

IBM Research

# Using Machine Learning to Learn about Brain



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#### **Collaborations and Recent Books**

- Computational Biology Center @ IBM Watson:
  - Guillermo Cecchi, James Kozloski, Jeremy Rice
- **IBM Watson**, other departments
  - Steve Heisig, Ravi Rao, Sasha Aravkin, Melissa Carroll
- Neurospin (France):
  - JB Poline, Bertrand Thirion et al
- Mt Sinai (New York):
  - Rita Goldstein
- Northwestern U. (Chicago)
  - A.V. Apkarian
- SUNY Stony Brook:
  - Jean Honorio (now at MIT), Dimitris Samaras
- Lehigh University:
  - Katya Scheinberg





#### **Functional Magnetic Resonance Imaging (fMRI)**







- Blood-oxygen-level-dependent (BOLD) signal related to brain activity while subject performs some task in scanner
- 4D 'brain movie': a sequence of 3D brain volumes
   3D voxels ~ 3x3x3 mm, time repetitions (TR) ~1-2s
- Challenge: high-dimensional, small-sample data

10,000 to 100,000 variables (voxels), but only 100s of TRs (samples), and less than 100 subjects

### What are we looking for in fMRI data?

Mainstream fMRI analysis objective:

discovering brain areas **relevant** to a mental state or a task

#### But how to measure 'relevance'?



- Ultimately: mutual information (but computationally intractable to evaluate on all voxel subsets)
- Simplest approximation: univariate (voxel-vise) correlations with the task (GLM approach)
   But informative multivoxel patterns are often missed (Haxby et al, many other studies, this work)
- □ This work: predictive accuracy of multivariate sparse models as a better proxy for relevance

#### Questions:

How is task-related information distributed in the brain?

Is there a sharp boundary between relevant vs. irrelevant brain areas?

Or is the information distribution through the brain almost 'holographic'?

#### **Our Goal: Interpretable Multivariate Predictive Models**



#### **Feature Selection**

[Carroll et al, Neuroimage 2009] [Rish et al, Brain Informatics 2010] [Rish et al, SPIE Med.Imaging 2012]

#### Sparse regression (LASSO, Elastic Net)

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda_2 \|\boldsymbol{\beta}\|^2 + \lambda_1 \|\boldsymbol{\beta}\|_1$$

#### **Feature Construction:**

#### - feature engineering (network properties etc.)

[Rish et al, PLoS One 2013, Cecchi et al, NIPS 2009] [Rish et al, SPIE Med.Imaging 2012]

#### - automated feature extraction: dictionary learning, deep learning, and so on

[Rish et al, ICML 2008], ongoing work



#### **Example: Pain Perception Studies**



14 healthy subjects presented with painful thermal stimuli while in fMRI scanner, and asked to rate their pain level (using a finger-span device).

#### Where are pain-related brain areas?

Can we predict pain perception and/or stimulus from fMRI?



### Example: Videogame Playing (PBAIC07)

- subjects play a videogame in a scanner
- 24 continuous response variables (convolved with HRF function)
  - Listening to Instructions
  - Annoyance
  - Anxiety
  - Looking at faces, etc.



Instructions variable:



Can we find brain areas involved in this task? Can we predict response variables from fMRI?

#### **Reversing GLMs: Predicting Mental State from Voxels**



Find a small number of the most relevant voxels (brain areas) Relevant ⇔ (jointly) predictive about task (vs. individually correlated)

#### Feature Selection via Sparse Regression: LASSO and Elastic Net

**ISSUE**: high-dimensional, small-sample problem

- solutions are overfit to data: poor generalization
- difficult to *interpret* (determine relevant voxels)

APPROACH:

- LASSO: adds  $l_1$ -norm regularization

 $\min_{\beta} ||\mathbf{y} - \mathbf{X}\beta||_2^2 + \lambda ||\beta||_1$ 

- selects relevant voxels (sparse solution  $\Leftrightarrow$  many zero coefficients)
  - improving LASSO: Elastic Net sparsity + grouping of correlated variables

$$\hat{\beta} = \arg\min_{\beta} ||\mathbf{y} - \mathbf{X}\beta||_2^2 + \lambda_1 ||\beta||_1 + \lambda_2 ||\beta||_2^2$$

*I*<sub>1</sub> keeps singularities at vertices ⇒ sparsity

*I*<sub>2</sub> enforces strictly convex edges ⇒ grouping effect



#### **Sparse Models Can Accurately Predict Mental States**

**PBAIC-07** Tasks Pain Rating Task 0.8 OLS (corr. with response) Ridge Predictive accuracy ).75 0.8 LASSO EN 0.1 Test Correl. 9.0 EN 2.0 07 ).65 OLS 0.2 ambda2=0.1 ambda2=1 lambda2=5 lambda2=10 Instructions VRFixation Regression Method Velocity 0.55 L 500 1000 1500 number of voxels [Rish et al. 2010] [Carroll et al. 2009]

Elastic Net: close to 0.8 prediction accuracy for pain ratings [Rish et al, BI-2010], as well as for several tasks in PBAIC-07 dataset [Carroll et al, Neuroimage 2009]

[SPIE Med.Imaging 2012], [Rish et al, BI 2010], [Carroll et al, Neuroimage 2009]

#### **Even Better Results: Combine Data-Driven and Analytical Models**

- Dynamical model (1<sup>st</sup> order, only 3 parameters) captures intersubject variability in pain response given stimulus
- Stimulus not available? Predict from fMRI, then apply the model!









Incorporating nonlinear dynamical model into sparse learning (via hidden stimulus variable) improves over 'direct' sparse regression – due to very high accuracy of analytical model !

[PLoS Comp Bio 2012]

### **But How is Predictive Information Distributed in the Brain?**

• Are there multiple sparse models that predict well?

Best sparse solution for PBAIC 'Instructions' task
↓
Voxels in a sparse solution predict well ⇒ task-relevant
↓
But does this mean ONLY these voxels are relevant?
Not necessarily – multiple good solutions may exist!



- Whole-brain exploration of relevant areas: find sparse solution, remove its voxels, find another one; repeat until no voxels are left:
  - 1. Run Elastic net to find one solution of size k = min(1000; # of remaining voxels)
  - 2. Remove the solution voxels from the data
  - 3. If no more voxels left, stop, otherwise Go to step 1
- How does the predictive power degrade as more voxels are removed?
- Is there a sharp transition between relevant and irrelevant voxels?

#### Full-Brain (Holographic) Information Distribution for Pain



- Surprisingly slow degradation of predictive accuracy!
- No sharp transition between relevant and irrelevant voxels

#### Pain-Predictive Solutions Are Spatially Distributed Throughout the Brain



Highly predictive solutions are spread throughout the brain:

later solutions DO NOT use voxels from same predictive areas as former ones

#### **Univariate Correlations DO NOT Properly Capture Voxel Relevance!**



 Exponential decay in relevance measured by univariate correlation with the task vs.
 linear decay for prediction accuracy

Still highly predictive solution #25 (0.52 accuracy vs. 0.67 of the 1<sup>st</sup> solution) has no voxels with individual correlation above 0.1!



#### **Visual Task: Similar Results to Pain**



- Similar to pain: linear decay of predictive accuracy (⇔relevance)

#### **PBAIC Tasks: Results Depend on the Task!**



- Solution relevance (accuracy) degrades faster than for pain, though for the 2 tasks in the top panel decay is still close to linear
- 3<sup>rd</sup> task (instructions): fast (exponential) decay; relevant voxels are a small fraction of the brain (NO holographic effect)
- Decay is slower for low grouping (small λ<sub>2</sub>), but this is likely an artifact of the method; larger λ<sub>2</sub> ⇔ are more reliable results





#### Relatively simple auditory task: listening to short instructions

#### More complex task: perceiving and rating pain





Sharp transition from highly relevant first two solutions (2000 voxels), to practically irrelevant remaining voxels (0.2 and lower accuracy) No such sharp transition, slow linear decay from best (on average) 0.65 accuracy (1<sup>st</sup> solution) to 0.5 (10<sup>th</sup> sol.) and 0.4 accuracy (24<sup>th</sup> solution, 23,000 voxels removed)

# **Sparse Regression and fMRI: Summary**

#### Main questions:

- How is task-related information distributed in the brain?
- □ Is there a sharp boundary between relevant vs. irrelevant brain areas?

#### Approach:

exploring solution space of multivariate sparse regression, where sparse solutions task-relevant voxel subsets/areas

#### Results:

- contrary to traditional univariate correlation (or GLM) approach, multivariate sparse regression reveals full-brain ('holographic') spread of task-relevant information
- tasks such as pain rating and visual rating seem to involve most of the brain rather than just specific areas (involvement measured by predictive accuracy)
- □ however, not all tasks are holographic (e.g., Instructions in PBAIC dataset is not)
- Hypothesis (requires further empirical investigation):
  - widespread activation (measured by multivariate predictive information) is more characteristic of complex tasks such as pain perception; simpler tasks have more clear separation between relevant and irrelevant brain areas.



## Overview

- Our goal: learning full-brain interpretable probabilistic network models
- Problem: full-brain networks, even edge-sparse, are hard to interpret; can we identify most relevant nodes/voxels?
- Proposed approach: variable (node) selection, besides the usual edge selection, using group-Lasso type of penalty
- Application: study of cocaine addicts vs. controls (Goldstein et al., 2007) performing a visual attention task with a monetary reward
- Results: significantly more interpretable and statistically more accurate networks that discover most important clusters of interacting voxels





### **Markov Networks (Markov Random Fields)**

$$X = \{X_1, ..., X_p\}, \quad G = (V, E)$$

$$P(\mathbf{X}) = \frac{1}{\mathbf{Z}} \prod_{C \in Cliques} \Phi_C(\mathbf{X}_C)$$

Lack of edge  $(i, j) \rightarrow$ conditional independence  $X_i \perp X_j | rest$ 

## Gausian Markov Random Fields (GMRFs)

Markov random field of jointly Gaussian variables

- $P(\mathbf{x}) = (2\pi)^{-\frac{P}{2}} \det(\Sigma)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x} \boldsymbol{\mu})^T \Sigma^{-1}(\mathbf{x} \boldsymbol{\mu})\right)$
- $\Sigma$  covariance matrix,  $\Sigma^{-1}$  precision (concentration) matrix
- Zeros in  $\Sigma$ : marginal independence
- Zeros in  $\Sigma^{-1} \Leftrightarrow$  conditional independence  $\Leftrightarrow$  lack of edge



#### Maximum Likelihood Estimation of the Inverse Covariance Matrix

Assume the data X are centered to have zero mean. Then:

 $\hat{\Sigma}^{-1} = \arg \max_{C \succ 0} \log p(C | \mathbf{X}) = \arg \max_{C \succ 0} \log p(\mathbf{X}, C) =$ 

 $= \arg \max_{C \succ 0} \log \det(C) - \operatorname{tr}(SC)$ 

where  $S = \frac{1}{N} \sum_{i=1}^{N} x_i^T x_i$  is the empirical covariance matrix (MLE of  $\Sigma$ )

Why not just use  $\hat{\Sigma}^{-1} = S^{-1}$ ?

- in small-sample case (n < p), S may not be even invertible
- even if it is, S<sup>-1</sup> almost never contains exact zeros
- needed: an explicit sparsity-enforcing constraint (regularization)

#### *I***<sub>1</sub>-Regularized Maximum Likelihood Problem**

# Primal: $\hat{\Sigma}^{-1} = \arg \max_{C \succ 0} \log \det(C) - \operatorname{tr}(SC) - \lambda ||C||_1$ (1)

#### Various algorithms:

- Approximation: LASSO for each node (Meinshausen&Buhlman, 2006)
- Block-coordinate descent: COVSEL (Banerjee et al, 2006), glasso (Friedman et al, 2007)
- Projected gradient (Duchi et al, 2008)
- Greedy ascent (Scheinberg and Rish, 2010)
- Alternating Linearization Method (Scheinberg et al, 2011)
- several more recent efficient techniques available

#### Various sparse structure, besides basic edge-sparsity:

- diagonal structure (Levina et al., 2008)
- block structure for known block-variable assignments (Duchi et al., 2008)
- unknown block-variable assignments (Marlin & Murphy, 2009; Marlin et al., 2009)
- spatial coherence (Honorio et al, 2009)
- common structure among multiple tasks (Honorio et al, 2010)

### Variable Selection in Gaussian MRFs

- Datasets with thousands of variables: fMRI, gene expression, stock prices, world weather
- Hypothesis: often, only a relatively few variables are interacting with each other, forming network clusters; the rest are not relevant



Goal: select these *important* nodes, and find their interaction pattern

#### Variable-Selection Regularizer: Block-Sparsity over Node's Neighbors



Variable-selection prior: block I1/lp norm, for  $p \in \{2,\infty\}$ 

$$||C||_{1,p} = \sum ||c_{n,1}, ..., c_{n,n-1}, c_{n,n+1}, ..., c_{n,N}||_p$$

 We use Block-Coordinate Descent (BCD) on the primal (not dual!): a sequence of quadratic subproblems with closed form solutions, see (Honorio et al, AISTATS 2012)

#### **Cocaine Addiction fMRI Data**

- fMRI dataset previously collected by (Goldstein et al, 2007)
  - 15 cocaine addicted subjects and 11 control subjects
  - 87 scans/TRs (3.5 s), 53x63x46 voxels
- Subsampling to reduce dimensionality: 4x4x4 voxel cubes ⇔869 nodes
- Task: visual attention, with monetary reward

Instructions were to press a response button (using the thumb of the dominant hand) with speed and accuracy upon seeing the target (red square) after a "Go" but not after a "No-go" instruction stimulus.

#### B. Each 3.5-sec trial (81 go and 81 no-go trials in each block):

Fixation	Instruction	Fixation	Trigger/Response	e Feedback
1000 ms	500 ms	1000 ms	500 ms	500 ms
+	"Go" or "No-go"	+		\$0.00 \$0.01 or \$0.45

#### **Results: Better Model Fit (Better Likelihood)**

- 1/3 of the data was used for training, 1/3 for validation and 1/3 for testing



Our methods (LI,L2) outperform competitors, e.g. Meinshausen-Buhlmann (MO,MA), graphical lasso (GL), scale-free networks (SF) and Tikhonov regularization (TR).

Variable-selection assumption seem to fit the data better than standard sparse GMRFs.

cocaine subjects control subjects





### Blue - positive interactions red - negative interactions

Our structures involve fewer connected variables (~**50 connected nodes**) and have higher log-likelihood than graphical lasso).

Where cocain GMRI leave

When performing classification of cocaine vs. control by using GMRFs, all methods obtain **84.6%** leave-one-subject-out accuracy

our  $\ell_{1,2}$  method

graphical lasso

#### **Discussion**



Blue - positive interactions red - negative interactions

In cocaine addicts, as compared to controls, we observe

- increased interactions between the visual cortex (left) and the prefrontal cortex (right)
- decreased density of interactions between the visual cortex with other brain areas

Note that the trigger for reward was a visual stimulus and that abnormalities in the visual cortex was reported in (Lee et al, 2003) when comparing cocaine abusers to control subjects

Also, prefrontal cortex is involved in decision making and reward processing, and abnormal monetary processing in the prefrontal cortex was reported in (Goldstein et al, 2009) when comparing cocaine addicted individuals to controls.

### Conclusions

- We introduced variable-selection into sparse Gaussian MRF learning
- Our models fit data better than competitors without variable selection
- Most importantly, our method produces much more interpretable networks
- Application: study of cocaine addicts vs. controls (Goldstein et al., 2007) performing a visual attention task with a monetary reward
- Results: significantly more interpretable and statistically more accurate networks that discover most important clusters of interacting voxels







 Not a localized dysfunction, spatially or mechanistically (e.g., unlike depression, epilepsy, stroke, Parkinson's)

 Hypothesized to be a disconnection syndrome [Wernicke 1906; Bleuler, 1911; Friston & Frith, 1995]

Our objective: discover schizophrenia 'biomarkers', i.e. brain activity patterns associated with this disorder

### **Experiment: Simple Auditory Task in fMRI Scanner\***



96 trials, with 32 sentences in French (native), 32 sentences in foreign languages, and 32 silence interval controls. Two runs.

- Patient Group (11 subjects)
  - Prone to auditory hallucinations
  - Native French speakers, right-handed, 3+ yrs. illness
- Normal Group (11 subjects)

\*M. Plaze, et al., Schizophrenia Research (2006)

### **Standard Approach: Univariate, Task-Related Activations**



- For each voxel, compute a score (e.g., correlation, or GLM coefficient) reflecting how well its activity matches the stimulus sequence
- Threshold the scores to select only statistically significant ones

However, no statistically significant differences were found across groups; also, classification based on activation features was close to chance level\*

\*G. Cecchi, et al., Neural Information Processing Systems (NIPS-2009)

#### **Network Features Greatly Outperform Task-Activation Features**

#### [NIPS 2009] [PLoS ONE2013]

Functional networks: (thresholded) voxel-level correlation matrices



No matter which classifier we used, network features outperformed local activations, thus serving as much better biomarkers.

Best results: specific combination of a degree feature + classifier

#### Schizophrenia and Networks: Summary

 Functional networks contain large amount of schizophrenia-related information that may not be present in task-related activations

 Network properties, as opposed to activations, allow for impressively high prediction accuracy (up to 93%) given a simple auditory task

 Simplest features (a dozen of top-ranked pairwise correlations) are most predictive among all network features we tried so far

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# **Beyond fMRI:**

# 'Mind-Reading' from Cheaper Sensors?







## **Text Analytics for "Computational Psychiatry"**

#### **Language is a window into the brain**" - M. Covington

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- 93% accuracy discriminating schizophrenics from manics based on syntactic speech graphs [PLoS One, 2012]
- nearly 100% accuracy predicting 1<sup>st</sup> psychotic episode ONE YEAR in advance (!!) via coherence and a few other features (ongoing work)
- 88% accuracy discriminating ecstasy and meth users from controls, using semantic features such as proximity to 'empathy' concept, etc., and graph features

[Neuropsychopharmacology, 2014]

# в I / walked / into a place, / and I / found / my grandma. / I / hugged / her / strongly, / I / woke up. About dreaming About waking Schizophrenia Control Mania



### **Current Work: Speech Coherence**



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https://www.youtube.com/watch?v=MXzwAXzUwwE



Phrase-to-phrase Coherence

### **Text coherence:**

Currently measured as the angle between vector representations of consecutive sentences (word vectors computed by LSA)



#### [Heisig et al, 2014]

### **Current Work: Speech Coherence**



https://www.youtube.com/watch?v=e2h-DgYcCtw

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Friend anymore money over there b)

https://www.youtube.com/watch?v=21z30aNO3cA



FEATURE	Example 1	Examp	le 2 toper	-
Lemmatized-Nodes	352	350	an <del>gerre par</del> t in the	
Lemmatized-Edges	985	1073		0
Lemmatized-Loop Len 1	8	4	the bachard	1
Lemmatized-Loop Len 2	44	64	was with the share of the share	
Lemmatized-Loop Len 3	284	442		/
Lemmatized-Loop Len 4	1712	2956	-	
			( <b>b</b> ,	F
Coherence:				

Phrase to phrase-median 0.2201 Alternate phrases-median 0.2895 0.0049 0.0045

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### **Goal: Mental State Detection to Improve Mental Function**

#### theguardian

News Sport Comment Culture Business Money Life & style

#### News World news New York

#### Train driver in deadly New York crash had 'severe' sleep disorder, NTSB says

- · Report found William Rockefeller had 'obstructive sleep apnea'
- Commuter train derailment in December 2013 left left four dead

Associated Press in White Plains, New York theguardian.com, Monday 7 April 2014 20.39 BST Jump to comments (29)



Metro-North engineer William Rockefeller Jr is loaded into an ambulance after a derailment in the Bronx borough of New York 1 December 1 2013. Photograph: Eric Thayer/Reuters

The driver of a New York commuter train that derailed at high speed last year, killing four people, had a serious sleep disorder that interrupted his rest dozens of times each night, federal investigators disclosed on Monday.



## Operator of train that jumped tracks at Chicago's O'Hare Airport fired

By Suzanne Presto and Greg Botelho, CNN updated 9:49 AM EDT, Sat April 5, 2014



Driver of O'Hare train derailment fired

STORY HIGHLIGHTS

• NEW: Official: No reason, based on schedule, that fatigue should have been a factor (CNN) -- The driver of a train that jumped the tracks last month at Chicago's O'Hare International Airport -- after having reportedly "dozed off" -- has been fired, a transit authority spokeswoman said Friday.

Can we avoid such tragic accidents by monitoring driver's mental state and performing preemptive actions in real-time?

#### [Heisig et al, 2014] Ongoing Work: Driver Cognitive Load from EEG



**EEG**: Raw waveform is FFTed to power in frequency bands (e.g., from NeuroSky or Muse device)





**Example**: Geographic EEG Plot of relaxation index. Merging onto a highway requires extra concentration. Sensitive software would not interrupt the driver prior to and during transit of this area.

### **Preliminary Results with Sparse Regression**

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- We used sparse regression (LASSO/Elastic Net) to predict Attention and Relaxation from 'raw' frequency band EEG data
- Accuracy measure: correlation between true and predicted signals
- Encouraging results:
   Attention: 0.91 correlation
   best model uses smoothed normalized Theta band
   β<sub>1</sub>
   Relaxation: 0.87 correlation

best model uses smoothed normalized hiAlpha, Theta, MidGamma

- Note that predictive model significantly outperforms the best singlevariable correlations:
  - □ Attention: highest correlation was (negative) 0.59 with sHiAlphaNorm
  - □ Relaxation: highest correlation was (positive) 0.71 with sHiAlphaNorm

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### **Towards "Augmented Human": Real-Time Mind-Reading from Cheap Sensors**

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# Links

Publication page:

http://researcher.watson.ibm.com/researcher/view\_person\_pubs.php?person=us-rish&t=1

Books:

Practical Applications of Sparse Modeling, I Rish, GA. Cecchi, A Lozano, A Niculescu-Mizil (editors), MIT Press, 2014.

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