An introduction to machine learning for fMRI

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what is machine learning?

- how to build computer systems that automatically improve with experience
what is machine learning?

- how to build computer systems that automatically improve with experience

- building models of data for
  - predicting numeric variables (regression)
  - predicting categoric variables (classification)
  - grouping data points (clustering)
  - ...

what is machine learning?

- how to build computer systems that automatically improve with experience

- building models of data for
  - predicting numeric variables (regression)
  - predicting categoric variables (classification)
  - grouping data points (clustering)
  - ...

- overlaps with applied statistics
why use it at all?

to tell a story about data

[adapted from slides by Russ Poldrack]
once upon a time there was a sample...

[adapted from slides by Russ Poldrack]
... and then came a beautiful model...

fit model by estimating parameters

RT = 503.7 - age\* -0.530

[adapted from slides by Russ Poldrack]
very suggestive, but...

\[ RT = 503.7 + \text{age}^* - 0.530 \]

Is RT really related to age?

[adapted from slides by Russ Poldrack]
is RT related to age?

Model:
\[ RT = b_0 + b_1 \times \text{age} + e \]

parameters in the population

[adapted from slides by Russ Poldrack]
is RT related to age?

Model:
\[ RT = b_0 + b_1 \cdot \text{age} + \epsilon \]

parameters in the population

parameters estimated from the sample

\[ b_{est} = (X'X)^{-1}X'y \]

[adapted from slides by Russ Poldrack]
is RT related to age?

Model:

\[ RT = b_0 + b_1 \times \text{age} + e \]

Hypothesis:
Is \( b_1 \) different from 0?

[adapted from slides by Russ Poldrack]
is RT related to age?

Null hypothesis: $b_1 = 0$
Alternative: $b_1 \sim= 0$

[adapted from slides by Russ Poldrack]
is RT related to age?

Null hypothesis: $b_1 = 0$
Alternative: $b_1 \sim= 0$

How likely is the parameter estimate ($\hat{b}_1 = -0.53$) if the null hypothesis is true?
is RT related to age?

Null hypothesis:  \(b_1 = 0\)
Alternative:  \(b_1 \sim= 0\)

How likely is the parameter estimate (\(b_1 = -0.53\)) if the null hypothesis is true?

We need a statistic with a known distribution to determine this!

[adapted from slides by Russ Poldrack]
is RT related to age?

the CLT tells us

\[ \hat{\beta}_1 \sim N(\beta_1, Var(\hat{\beta}_1)) \]

but we don’t know

\[ Var(\hat{\beta}_1) \]

[adapted from slides by Russ Poldrack]
is RT related to age?

the CLT tells us

\[ \hat{\beta}_1 \sim N(\beta_1, Var(\hat{\beta}_1)) \]

but we don’t know \( Var(\hat{\beta}_1) \)

we do know

\[ t = \frac{\hat{\beta}_1}{\sqrt{Var(\hat{\beta}_1)}} \sim T_{N-p} \]

[adapted from slides by Russ Poldrack]
is RT related to age?

$t(10) = -4.76$

How likely is this value in this $t$ distribution?

$p < .001$

[adapted from slides by Russ Poldrack]
what can we conclude?

- in this sample
  - p < 0.001 - there is a relationship between age and RT
  - R² - age accounts for 69% of variance in RT

- very unlikely if no relationship in the population

- the test does not tell us how well we can predict RT from age in the population

[adapted from slides by Russ Poldrack]
what happens with a new sample?

draw a new sample from the same population

compute the R2 using parameters estimated in the original sample

R² (original sample) = 0.694
R² (new sample) = 0.495

[adapted from slides by Russ Poldrack]
what happens with a new sample?

repeat this 100 times…

using model parameters estimated from the original sample

average $R^2 = 0.578$

a measure of how good the model learned from a single sample is

[adapted from slides by Russ Poldrack]
the learning perspective

When we estimate parameters from a sample, we are **learning** about the population from **training** data.

[adapted from slides by Russ Poldrack]
the learning perspective

When we estimate parameters from a sample, we are **learning** about the population from **training** data.

How well can we measure the prediction ability of our learned model? Use a new sample as **test** data.

[adapted from slides by Russ Poldrack]
test data and cross-validation

If you can’t collect more split your sample in two...

[adapted from slides by Russ Poldrack]
test data and cross-validation

If you can’t collect more split your sample in two...

k-fold cross-validation:
- split into k folds
- train on k-1, test on the left out
- average prediction measure on all k folds
- several variants: all possible splits, leave-one-out

[adapted from slides by Russ Poldrack]
leave-one-out cross-validation

regression lines on each training set

original sample
$R^2 = 0.694$

leave-one-out on original
$R^2 = 0.586$

mean over 100 new samples
$R^2 = 0.591$

[adapted from slides by Russ Poldrack]
As model complexity goes up, we can always fit the training data better.

What does this do to our predictive ability?

[adapted from slides by Russ Poldrack]
polynomials of higher degree fit the training data better...
model complexity

polynomials of higher degree fit the training data better...

... but they do worse on test data: overfitting

[adapted from slides by Russ Poldrack]
model complexity

if the relationship in the population were more complicated

[adapted from slides by Russ Poldrack]
model complexity

if the relationship in the population were more complicated we could use CV to determine adequate model complexity

(this would need to be done with nested CV, CV inside the training set)
what is machine learning, redux

- **generalization**: make predictions about a new individual

- A model that generalizes captures the relationship between the individual and what we want to predict

- Cross-validation is a good way of
  - measuring generalization
  - doing model selection (there are others)
what is machine learning, redux

- generalization: make predictions about a new individual

- a model that generalizes captures the relationship between the individual and what we want to predict

- cross-validation is a good way of
  - measuring generalization
  - doing model selection (there are others)

- “all models are wrong but some are useful”
  George Box
what does this have to do with fMRI?

In this talk:

- prediction is classification
- generalization is within subject (population of trials)
- how to draw conclusions with statistical significance
- what has it been used for?
two questions

**GLM:** are there voxels that reflect the stimulus?

stimulus $\rightarrow$ fMRI activation (single voxel)

contrast of interest $\rightarrow$ GLM
two questions

**GLM:** are there voxels that reflect the stimulus?

- Stimulus $\rightarrow$ fMRI activation (single voxel) $\rightarrow$ GLM $\rightarrow$ contrast of interest

**Classifier:** do voxels contain information to predict?

- Stimulus $\rightarrow$ fMRI activation (multiple voxels) $\rightarrow$ what is the subject seeing?
case study: two categories

- subjects read concrete nouns in 2 categories
  - words name either tools or building types
  - trial:
    - see a word
    - think about properties, use, visualize
    - blank

3 seconds
8 seconds

[data from Rob Mason and Marcel Just, CCBI, CMU]
case study: two categories

- subjects read concrete nouns in 2 categories
  - words name either tools or building types
  - trial:
    - see a word
    - think about properties, use, visualize
    - blank

- goal: can the two categories be distinguished?
- average images around trial peak to get one labelled image

[data from Rob Mason and Marcel Just, CCBI, CMU]
the name(s) of the game

average trial image

example

voxels (features)  class label

tools
the name(s) of the game

average trial image

14 examples

tools
labels = example group

example

voxels (features)

class label

/tools/
the name(s) of the game

average trial image

example

voxels (features)

class label

tools

14 examples

example group

dataset

84 examples

average trial image

tools

tools

labels = 

labels

group 1

group 6

84 examples
classifying two categories

<table>
<thead>
<tr>
<th>training data (42)</th>
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classifying two categories

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| group 6        | ...    | classifier
classifying two categories

training data (42)  labels

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predicted labels  true labels

=  vs
classifying two categories

training data (42)  

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labels

| true labels |

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+ classifier

predicted labels  

true labels  

accuracy estimate  

= #correct/42  

= 0.65
a classifier

- is a function from data to labels
- parameters learned from training data
a classifier

- is a function from data to labels
- parameters learned from training data

- want to estimate its true accuracy
  - “probability of labelling a new example correctly”
- estimation is done on the test data
  - it is finite, hence an estimate with uncertainty
a classifier

- is a function from data to labels
- parameters learned from training data

- want to estimate its true accuracy
  - “probability of labelling a new example correctly”
- estimation is done on the test data
  - it is finite, hence an estimate with uncertainty

- null hypothesis: “the classifier learned nothing”
what questions can be tackled?

- is there information? (pattern discrimination)
- where/when is information present? (pattern localization)
- how is information encoded? (pattern characterization)
“is there information?”

- what is inside the black box?
- how to test results?
- from a study to examples
what is inside the box?

- simplest function is no function at all
- “nearest neighbour”
what is inside the box?

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- simplest function is no function at all
- “nearest neighbour”

requires example similarity measure

- euclidean, correlation, …
what is inside the box?

- next simplest: learn linear discriminant
what is inside the box?

- next simplest: learn linear discriminant
- note that there are many solutions...
what is inside the box?

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what is inside the box?

- next simplest: learn linear discriminant
- note that there are many solutions...
linear classifiers

If weight0 + weight1 x voxel 1 + weight2 x voxel 2 + ... + weight n x voxel n > 0 then tools

otherwise buildings
linear classifiers

Various kinds

Gaussian Naive Bayes
Logistic Regression
Linear SVM

differ on how weights are chosen

If \[ \text{weight}_0 + \text{weight}_1 \times \text{voxel}_1 + \text{weight}_2 \times \text{voxel}_2 + \ldots + \text{weight}_n \times \text{voxel}_n \] > 0 tools

otherwise buildings
linear classifiers

If \( \sum_{i=1}^{n} \text{voxel } i \cdot \text{weight}_i > 0 \) tools

otherwise buildings

linear SVM weights:
linear classifiers

If $\sum weight_i \cdot x_i > 0$ tools

otherwise buildings

linear SVM weights:

weights pull towards tools

weights pull towards buildings
nonlinear classifiers

- linear on a transformed feature space
nonlinear classifiers

- linear on a transformed feature space
- neural networks: new features are learnt

Diagram:
- Tools vs buildings
- Voxel 1 and Voxel 2
nonlinear classifiers

- linear on a transformed feature space!

- neural networks:
  new features are learnt

- SVMs
  new features are (implicitly) determined by a kernel

\[
\begin{align*}
\text{tools vs buildings} & \quad \text{voxel 1} \quad \text{voxel 2} \\
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nonlinear classifiers

reasons to be careful:

- too few examples,
  too many features
- harder to interpret
nonlinear classifiers

reasons to be careful:

- too few examples,
- too many features
- harder to interpret

- overfitting

[from Hastie et al, 2001]
## How do we test predictions?

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<td>group 6</td>
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</table>

classifier

\[ \text{predicted labels} \] vs \[ \text{true labels} \]
how do we test predictions?

Predicted labels

tools
buildings
buildings

...

tools
buildings
tools
how do we test predictions?

<table>
<thead>
<tr>
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<th>Predicted labels</th>
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<td>tools</td>
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#correct out of #test
how do we test predictions?

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- null hypothesis:
  
  “classifier learnt nothing” → “predicts randomly”
how do we test predictions?

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- null hypothesis:
  
  “classifier learnt nothing” → “predicts randomly”

- intuition:
  
  - a result is significant if very unlikely under null
how do we test predictions?

- $X = \#\text{correct}$
- $P(X|\text{null})$ is binomial(#test,0.5)
- p-value is $P(X\geq\text{result to test}|\text{null})$

distribution under null (0.05 p-value cut-off)
how do we test predictions?

- \( X = \) #correct
- \( P(X|\text{null}) \) is binomial(#test,0.5)
- p-value is \( P(X\geq\text{result to test}|\text{null}) \)
- lots of caveats:
  - accuracy is an estimate
  - few examples \( \rightarrow \) very uncertain
  - can get a confidence interval
  - must correct for multiple comparisons

distribution under null
(0.05 p-value cut-off)
what questions can be tackled?

- is there information?  
  (pattern discrimination)
- where/when is information present?  
  (pattern localization)
- how is information encoded?  
  (pattern characterization)
case study: orientation

[Kamitani & Tong, 2005]

subjects see gratings in one of 8 orientations
case study: orientation

subjects see gratings in one of 8 orientations

voxels in visual cortex respond similarly to different orientations

[Kamitani & Tong, 2005]
case study: orientation

subjects see gratings in one of 8 orientations

yet, voxels can be combined to predict the orientation of the grating being seen!
features

- case study #1, features are voxels
- case study #2, features are voxels in visual cortex
features

- case study #1, features are voxels
- case study #2, features are voxels in visual cortex

- what else could they be?
  voxels at particular times in a trial,
  syntactic ambiguity study
features

- you can also synthesize features
  - Singular Value Decomposition (SVD)
  - Independent Component Analysis (ICA)

\[
\text{examples} \quad \text{dataset} \quad = \quad Z \quad \text{basis images} \\
\text{voxels} \quad \text{new features} \quad \text{voxels}
\]
### features

- you can also synthesize features
  - Singular Value Decomposition (SVD)
  - Independent Component Analysis (ICA)

\[
\text{dataset} \quad \begin{array}{c}
\text{examples} \\
\text{voxels}
\end{array} = \begin{array}{c}
\text{basis images} \\
\text{voxels}
\end{array} \quad \begin{array}{c}
\text{Z} \\
\text{new features}
\end{array}
\]

- reduces to \#features < \#examples
- a feature has a spatial extent: basis image
- learn on the training set, convert the test set
example construction

- an example
  - can be created from one or more brain images
  - needs to be amenable to labelling
example construction

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  - can be created from one or more brain images
  - needs to be amenable to labelling

- some possibilities
  - the brain image from a single TR
  - the average image in a trial or a block
  - the image of beta coefficients from deconvolution
example construction

- an example
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- some possibilities
  - the brain image from a single TR
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  - the image of beta coefficients from deconvolution

- caveats
  - remember the haemodynamic response time-to-peak
  - images for two examples not separate “enough”
    - in test set, lowers the effective #examples in statistical test
    - in between train and test set, “peeking” / ”circularity”
  - read [Kriegeskorte et al. 2009] (“double dipping”)
localization

- key idea #1
  test conclusions pertain to whatever is fed to the classifier
localization

- key idea #1
  test conclusions pertain to whatever is fed to the classifier

- key idea #2
  one can predict anything that can be labelled:
  stimuli, subject percepts, behaviour, response, …
localization

- key idea #1
  test conclusions pertain to whatever is fed to the classifier

- key idea #2
  one can predict anything that can be labelled:
  stimuli, subject percepts, behaviour, response, ...

so what criteria can we use?
- location
- time
- voxel behaviour or relationship to label
  - aka “feature selection”
feature (voxel) selection

- what does it look like

<table>
<thead>
<tr>
<th>training data (42)</th>
<th>labels</th>
</tr>
</thead>
<tbody>
<tr>
<td>group 1</td>
<td>...</td>
</tr>
<tr>
<td>group 3</td>
<td>...</td>
</tr>
<tr>
<td>group 5</td>
<td>...</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>test data (42)</th>
</tr>
</thead>
<tbody>
<tr>
<td>group 2</td>
</tr>
<tr>
<td>group 4</td>
</tr>
<tr>
<td>group 6</td>
</tr>
</tbody>
</table>

+ classifier = vs
feature (voxel) selection

- what does it look like

\[
\begin{array}{c|c}
\text{group 1} & \text{…} \\
\text{group 3} & \text{…} \\
\text{group 5} & \text{…} \\
\hline
\text{test data (42)} & \text{labels} \\
\end{array}
\]

\[
\begin{array}{c|c}
\text{group 2} & \text{…} \\
\text{group 4} & \text{…} \\
\text{group 6} & \text{…} \\
\hline
\text{training data (42)} & \text{predicted labels} \quad \text{true labels} \\
\end{array}
\]

\[
\text{classifier} = \text{predicted labels} \quad \text{vs} \quad \text{true labels}
\]
feature (voxel) selection

- what does it look like

- classifier

\[
\begin{align*}
\text{training data (42)} & \quad \text{labels} \\
\text{group 1} & \quad \text{group 3} & \quad \text{group 5} \\
\text{test data (42)} & \quad \text{predicted labels} \quad \text{true labels} \\
\text{group 2} & \quad \text{group 4} & \quad \text{group 6} \\
\end{align*}
\]
feature (voxel) selection

- what does it look like

```
training data (42)         labels

group 1
group 3
group 5

---

test data (42)

---

group 2
group 4
group 6

+

classifier

= predicted labels vs true labels
```

- great for improving prediction accuracy
- but
  - voxels often come from all over the place
  - very little overlap in selected across training sets
feature (voxel) selection

- look at the training data and labels
feature (voxel) selection

- look at the training data and labels
- a few criteria:
  - difference from baseline
feature (voxel) selection

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- a few criteria:
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  - difference between classes (e.g. ANOVA)
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  - preferential response to one class
feature (voxel) selection

- look at the training data and labels
- a few criteria:
  - difference from baseline
  - difference between classes (e.g. ANOVA)
  - preferential response to one class
  - stability
  - ...

![Charts showing data distribution for A, B, and C in different runs.](chart.png)
case study: category reinstatement

- items from 3 categories: faces, locations, objects
- classifier trained during study of the grouped items
- detect category reinstatement during free recall (test)

[Polyn et al 2005]
temporal localization

voxel influence on reinstatement estimate

[Polyn et al 2005]
temporal localization

key ideas:
- trained classifiers may be used as detectors to localize the time at which information is present
- test examples can be temporally overlapping
- it is feasible to decode endogenous events
what questions can be tackled?

- is there information?  
  (pattern discrimination)
- where/when is information present?  
  (pattern localization)
- how is information encoded?  
  (pattern characterization)
classifier dissection

- a classifier learns to relate features to labels
- we can consider not just what gets selected but also how the classifier uses it
- in linear classifiers, look at voxel weights
classifier dissection

- weights depend on classifier assumptions
- less of an issue if feature selection is used

weights are similar, but accuracy difference 15%
classifier dissection

- assumption effects on synthetic data

```
SVM

GNB
```

see [Pereira, Botvinick 2010]
case study: 8 categories

subjects see photographs of objects in 8 categories
- faces, houses, cats, bottles, scissors, shoes, chairs, scrambled
- block: series of photographs of the same category

[Haxby et al., 2001]
case study: 8 categories

nearest neighbour classifier

- all category pair distinctions
- selects voxels by location
  - fusiform gyrus
  - rest of temporal cortex
- selects voxels by behaviour
  - responsive to single category
  - responsive to multiple

logic:
- restrict by location/behaviour
- see if there is still information

[Haxby et al., 2001]
classifier dissection

1) whole-brain logistic regression weights

faces
classifier dissection

1) whole-brain logistic regression weights

faces

houses
classifier dissection

1) whole-brain logistic regression weights

faces

houses

chairs
classifier dissection

2) feature selection

faces
classifier dissection

2) feature selection

faces

top 1000 voxels
classifier dissection

whole brain classifier

- accuracy 40% in this case
- many more features than examples => simple classifier
- messy maps (can bootstrap to threshold)
classifier dissection

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- accuracy 80% in this case
- sparse, non-reproducible maps
- different methods pick different voxels
classifier dissection

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- sparse, non-reproducible maps
- different methods pick different voxels

a lot of work
[Mitchell et al 2004], [Norman et al 2006], [Haynes et al 2006],
[Pereira 2007], [De Martino et al 2008], [Carrol et al 2009],
Pereira et al 2009]
classifier dissection

neural network
- one-of-8 classifier
- temporal cortex

learned model
- hidden units
- activation patterns across units reflect category similarity

[Hanson et al., 2004]
classifier dissection

neural network
- one-of-8 classifier
- temporal cortex

learned model
- hidden units
- activation patterns across units reflect category similarity
- sensitivity analysis
  - add noise to voxels
  - which ones lead to classification error?

[Hanson et al., 2004]
classifier dissection conclusions

- if linear works, you can look at weights
  - but know what your classifier does (or try several)
  - read about bootstrapping (and [Strother et al. 2002])
classifier dissection conclusions

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- voxel selection
  - may be necessary in multiclass situations
  - try multiple methods and **look** at the voxels they pick
  - voxels picked may be a small subset of informative ones
  - report all #s of voxels selected or
    use cross-validation on training set to pick a # to use
classifier dissection conclusions

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- nonlinear classifiers
  - worth trying, but try linear + voxel selection first
  - look at [Hanson et al. 2004] and [Rasmussen et al. 2011]
    for ways of gauging voxel influence on classifier
information-based mapping (searchlights) [Kriegeskorte 2006]

- focus the classifier on small voxel neighbourhoods
- more examples than features
- can learn voxel relationships (e.g. covariance matrix)
- can train nonlinear classifiers

classifier = predicted labels

classifier = predicted labels

voxel accuracy
information mapping

- on 8 categories, yields an accuracy map

- also local information: covariance, voxel weights
information mapping

- on 8 categories, yields an accuracy map
- also local information: covariance, voxel weights
- can be thresholded for statistical significance
information mapping

- “H0: chance level” deems many voxels significant
- what does accuracy mean in multi-class settings?
  - confusion matrix
  - for each class, what do examples belonging to it get labelled as?

8 classes

Accuracy

0.76

Faces
Houses
Cats
Shoes
Bottles
Chairs
Scissors
Scrambled

1.0
0.5
0.0

122
information mapping

- contrast each pair of classes directly
- threshold accuracy to a binary image

face v house
face v cats
...
...
scrambled v chairs

count# pairs significant

voxels
information mapping

- each voxel has a \textit{binary profile} across pairs
- how many different ones?

face v house
face v cats
...
...
scrambled v chairs

count\# pairs significant
information mapping

- A binary profile is a kind of confusion matrix
- Only a few hundred profiles, many similar
- Cluster them!

houses versus all else

faces and cat versus all else

[Pereira & Botvinick, KDD 2011]
information mapping

- a map of accuracy works well in 2 class situation
- some classifiers seem consistently better
  see [Pereira&Botvinick 2010] for details
- easy to get above chance with multiway prediction
  so reporting accuracy or #significant is not enough
- consider reporting common profiles or
  grouping classes into distinctions to test
what questions can be tackled?

- is there information? (pattern discrimination)
- where/when is information present? (pattern localization)
- how is information encoded? (pattern characterization)
to get started

- **MVPA toolbox (in MATLAB)**
  http://code.google.com/p/princeton-mvpa-toolbox

- **PyMVPA (in Python)**
  http://www.pymvpa.org

- support the whole workflow
  - cross-validation, voxel selection, multiple classifiers,…
  - helpful mailing lists (most people are on both)
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- **Searchmighth (in MATLAB, shameless plug)**
  - http://minerva.csbmb.princeton.edu/searchmighth
  - special purpose toolbox for information mapping
  - can be used with MVPA toolbox
Thank you!
questions?