Low-rank logistic regression for supervised network decomposition

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***Abstract*—Neuroimaging methods tend to focus on either structure discovery or cognitive modulation. Predicting cognitive processes however hinges on the neurobiological pertinence of the constructed feature space. We therefore propose to the solve the unsupervised dimensionality reduction and supervised task classification in an identical optimization problem. Using Human Connectome Project (HCP) data (n=498), optimal low-rank projections and logistic-regression models are identified in a same gradient descent. Brain network decompositions are thus exposed that explain task-descriminative spatial patterns. This is compared against separate decomposition (i.e., ICA and sparse PCA) and classification by logistic regression in independent data splits. RESULTSoutperformes We thus provide modes of brain signal variation extracted for cognitive interpretability.**

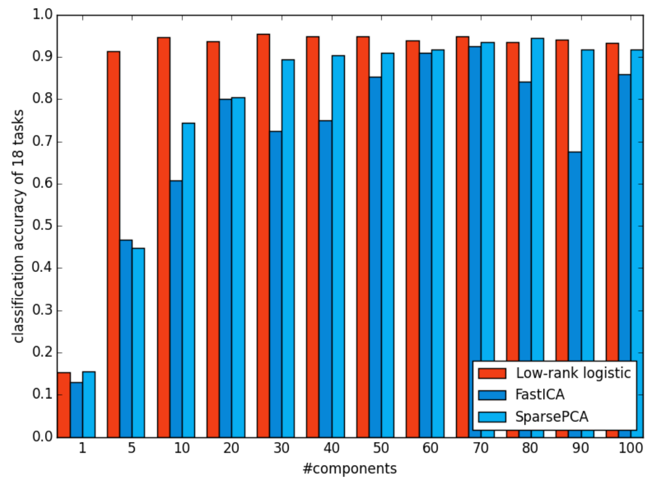
***Index Terms*—Dimensional reduction; brain networks; machine learning; brain imaging**

I. Introduction

Neuroimaging methods can be grouped by focus on discovering neurobiological structure or discovering the neural correlates associated with cognitive processes. To reveal coherent spatial structures across time, independent component analysis (ICA; (1)) is frequently used to decompose BOLD signals into a set of fluctuation patterns. The ensuing spatial patterns are believed to represent neural networks of functionally interaction brain regions. Similarly, sparse PCA (SPCA; (2)) has recently been used to separate BOLD signals into parsimonious network components with less distributed regions. Rather than partially overlapping spatial patterns, most clustering approaches used in neuroimaging (e.g., k-means, hierarchical, or ward clustering; (3)) yield non-overlapping regions of coherent connectivity or task activation. Clustering of brain regions or the entire brain is increasingly used to locate functionally distinct neurobiological compartments (4). As another example, graph analyses (5) use predefined regions to study high-level network properties. All these approaches are completely *unsupervised* in characterizing neurobiological structure without any relation to psychological processes.

To investigate, however, the neural correlates underlying mental operations, the general linear model (GLM; (6)) is the prevalent approach. The contribution of individual voxels is estimated according to a design matrix of experimental conditions. Psychophysiological interactions (PPI; (7)), on the other hand, elucidate the functional interactions between brain regions as a function of experimental conditions. As a final example, dynamic causal modeling (DCM; (8)) quantifies directed, cognitive-task-driven influences between regions by treating the brain as a nonlinear dynamic system with unknown neuronal states. This second set of *supervised* approaches operates in single voxels or investigator-provided region definitions to localize the neural underpinnings of psychological processes.

Yet, special interest lies in the data-driven discovery of neurobiological structure that explains differences in cognitive conditions. Integrating unsupervised discovery and supervised classification should preferentially identify neurobiological structure that allows for the best predictive models. We propose such an approach based on conjoint gradient-descent to optimize linear decomposition and multi-task disambiguation.



Integrated versus serial decomposition and classification Depicts the out-of-sample performance of 18-task classification based on HCP task activity maps. Data reduction and classification was performed simultaneously (Low-rank logistic regression, red) or serially (ICA and SparsePCA, blue)

II. Methods

Data was drawn from 498 unrelated, healthy HCP participants. All provided informed consent to the Washington University in St. Louis institutional review board. HCP tasks were selected that feature known suitability as localizers and reliability across participants (9). Mostly block-design, but also event-related, paradigms were administered on 1) working memory/cognitive control processing, 2) incentive processing, 3) visual and somatosensory-motor processing, 4) language processing (semantic and phonological processing), 5) social cognition, 6) relational processing, and 7) emotional processing. All data were acquired on the same Siemens Skyra 3T scanner. Whole-brain EPI acquisitions were acquired with a 32 channel head coil (TR=720ms, TE=33.1ms, flip angle=52, BW=2290Hz/Px, in-plane FOV=280 $\times$ 180mm, 72 slices, 2.0mm isotropic voxels). The minimally preprocessed pipeline (10) includes gradient unwarping, motion correction, fieldmap-based EPI distortion correction, brain-boundary-based registration of EPI to structural T1-weighted scan, non-linear (FNIRT) registration into MNI space, and grand-mean intensity normalization. Activation maps were spatially smoothed by a Gaussian kernel of 4mm (FWHM). A general linear model (GLM) was implemented by FILM from the FSL suite with model regressors from convolution with a canonical hemodynamic response function and from temporal derivatives. HCP tasks were conceived to modulate activation in a maximum of different brain regions and neural systems. Indeed, at least 70% of the participants showed consistent brain activity in contrasts from the task battery, which certifies excellent coverage (9). In sum, the HCP task dataset incorporated 8650 first-level activity maps from 18 diverse paradigms administered to 498 participants. All maps were downsampled to a common 36x43x36 space of 5mm isotropic voxels and gray-matter masked (at least 10%). All analyses were based on task maps of 13,657 voxels representing Z values in gray matter.

Unsupervised and supervised learning were combined into a low-rank logistic regression problem. The 13,657 z values from each activity map were subject to a first linear projection into Z latent components (i.e., 1, 5, 10, .., 100). These hidden brain networks loadings were subsequently projected into the 18 class space for multinomial logistic regression. The goal was to find the two weight matrices (input-to-hidden: 13,657 x Z and hidden-to-output: Z x 18) and their corresponding bias vectors. Non-linearities were not applied on the transformation results. Weights and biases were initialized by Gaussian random noise. Gradient descent updated these matrices and vectors in each iteration (100 samples per batch, 250 epochs). Using the chain rule, the partial derivates for the update were computed for the transformation into the latent space and the subsequent transformation into the class space. We choose the RMSprop algorithm (11) with an initial learning rate of 0.01. Early stopping ensured that the best weight matrices/vectors were retained in each epoch cycle. This was evaluated by the prediction accuracy on a validation set (10% of the training data) at each iteration.

This approach was benchmarked against independent dimensionality reduction and learning of a classification function. Data reduction was performed on one half of the data by ICA and SPCA. ICA unmixed the BOLD signals into separate spatial components by minimizing their mutual information (12). This iterative blind source separation was realized by a parallel FASTICA implementation (200 maximum iterations, per-iteration tolerance of 0.0001, initialized by a random mixing matrix, preliminary whitening). SPCA separated the BOLD signals into network components with few regions, which scales well to large datasets (2). This regression-type optimization problem constrained by ℓ_1-penalty in an implementation without orthogonality assumptions (1000 maximum iterations, per-iteration tolerance of $1 * 10^{-8}$, sparsity alpha=1, ridge-shrinkage at 0.01, Lasso path computed with coordinate descent). Each linear decomposition revealed the specified number of latent network components in one half the HCP data. The extracted hidden network components were subsequently used to reduce the remain half of task maps to a considerably smaller number of component loadings. 13,657 voxels were thus condensed into 1, 5, 10, .., 100 measures of network involvement using ridge regression (regularization alpha parameter=0.001, using Cholesky solver). Multinomial logistic regression was finally performed on the brain network loadings to learn classifying the 18 cognitive tasks. Importantly, in all approaches, the final classification models were tested on an unseen test set (10% of data).

All analysis scripts that produced the results are accessible online (http://github.com/banilo/prni2015).

III. Results

Low-rank regression outperformed serial ICA/SparsePCA and logistic regression.

IV. Discussion

-hypothesis space includes sparse PCA and PCA but not ICA since no linearity

- if linearity, then would be closer to the notion of 1-hidden layer neural network rather than low-rank logistic regression

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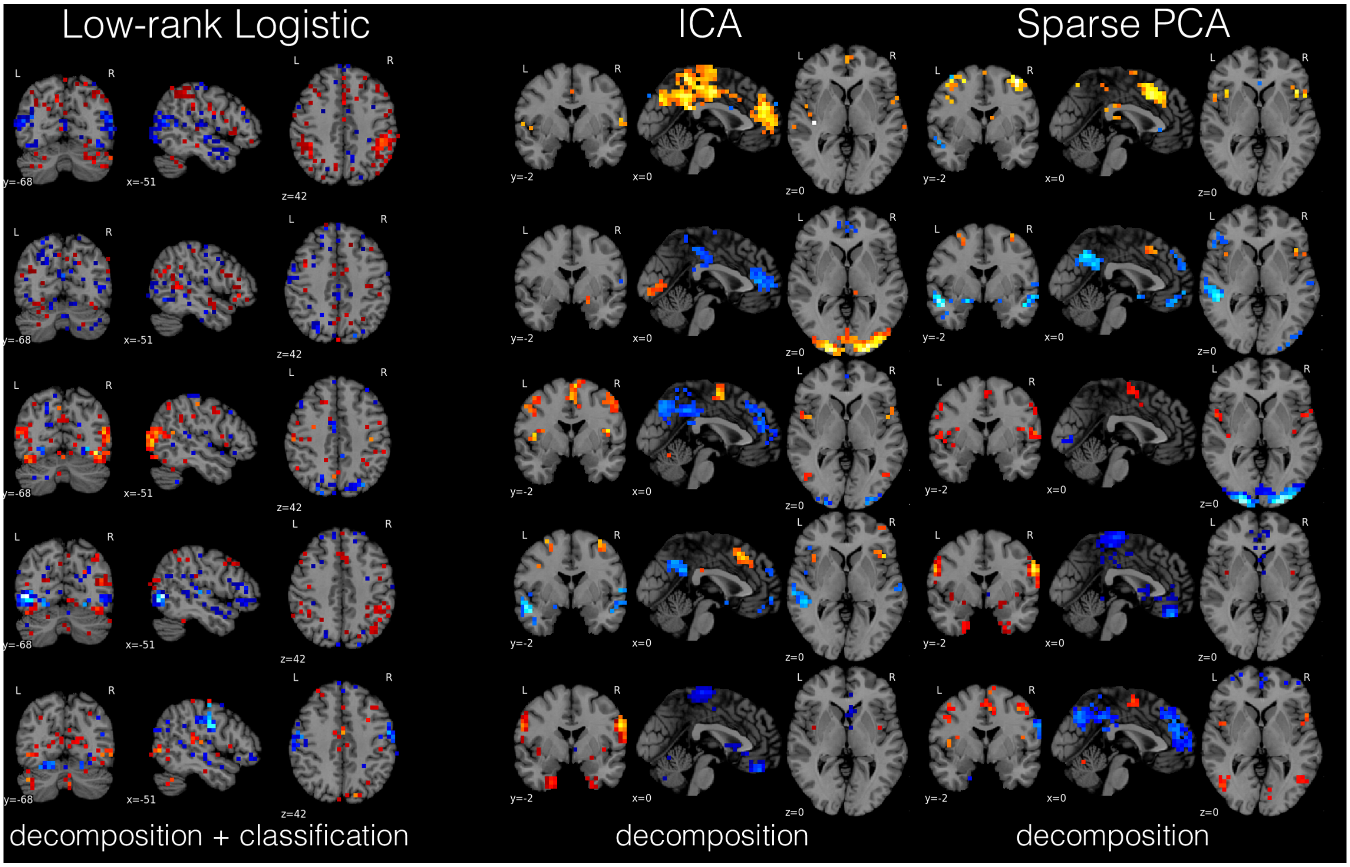

Fig. 1. **Decomposition into 5 networks**

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