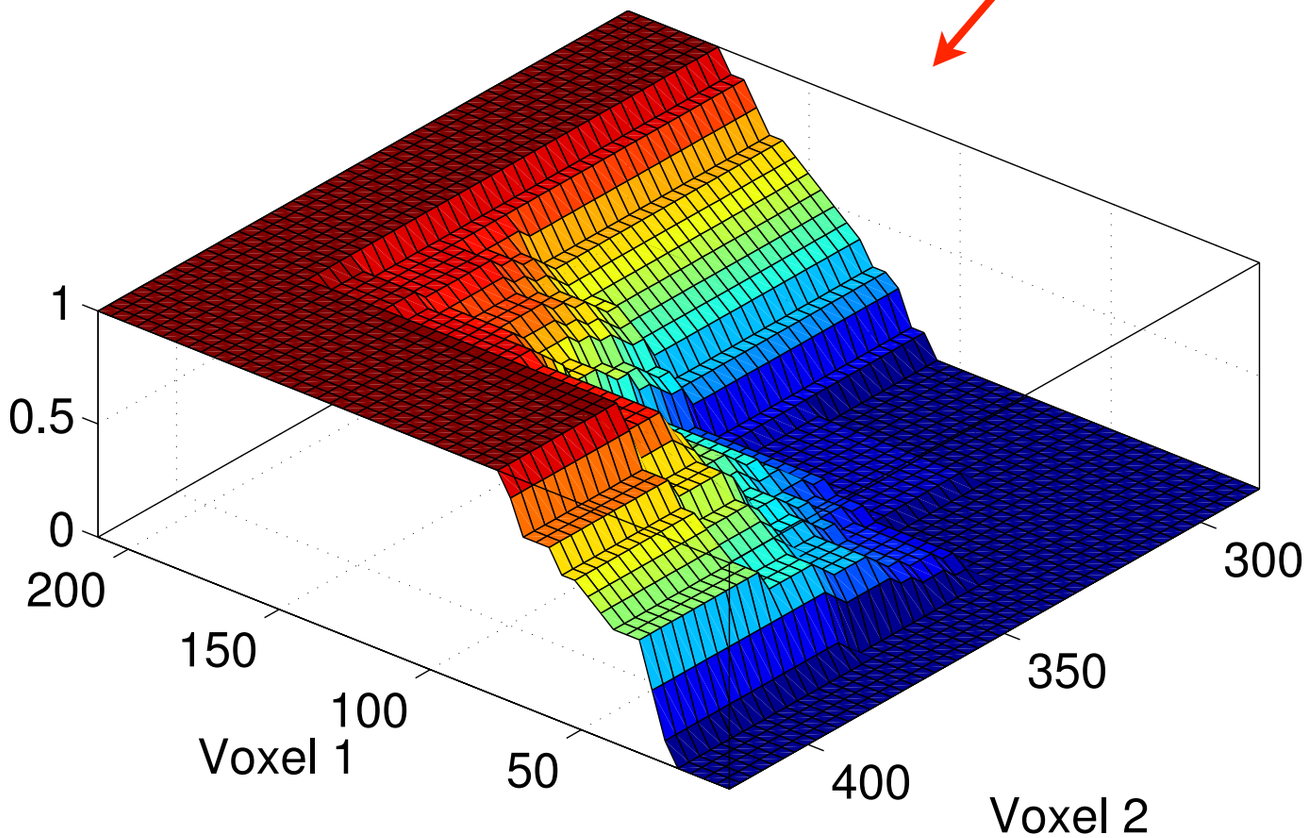
```
>adabag::bagging
>>stats::TreeBagger, PRoNTo::machine_RT_bin
>>>sklearn::RandomForestClassifier
```

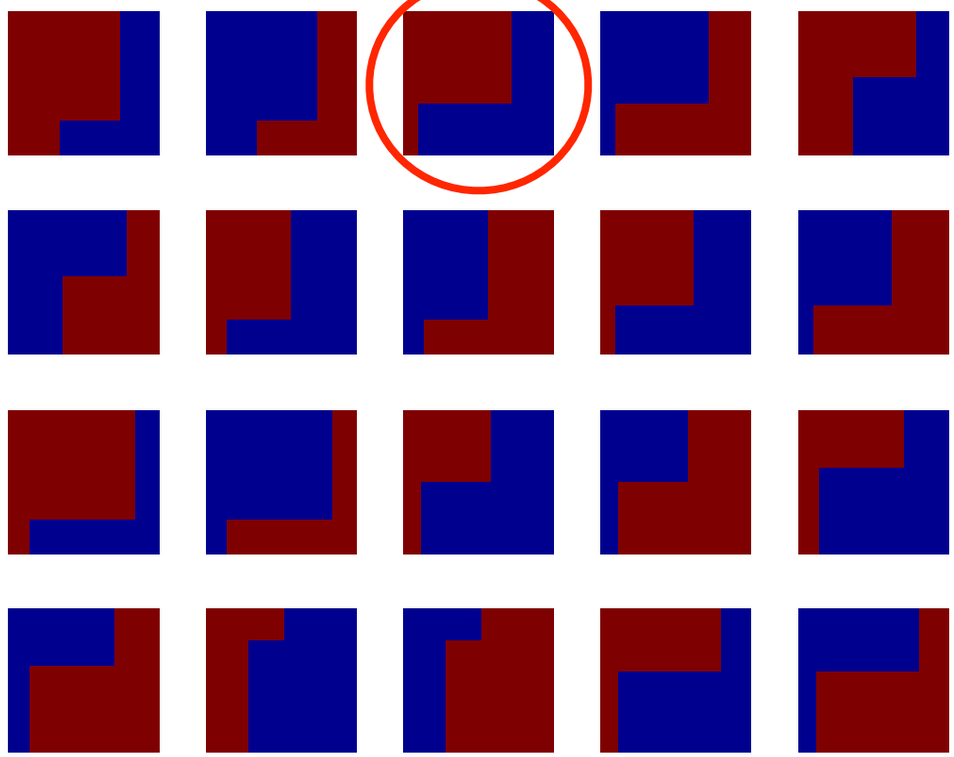
Random projection: [Ho, 1998]

RFs can be seen as probabilistic models

The leaf of each tree b can be seen as a posterior (multinomial distribution) $p_b(y|\mathbf{x})$

Ensemble probability: $p(y|\mathbf{x}) = \frac{1}{B}\sum_b p_b(y|\mathbf{x})$



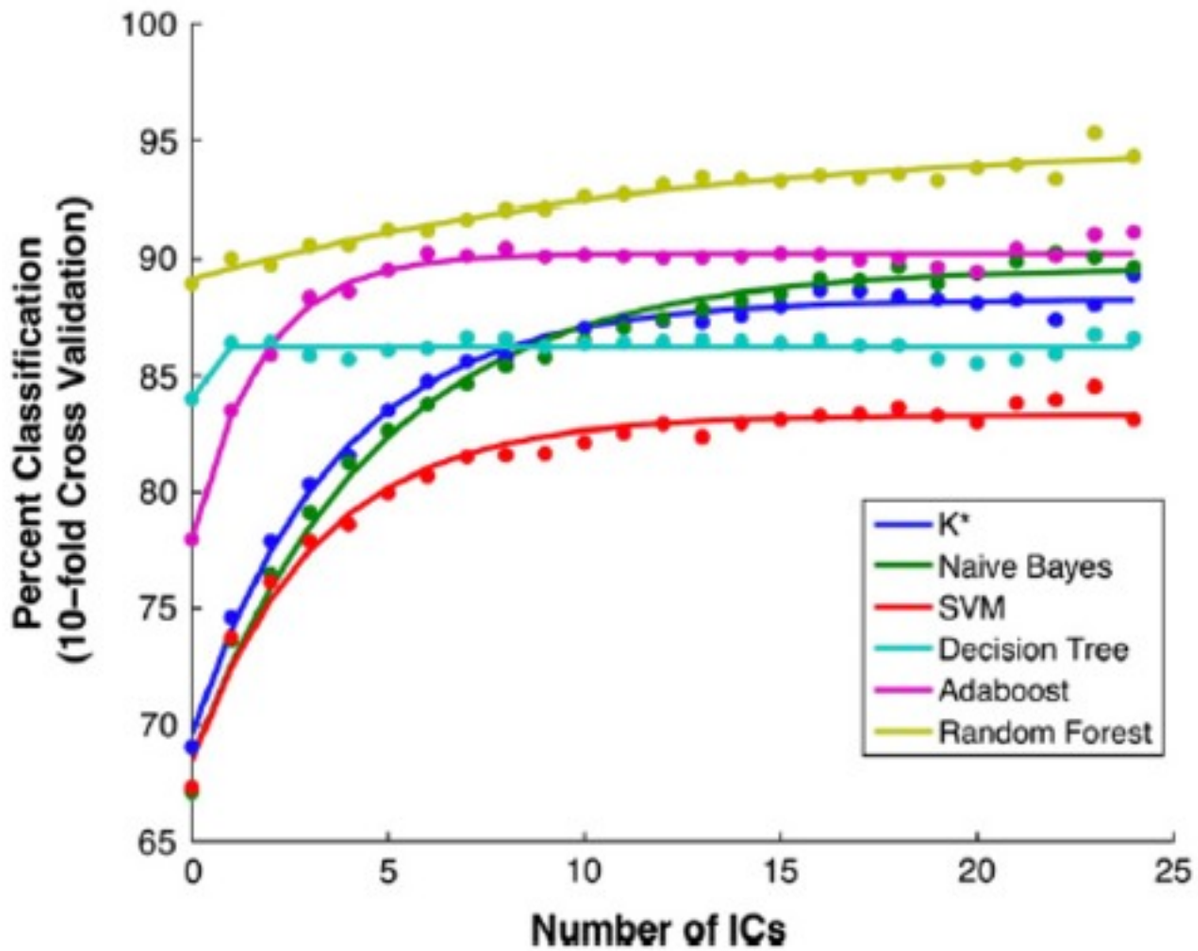


More trees = smoother posterior = less over-confidence

RF works for fMRI classification (1)

Data: event related fMRI, belief vs disbelief in statements, 14 subjects

Features: ICA timecourse value at button press



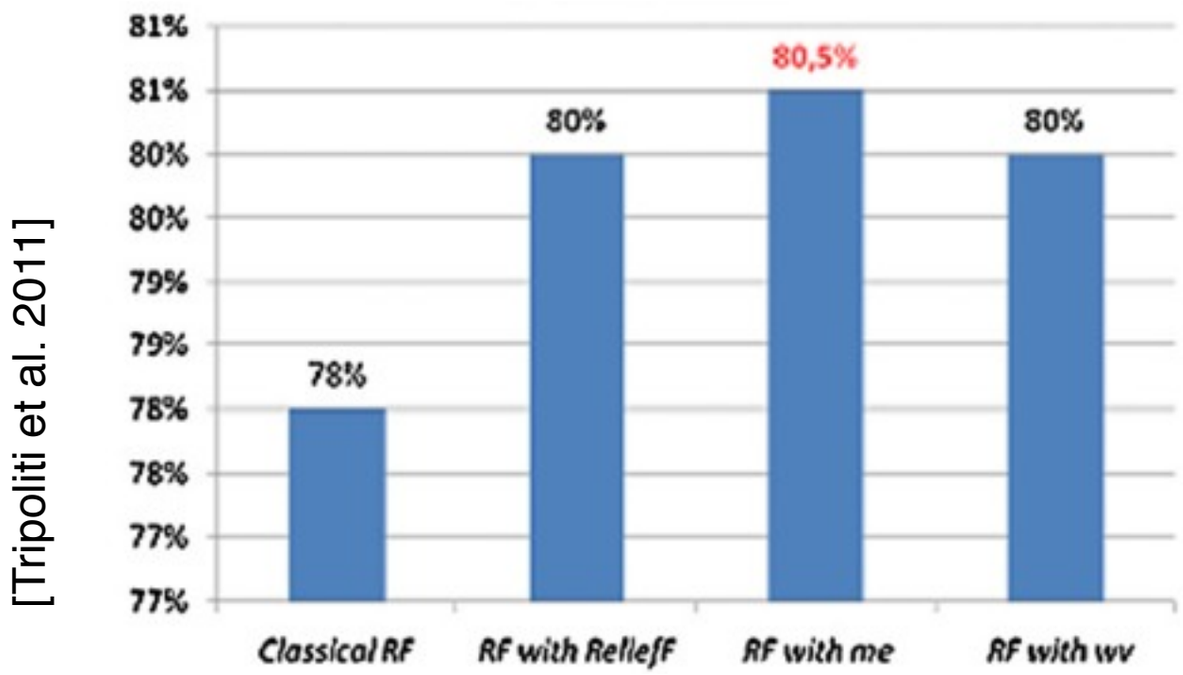
[Douglas et al. 2011]

RF works for multimodal classification

Data: 14 HC young, 13 AD old, 14 HC old. Visual stimulation + keypress. fMRI.

Features: fMRI GLM activation-related (n suprathreshold voxels, peak z-score,...), RT, demographics... + feature selection

Classifiers: RF + variants of split criterion. Group classification.



[Tripoliti et al. 2011]

activation features only

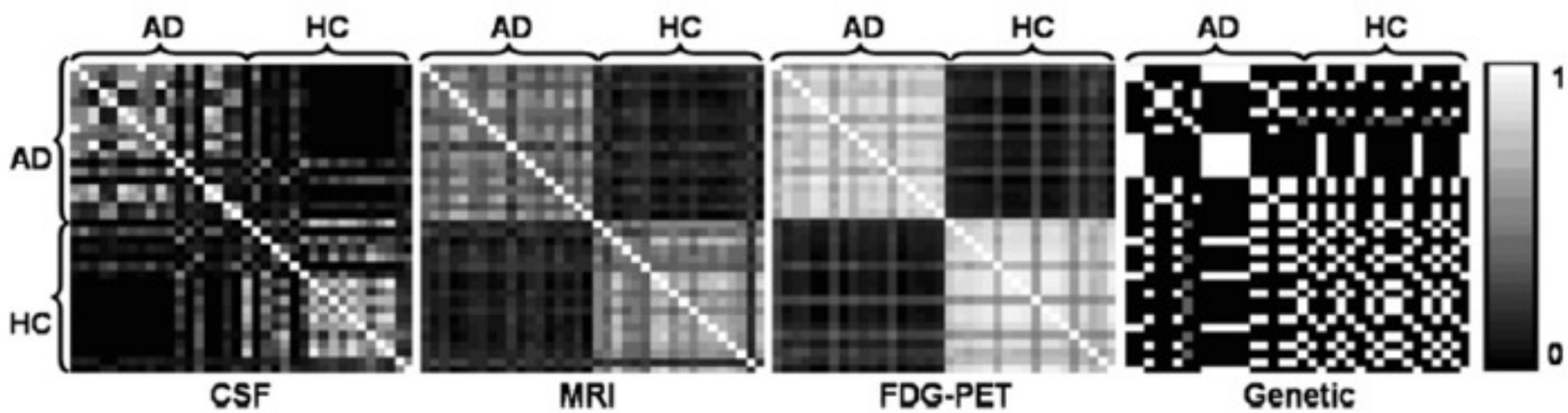
97-99% acc

+ other features

RF really works for multimodal classification

Data: ADNI, 37 AD, 75 MCI, 35 HC. MRI, FDG-PET, CSF measures, 1 SNP

Features: RF as kernel + MDS



		CSF	MRI	FDG-PET	Genetic	Combined embedding	Concatenated features
AD/HC	Acc. (%)	76.1 (0.8)	82.5 (0.7)	86.4 (0.7)	72.6 (0.9)	89.0 (0.7)	86.2 (0.7)
	Bacc. (%)	76.3 (1.3)	82.1 (1.4)	86.5 (1.2)	72.7 (1.3)	89.0 (1.2)	87.1 (1.1)
	Sens. (%)	72.8 (1.3)	88.6 (1.2)	85.8 (1.2)	71.3 (1.3)	87.9 (1.2)	85.1 (1.4)
	Spec. (%)	79.8 (1.4)	75.6 (1.5)	87.1 (1.3)	74.1 (1.4)	90.0 (1.1)	86.1 (1.3)
	k	13	22	9	2	18	–
MCI/HC	Acc. (%)	61.7 (0.8)	67.3 (1.0)	53.5 (0.7)	73.8 (0.5)	74.6 (0.8)	66.3 (0.8)
	Bacc. (%)	61.7 (1.3)	69.1 (1.4)	60.2 (1.2)	60.7 (0.9)	72.7 (0.8)	65.3 (1.1)
	Sens. (%)	61.6 (1.1)	64.3 (1.3)	42.3 (1.1)	94.7 (0.5)	77.5 (1.0)	68.5 (1.5)
	Spec. (%)	61.8 (1.5)	73.9 (1.4)	78.0 (1.3)	26.6 (1.2)	67.9 (1.7)	66.9 (1.3)
	k	25	47	35	2	20	–
pMCI/sMCI	Acc. (%)	52.1 (1.0)	58.4 (1.0)	53.0 (1.0)	43.5 (0.9)	58.0 (0.9)	53.0 (1.1)
	Bacc. (%)	52.7 (1.7)	58.3 (1.7)	52.8 (1.7)	41.2 (2.4)	57.9 (1.7)	57.3 (1.9)
	Sens. (%)	57.9 (1.6)	56.9 (1.6)	50.6 (1.8)	27.4 (2.0)	57.1 (1.8)	49.6 (1.4)
	Spec. (%)	47.5 (1.7)	59.7 (1.8)	54.9 (1.6)	55.0 (2.7)	58.7 (1.5)	53.5 (1.7)
	k	21	38	35	1	29	–

[Gray et al 2013]

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Extremely Randomised Trees increase diversity

Tree variance is due in large part to cutpoint choice. We can generate even more diversity with Extra-trees

Select both K voxels *and cutpoints* at random, pick best*.

Stop growing when leaves are small

When K=1, called *totally randomized trees*

+ Accuracy and variance reduction competitive with and sometimes better than RF, faster than RF

Extra-trees: [Geurts et al., 2006]

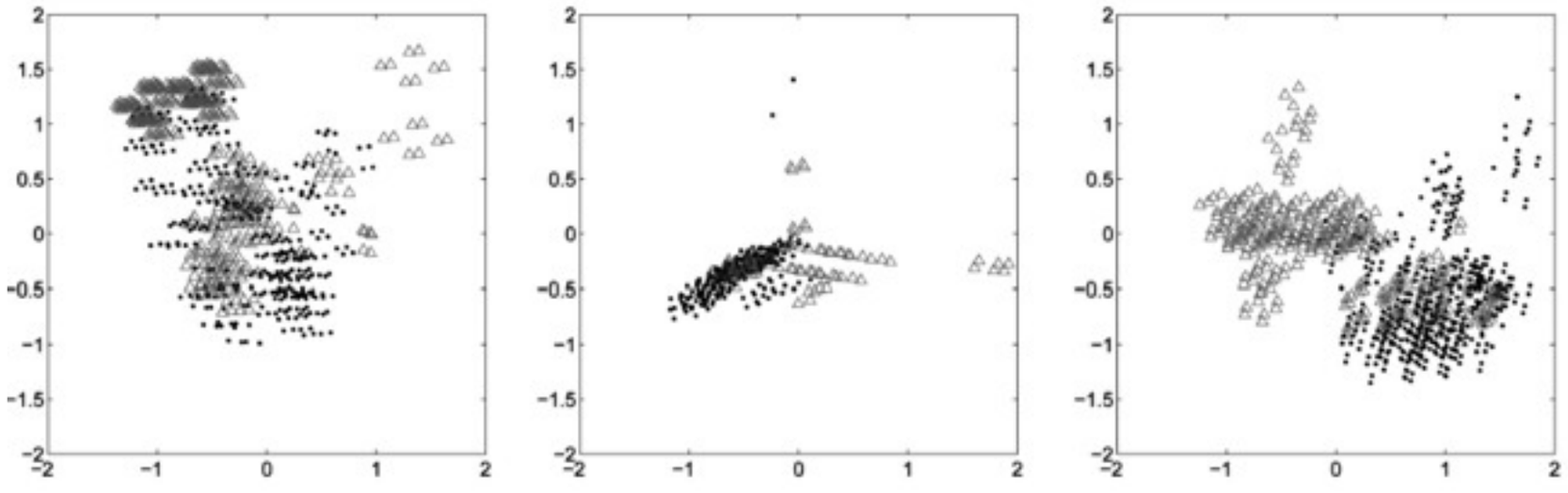
*Dietterich 1998 - the opposite: select top-K best splits, then pick at random


```
>extraTrees::extraTrees
>>PRoNTo::machine_RT_bin
>>>sklearn::ExtraTreesClassifier
```

Rotation forests do subspace PCA

We can also generate random rotations of the data to add diversity. For each tree:

1. Project training data **X** into M random non-overlapping subspaces, each of size K
2. For each subspace: choose a subset of classes, draw 75% bootstrap, do PCA



[Rodriguez et al. 2006]

3. Rearrange PCs into a block-diag matrix **R** and project whole training set to **XR**.
4. Train the tree


```
>Weka via rJava
>>Weka via writeARFF or Java
>>>?
```

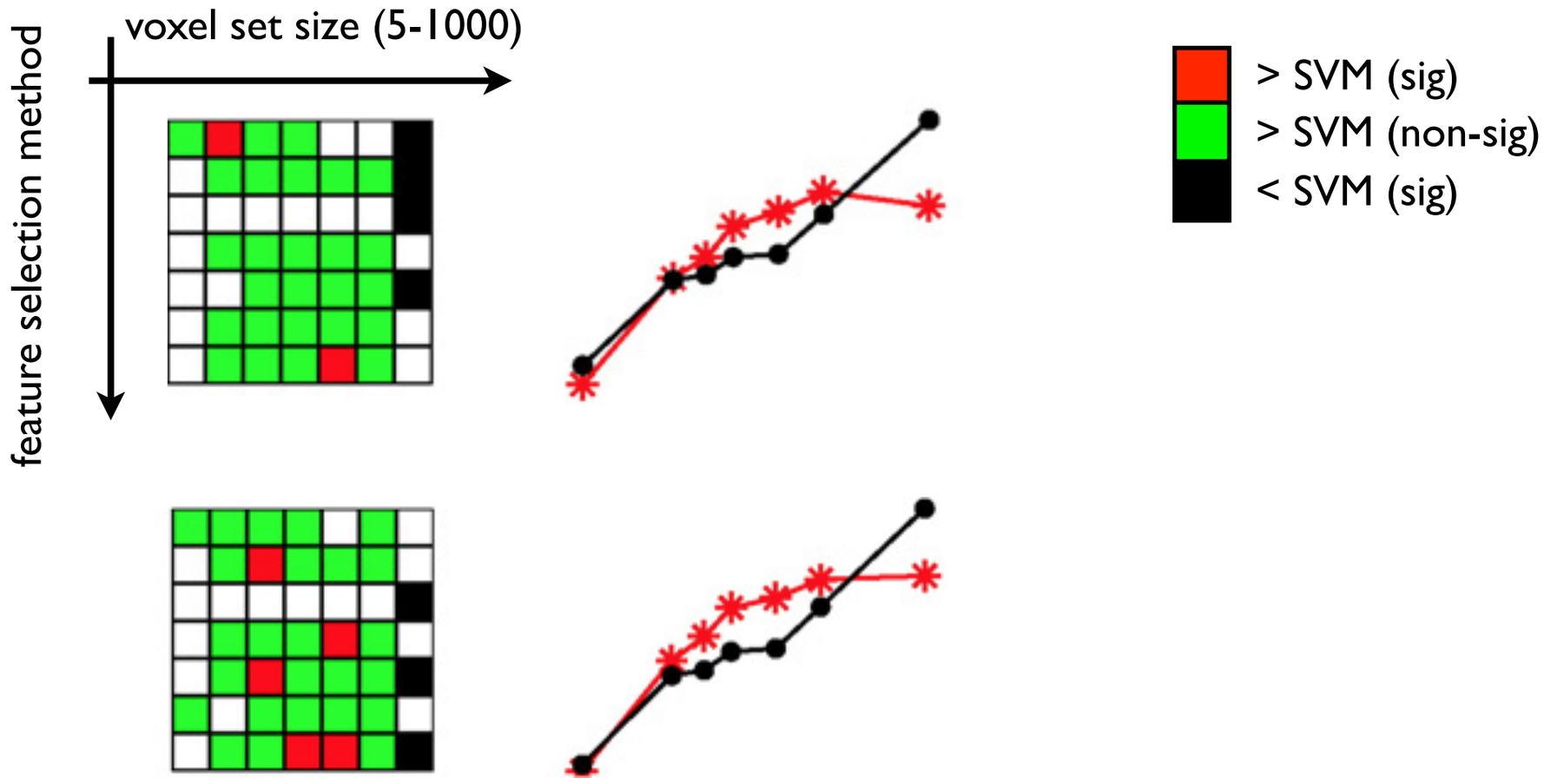
RotFor works for fMRI

Data: Haxby (8 classes, 90 points per class, 43K voxels)

Tests: feature selection, ensembles vs SVM

RF (1000)

RotFor



[Kuncheva&Rodriguez 2010]

Ensemble of FTs may improve accuracy

PCA-derived features are multivariate in the original space, so in fact RotFor does axis-parallel (univariate) cuts on MV data...

We can also try slightly more stable MV trees instead of univariate trees (trade diversity for accuracy)

On 62 UCI low-dimensional datasets, it seems that Bagging + FT-leaves works about the same as RotFor + univariate tree* . All other ensembles of univariate trees perform worse...

On high-dimensional fMRI connectivity data**, and low-dimensional graph/vertex attribute representations of fMRI connectivity***, bags of FTs work quite well

*[Rodriguez et al, 2010]

[Richiardi et al, 2011a] *[Richiardi et al, 2011b]

Trees ensembles vs SVMs

	SVM	Tree ensembles
Interpretability	+	+-
Irrelevant voxels	+-	+
Input scaling	-	+
Speed	+ (linear)	+ (parallel)
Generalisation error	++	++
Information Mapping	+-	++ (see later)

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More trees is generally better

For many tree ensembles, more trees (L) lead to more decrease in variance

- Typically use several hundreds to reach plateau (Langs: 40K)
- Large L "better approximates infinity" than small L
- For RF, the out-of-bag error estimate's bias decreases a lot with increasing trees - bootstrapping uses ~2/3 of data for each tree, more trees leads to better OOB estimate
- This also gives a much smoother posterior distribution

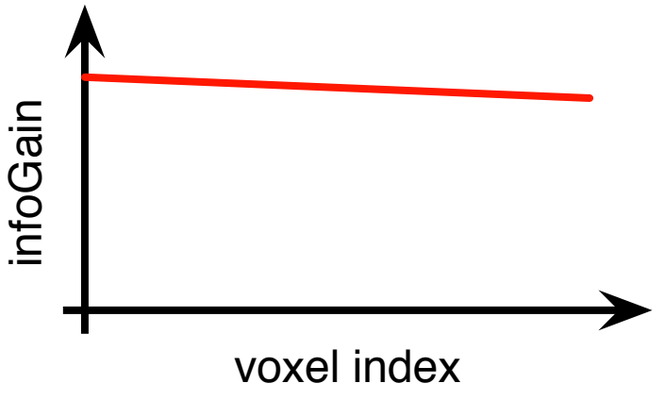
For multivariate trees, use fewer trees

- 10-30 works well empirically on very different datasets

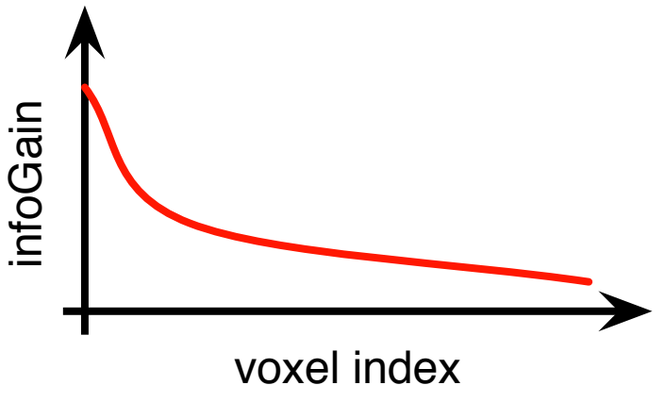
Projection dimension depends on distribution of informativeness

Low-dim results

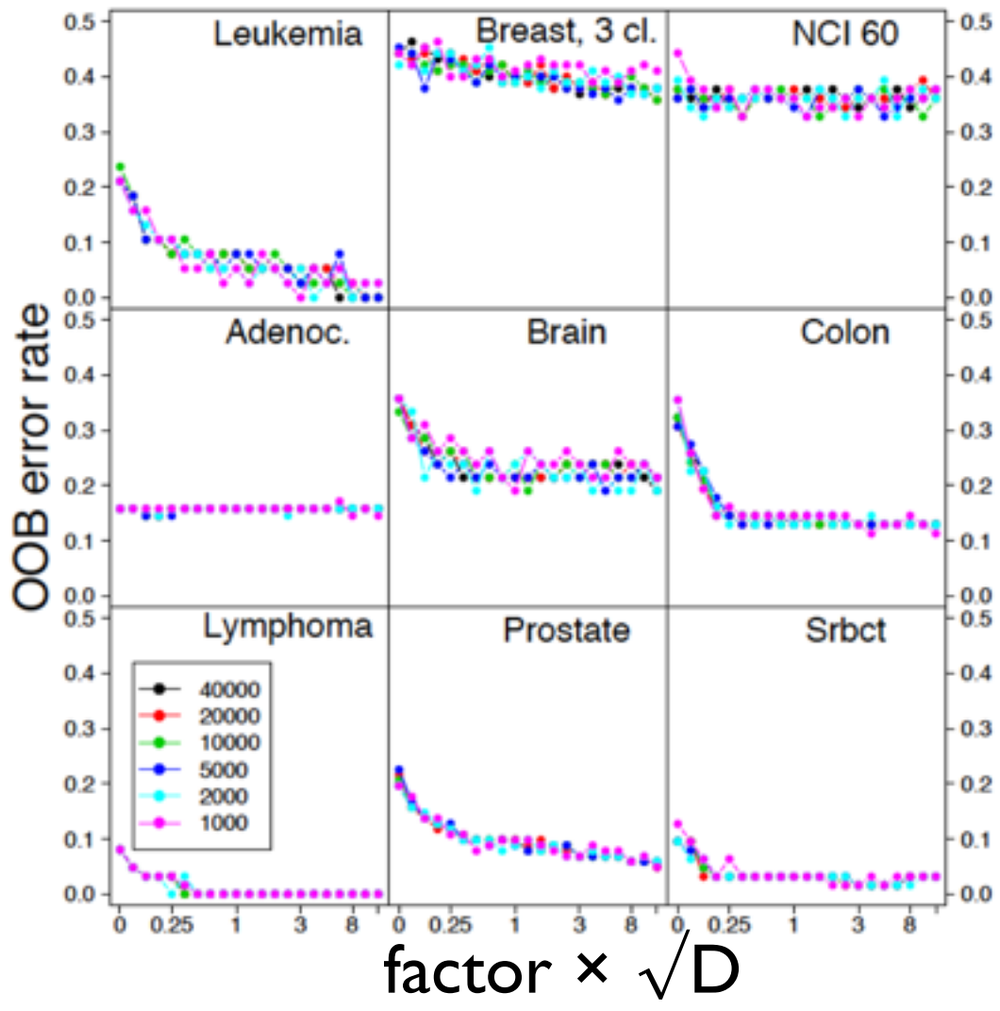
The optimal projection dimension, K, depends on the presence of irrelevant voxels



many useful voxels
- use small K



information concentrated in few voxels - use large K



D=2-10K, N=40-100, C=2-8

see e.g. [Geurts et al. 2006] for details

[Diaz-Uriarte et al., 2006]

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Tree ensembles directly provide information maps

The split criterion and related measures are natural indicators of the 'usefulness' of voxels in the discrimination task

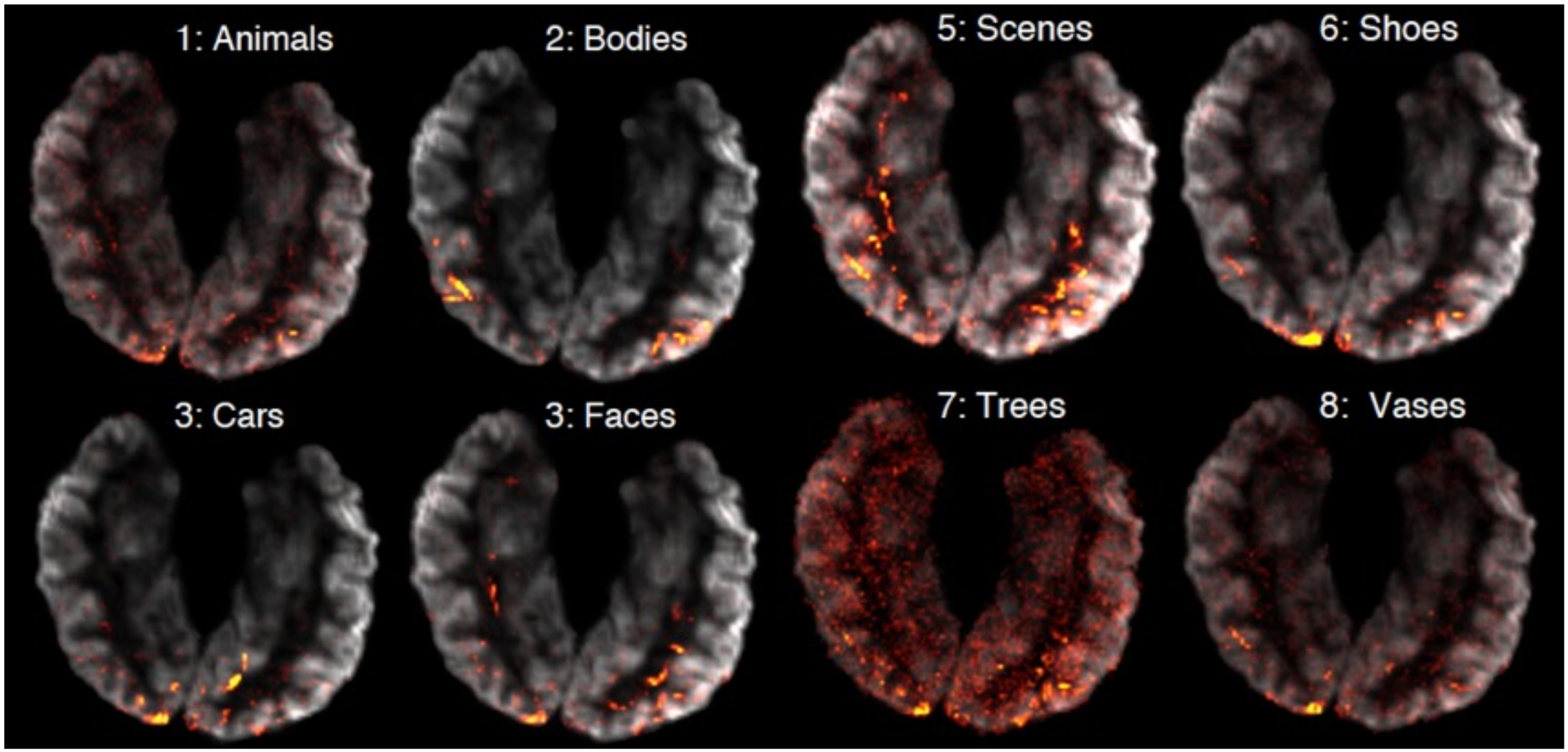
But they are unsigned

They are computed at each node of the tree, so we can aggregate them over trees to get stable estimates

Different ensembles provide different information maps, and we can use other data than split criteria to map

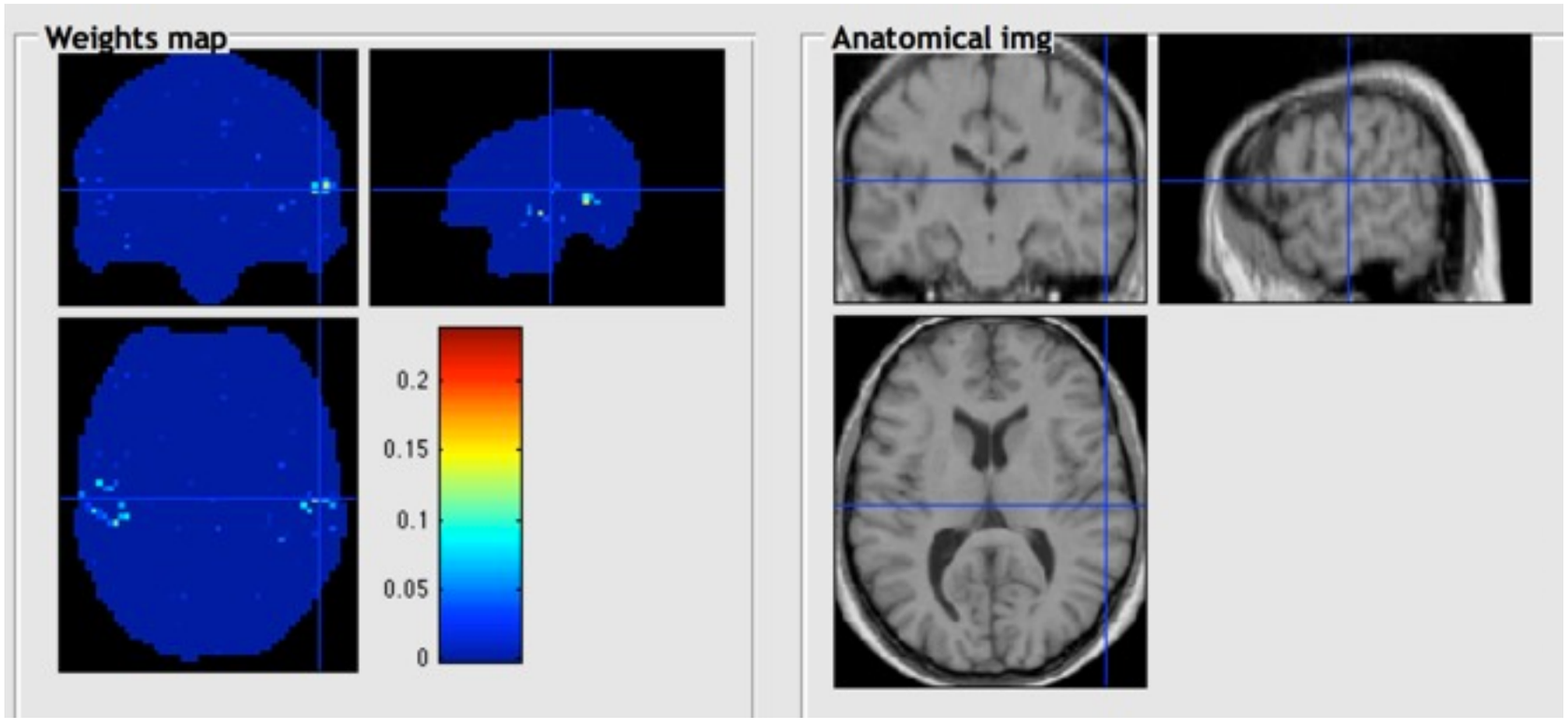
Information mapping: RF/Gini importance

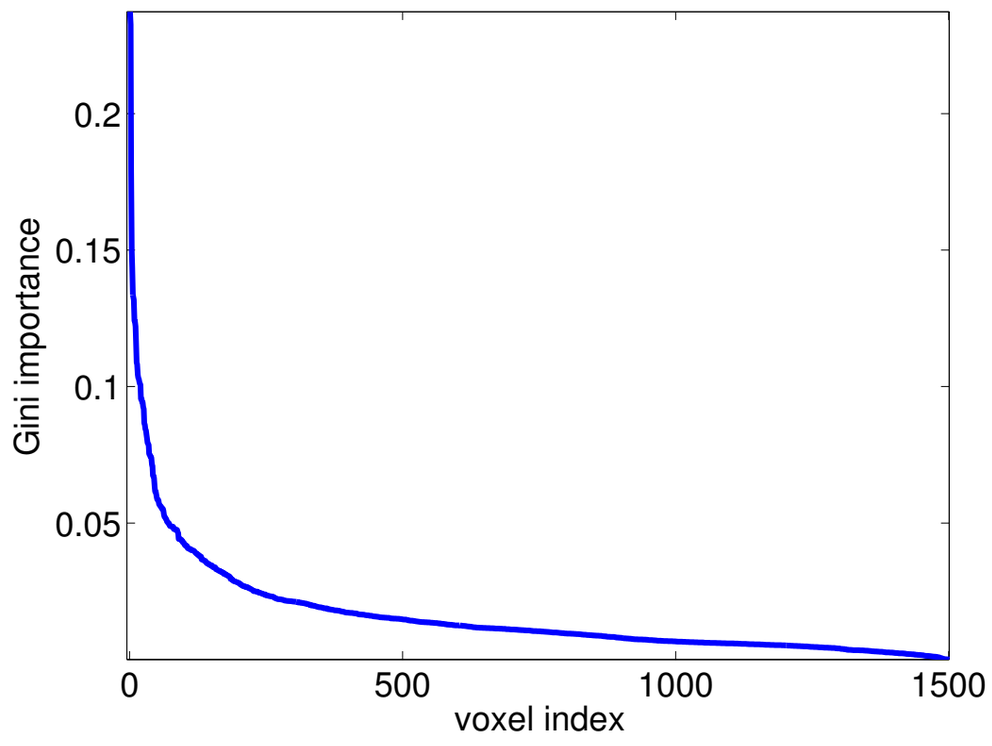
GI of a voxel: infoGain (compute with Gini impurity) for this voxel, averaged over all trees in ensemble



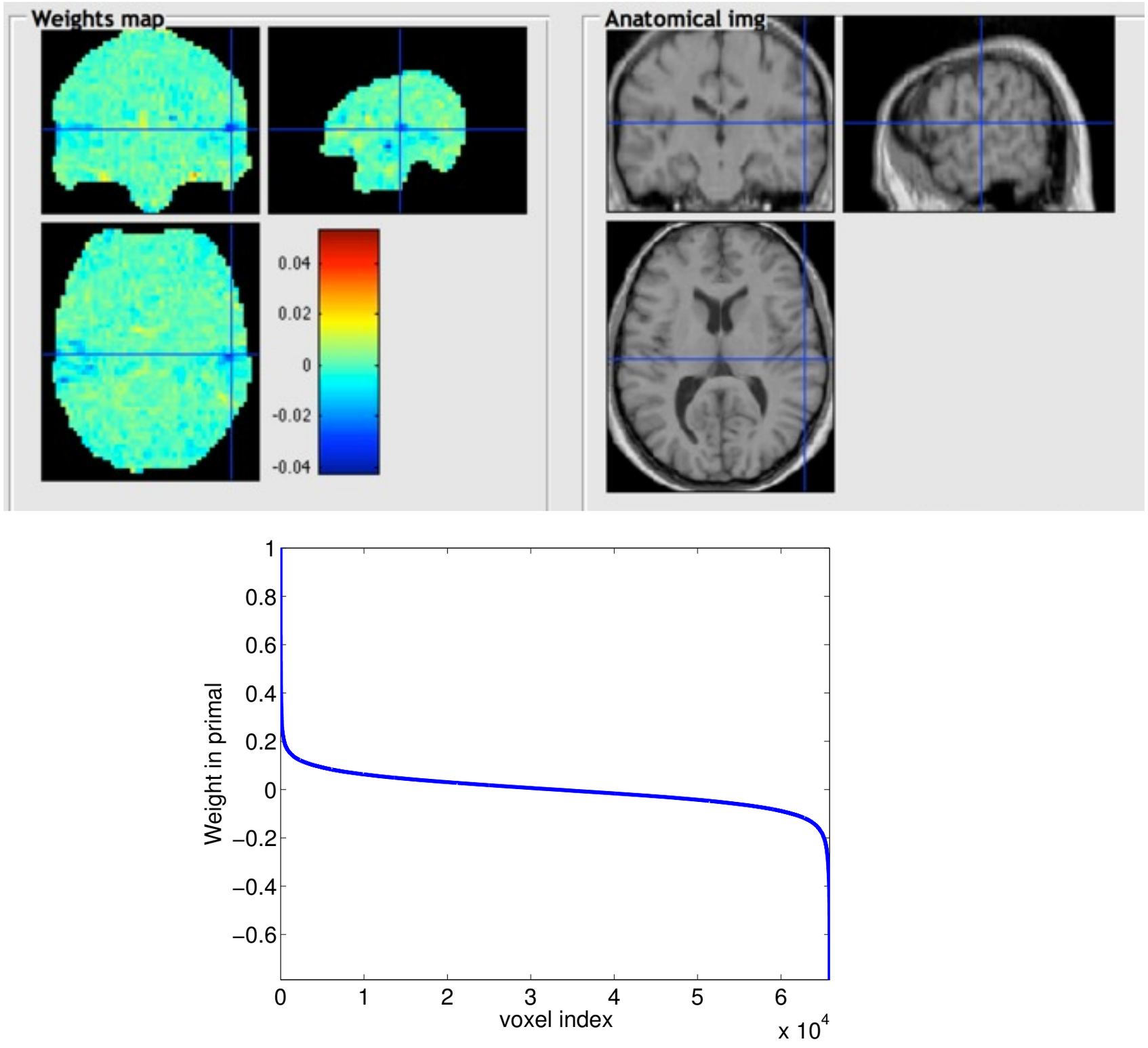
[Langs et al., 2011]

Information mapping: RF/GI/var



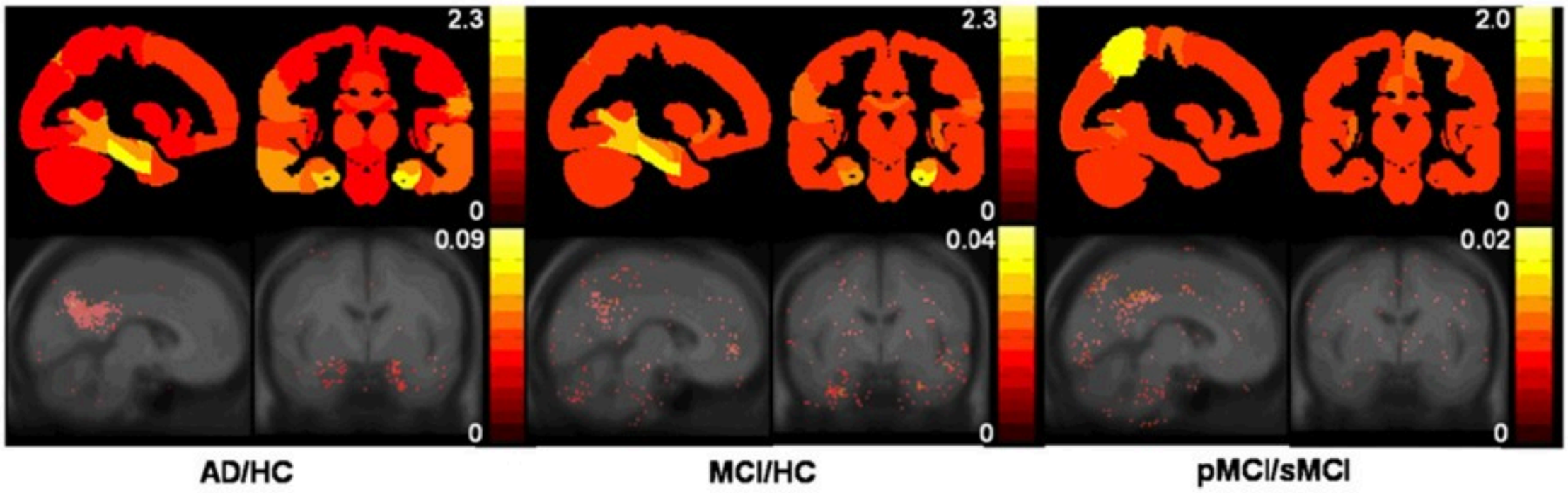


Information Mapping: L_2 SVM



Information mapping - Regional GI

Data: ADNI, 37 AD, 75 MCI, 35 HC. MRI, FDG-PET, CSF measures, 1 SNP



[Gray et al 2013]

Information mapping: RF/Variable importance

VI of a voxel*: average loss of accuracy on OOB samples when randomly permuting values of the voxel

This is suboptimal with correlated voxels

Permuting one single variable ignores correlations

With several relevant & correlated voxels, they could be deweighted because removing one does not deteriorate accuracy

VI is well-correlated with GI**

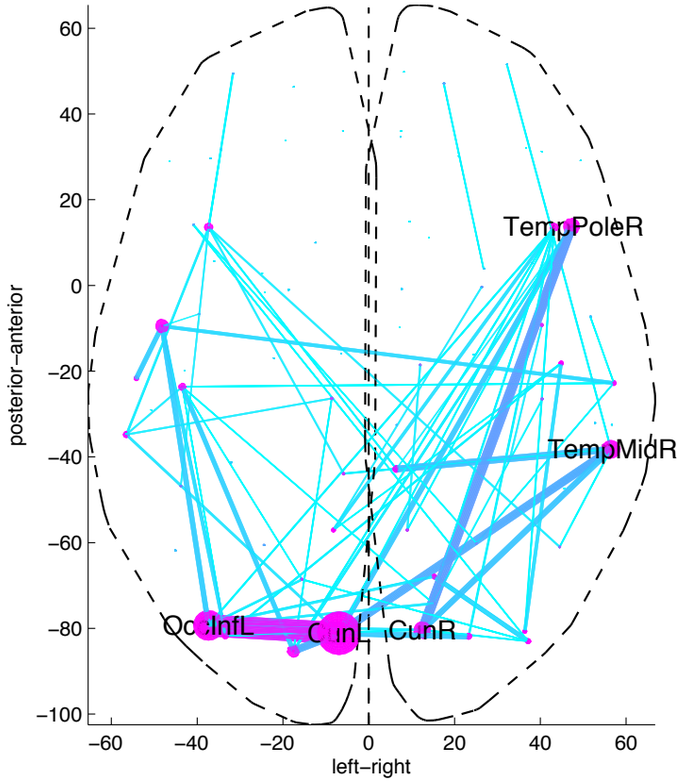
More on this later

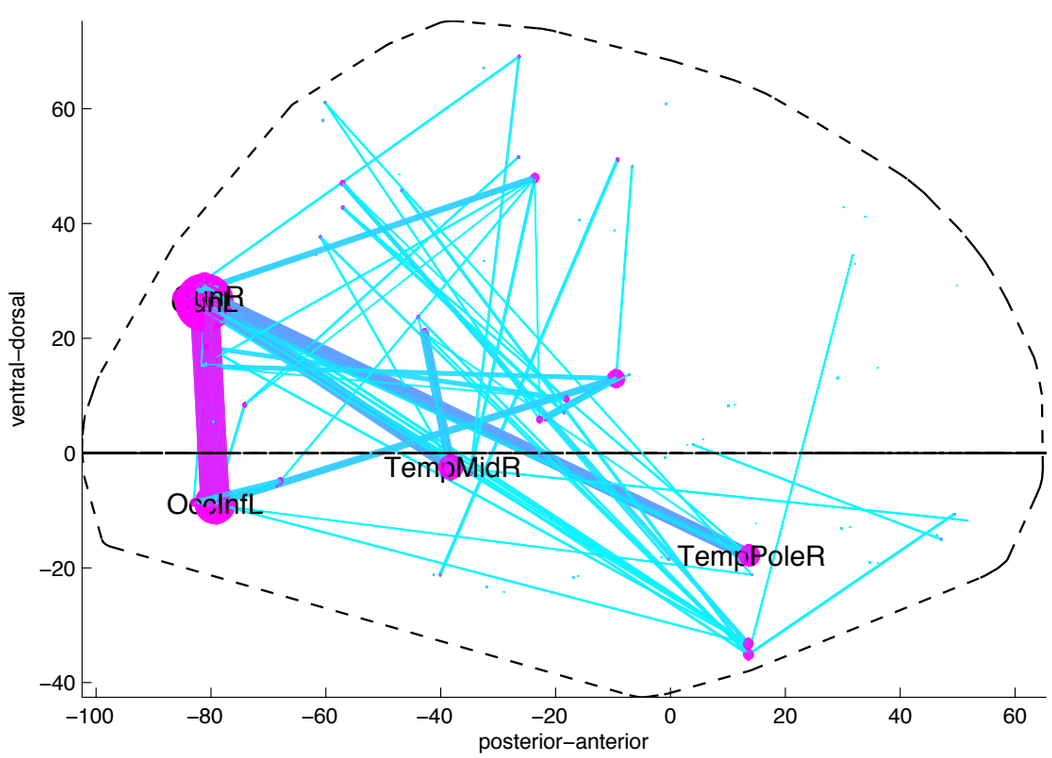
*[Breiman, 2001] **[Strobl et al., 2007]

Information mapping: bag of FTs

Leaves in an FT can be regression models

- These can be trained using any method, in practice LogitBoost (iterative reweighting) works well
- The importance of a voxel is its average regression weights across trees and folds



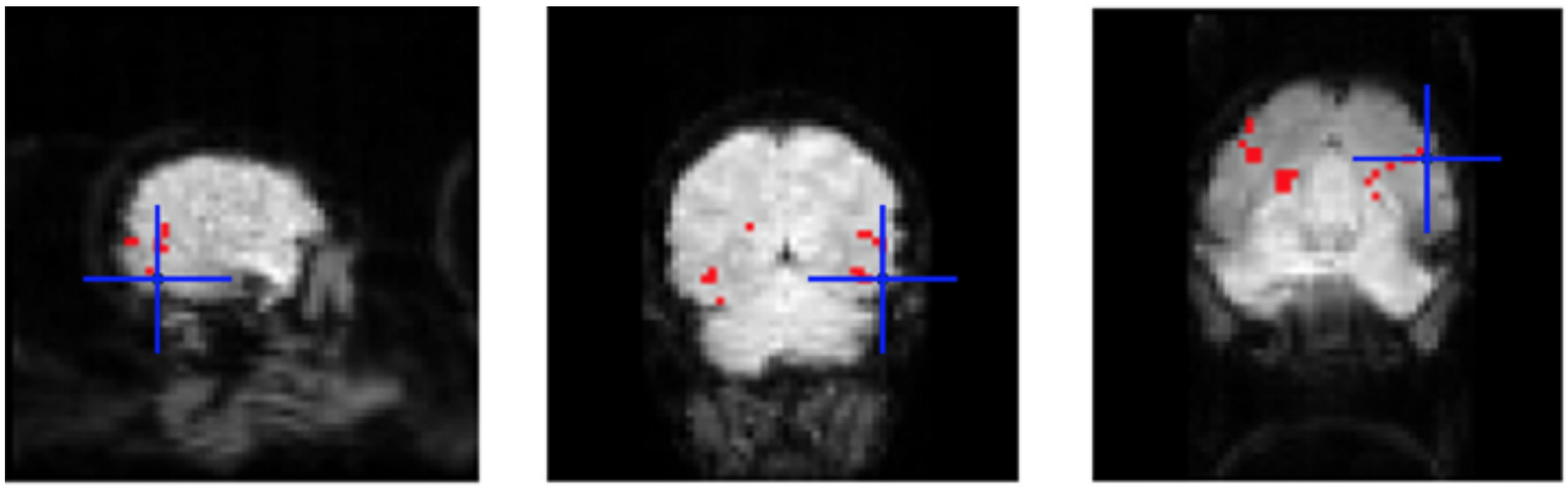


[Richiardi et al. 2011a]

Information mapping from accuracy

Finally we could also map results directly from classifier with best accuracy

Here: Haxby data, *SVM-RFE 200*, RF1000, intersection of *selected features* across 10 folds, one slice



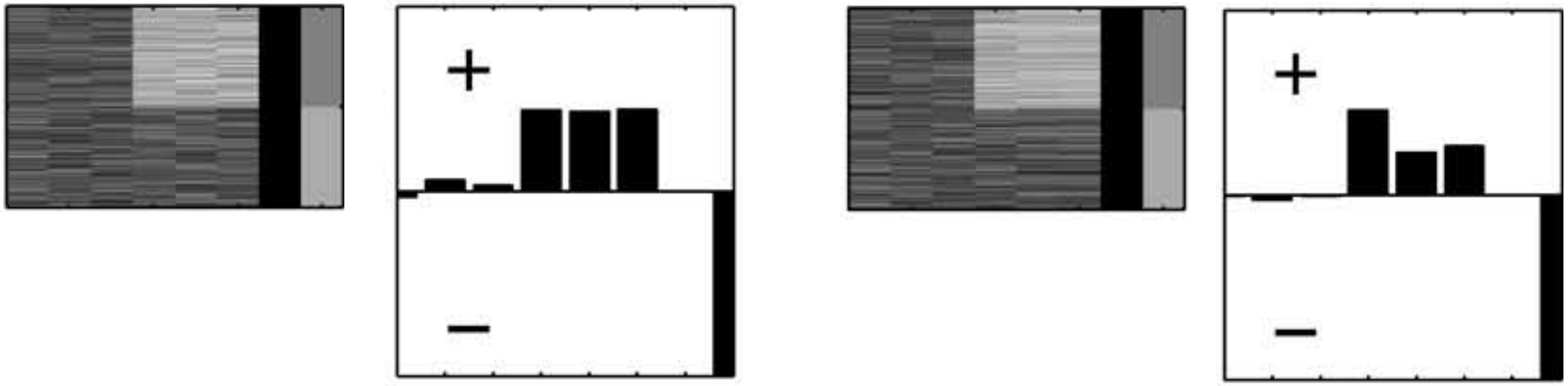
[Kuncheva et al. 2010]

Tutorial agenda

Lecture	**Practical**
Basics	Datasets
Growing trees	Matlab/ PRoNTo
Ensembling	
The random forest	Python/Scikit
Other forests	
Tuning your forests	
Information mapping	
Correlated features	

Correlated features are picked up by tree ensembles

With regularisers in SVMs, correlated features will be deweighted (L_2) or left out (L_1)



[Pereira & Botvinick, 2011]

Tree ensembles have grouping effect*, where correlated but informative features can survive with high weight

Empirically this seems to depend on tree depth...

*[Langs et al., 2011]

There are ways of dealing with correlated features

Several proposals from bioinformatics have attempted to tackle the GI/VI measure bias

Conditional Variable Importance only permutes a correlated variable within observations where its correlands have a certain value (accounts for correlation structure)

Permutation IMPortance fixes for under-importance of grouped vars by permuting class labels, then constructing a null distribution of GI values

These methods can be used in neuroimaging directly...

Cond. Var. Imp. [Strobl et al, 2008]
PIMP [Altmann et al., 2010]

`>party::cforest`

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Datasets

1. SINGLE SUBJECT: SPM Auditory - "Mother of All Experiments" - 1 subject, 2T scanner, TR=7s, 6 blocks of 42 s rest, 42s auditory stimulation.
Task: two-class intra-subject decoding: auditory vs rest.

2. GROUP COMPARISON: Buckner checkerboard - 41 subjects from three groups, young (18-24), elderly healthy (66-89) and elderly demented (age 68-83). Four runs per subject, 128 volumes per run with TR=2.68s.
Task: classify young (n=28) versus old (n=30) group based on 'first level' beta maps

Original auditory data at www.fil.ion.ucl.ac.uk/spm/data/auditory/

[Buckner et al., 2001]
Original visual data at fmridc.org

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Datasets

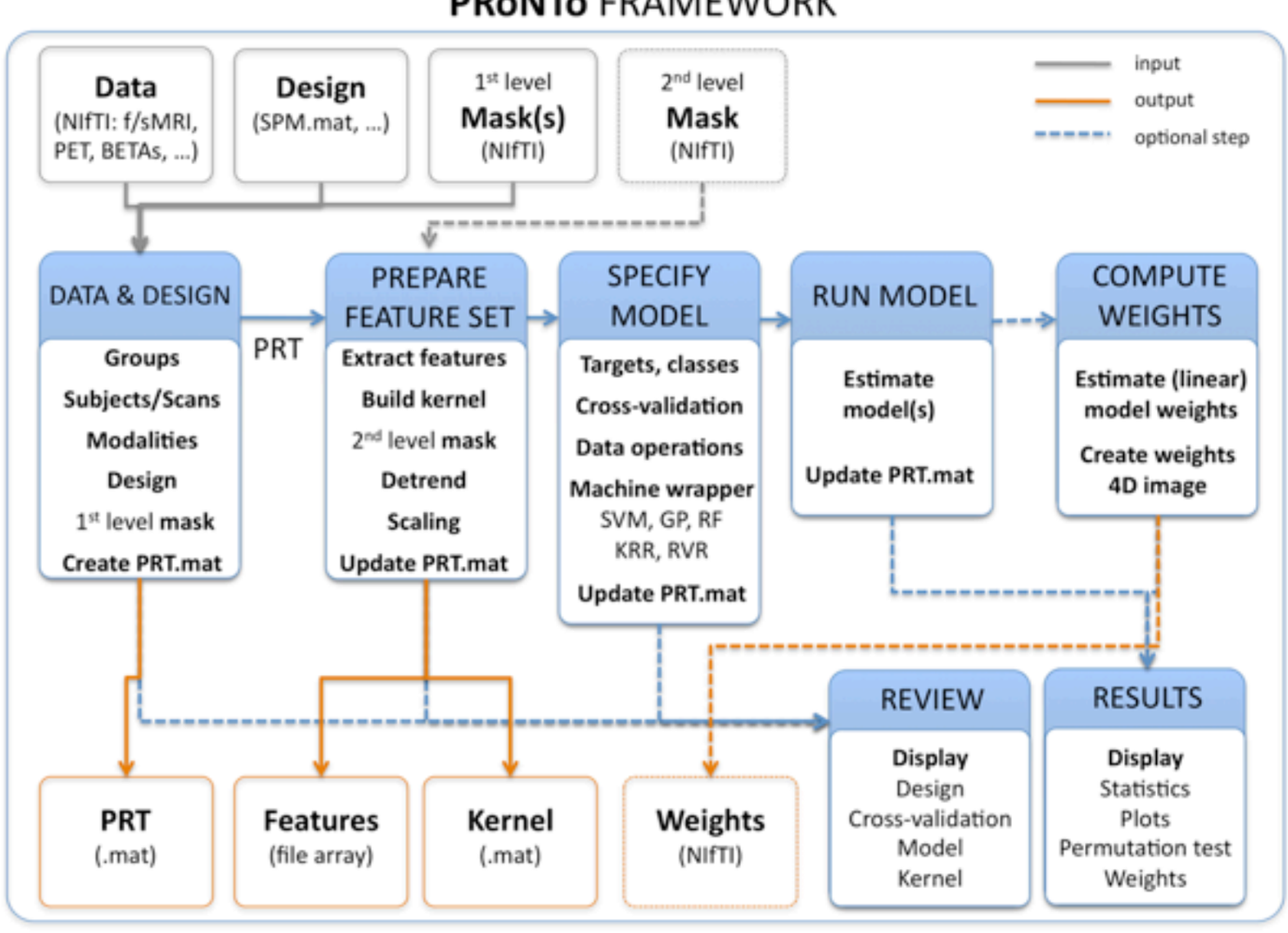
Matlab/ PRoNTo

Python/Scikit

The PRoNTo toolbox

Matlab code, open source, GUI / batch / scripting

Users can quickly test machine learning methods without coding



http://www.mlnl.cs.ucl.ac.uk/pronto/

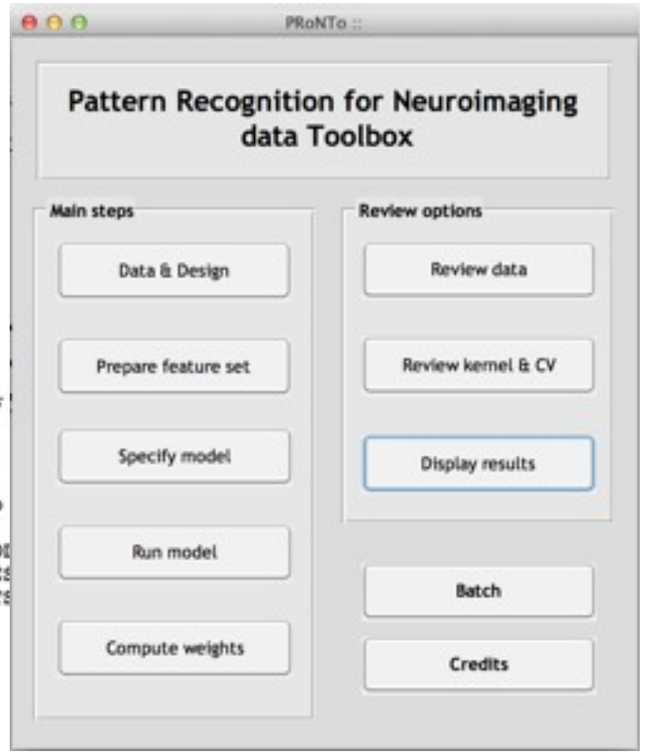
Start PRoNTo

1. Make sure your path is setup properly

```
>> which spm
>> which pronto
```

2. Start PRoNTo

```
>> pronto
```




```
PRoNTo v1.1b - http://www.mlnl.cs.ucl.ac.uk/pronto

THIS IS AN UNSUPPORTED BETA BRANCH FOR NON-KERNEL CO
INTENDED FOR THE PRNI 2013 TUTORIAL ON TREE ENSEMBLES
IT DOES NOT CONTAIN THE LATEST FIXES AND IMPROVEMENTS
AND IS NOT RECOMMENDED FOR GENERAL USE.

SVM path: OK
GP path: OK
RF path: OK
PRoNTo present working directory:
```

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Matlab/
PRoNTo

**Python/
Scikit**

Scikit-learn / niPy

A very good alternative for python fans is to use Scikit-learn + niPy. It has RF, Extra-trees, and others

For people that missed Gaël's tutorial at PRNI 2011: http://nisl.github.io/

PyMVPA also has access to Extra-trees and RF

Conclusions

Tree ensembles can offer competitive decoding performance with SVMs, and are good for multimodal classification

They produce information maps which are typically sparser than L_2 SVMs (is this good or bad?), and can have different interpretation

Implementations abound in the language of your choice, including R, Matlab, Python

So... take a walk in the forest for your next project

Thanks

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Montefiore Institute, U. of Liège
P. Geurts
FIL, UCL
G. Rees
PRoNTo team members @ UCL, KCL, U. Liège, NIH
J. Ashburner, C. Chu, A. Marquand, J. Mourao-Miranda, C. Phillips, J. Rondina, M. J. Rosa, J. Schrouff + João de Matos Monteiro
Computer Vision Group, U. Freiburg
A. Abdulkadir

MARIE CURIE ACTIONS

Modelling and Inference on Brain networks for Diagnosis, MC IOF #299500

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