Exploring Working Memory Task Predictability using fMRI Data

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Abstract

In our quarter-one project, our group performed a first-level analysis of functional magnetic resonance imaging (fMRI) data. This consisted of analyzing brain data in a 4-dimensional array and identifying areas of significant activation. In this project, we use voxel weights generated from individual first-level analysis to train various machine learning models to classify task types based on fMRI brain imaging data. With this model, we can address gaps in neuroscience literature on whether visual working memory tasks with varying task strategies use fundamentally different neural circuitry. Furthermore, it could suggest that models are able to "read minds" of individuals under different tasks. Multivoxel pattern analysis (MVPA) is an increasingly popular method of analyzing fMRI brain imaging by retaining the information of each voxel in the brain. However, recent work on MVPA was typically limited to Support Vector Machines (SVMs). With our project, we hope to explore other popular machine learning models to classify task type, look into the interpretability of models for task fMRI classification, and explore the use of confounds within brain imaging data to build more accurate models using the full fMRI data.

Code: https://github.com/yunchen-hung/fmriWorkingMemoryProject

1 Introduction

Multivoxel pattern analysis (MVPA) has been an increasingly popular method of functional magnetic resonance imaging (fMRI) brain imaging analysis in recent years. Instead of studying univariate analysis such as averaging activity across the entire brain, MVPA compares patterns of activation in clusters of voxels. It has also been considered as a method of "mind reading", as MVPA allows the decoding of representational states within the brain. A review study by (Mahmoudi et al. 2012) noted the effectiveness of Support Vector Machines (SVM) in MVPA of functional imaging data as a supervised classification problem, as it was equipped to deal with high dimensional data and flexibility in modeling various types of data. Recent literature by (Aglieri et al. 2021) performed MVPA on task fMRI data to decode which speaker participants were recalling in a speaker recognition task. They were able to identify temporal and extra-temporal regions associated with the task, displaying the capability of using SVM on task fMRI data in understanding the neural correlates involved in a task. Similarly, (Hof et al. 2021) trained SVMs on a task fMRI data to develop a sexual image classifier. They were able to distinguish between brain regions associated with response to sexual images and general response areas with high accuracy with MVPA. However, k-nearest neighbors (kNN), Gaussian Naive Bayes, and Logistic Regression are also potential models of interest for fMRI classification (Pereira, Mitchell and Botvinick 2009).

In our project, we specifically look into whether we can identify which visual working memory task subjects are performing based on their brain imaging data. The motivation for this lies in the fact that the two tasks within this dataset are highly similar to one another, with the only difference being the memory test section (For more information, refer to the dataset description section 2.1). Past neuroscience studies have yet to look into whether the neural pathways throughout the act of temporarily maintaining or storing perceptual information are different given different task strategies. We are interested in using modern machine learning methods to see if the neural correlates involved throughout the duration of the two memory tasks can be clearly separated and classified. We hypothesize that if the model accuracy is high, then it suggests that the neural circuitry behind the two tasks are different enough to be discriminated.

We aim to compare popular MVPA models such as kNN, Logistic Regression, and Naive Bayes to our baseline model of linear SVMs. In our quarter-one project, we took working memory task fMRI data and identified regions of significant activation in response to the various tasks. This was done by performing a voxel-wise linear regression on a dataset containing brain scans over time for each subject. Continuing forward, we will refer to this process as performing a first-level analysis of the data. Through these first-level analyses, we found that there are various differences in the activation depending on the corresponding task. This begs the question: are these differences in activation significant enough that we can distinguish between the tasks from the resulting fMRI data alone? Our supervised models are trained on the beta weights generated from first-level analysis for a full brain image in all runs (where a run is one trial of the task). This allows for easier interpretation as we can know which regions of the brain are used for each task. These models will then be evaluated through various metrics, such as accuracy, precision, and recall. We also explore the effect of confounds, such as noise within the white matter, and movements during fMRI scans, on model accuracy, as it may contain important information about the subjects ability to do each task.

Additionally, through training and comparing various machine learning models, we can further strengthen or improve the current literature on the optimal model for task fMRI classification with MVPA. Furthermore, we aim to focus more on increasing the interpretability of these models to not only aid other neuroscientists in understanding the black box of models, but also provide data scientists with more biologically accurate methods of performing MVPA on other task fMRI brain imaging data.

2 Methods

2.1 Dataset Description

The dataset in our project was sourced from the paper (Kiyonaga, Scimeca and D'Esposito 2018). Subjects were asked to perform two different visual working memory tasks, and they would alternate between each task for 4 runs each for a total of one hour in a functional magnetic resonance imaging (fMRI) machine. The two tasks were fairly similar but for the memory recall part. Subjects were asked to memorize three differently colored patches, then after a delay they were cued to recall the color of one of the squares by using a color wheel (task 'colorwheel') or performing a binary response (task 'samedifferent'). Due to the different levels of abstraction for each task, it is hypothesized that they may be using different areas of the brain to perform a memory task. However, whether the neural circuitry is distinguishable enough from each other is unknown.

In our model training, we selected 29 subjects who had little to no problems during their brain scan. Each subject had 4 runs for both tasks, making it about 116 runs total for each task. However, a few subjects had problems with their preprocessing. For instance, a few subjects had a missing events file, rendering that data unusable. The final total number of runs per task is about 95 runs each. The raw BIDS formatted data was preprocessed with fMRIprep pipeline. The specific methods used can be found in Appendix A.2, which is sourced directly from the preprocessing boilerplate.

2.2 First-Level Analysis

To increase mechanistic interpretability, we chose to extract the significance of every weight within a subject's brain through the analysis of beta weights. We performed a first-level analysis on individual participants by fitting a General Linear Model (GLM) for each run within two visual tasks. Our function took in information on the subject ID and task type to calculate the design matrix with the subject's events file and brain imaging data. The events file stored information about the onset offset of cues and probes within the experiment. For the first level analysis model, we selected spm and its time derivatives for the hemodynamic response function, with a repetition time of 2 seconds. Moreover, we smoothed the data with a Gaussian kernel width of 6 millimeters and used all but one of the available CPU cores to compute each first-level analysis.

After performing the first level analysis, the files containing the beta weights were then stored on our DSMLP server to allow for easy and efficient access. Once this was done, we then extracted the files directly to train our model. However, in the future, we would like to experiment with further data processing techniques in the form of dimensionality reduction. The number of features within each sample would be reduced either through principal component analysis (PCA) or by compressing related groups of voxels into clusters. This would reduce the size of each sample, potentially reducing the amount of overfitting (from the large amount of features per sample) and improving general efficiency.

2.3 Model Building

For each individual run in our dataset, our 'X' feature vector contained 902629 values and our 'y' vector contained the task type for each run. To build the model, different approaches were considered for building the training and test sets. One approach involved splitting the dataset into 3 groups:

a training set containing 60% of the sample size, a validation set containing 20%, and a test set containing 20%. To achieve this, scikit-learn's train test split module was used twice. The first usage was to split the data into two groups consisting of 80% and 20% of the total data. Following this, the larger set was split once again into two groups containing 60% and 20% of the total data. The purpose of each set was as follows:

- Training set: used to train the separate models and hyperparameters
- Validation set: used to evaluate which set of hyperparameters produces the best model
- Testing set: used for the final evaluation of the best-performing model

Another approach was considered for splitting the data into train and test sets. This approach involved organizing each set by each subject's run number. As stated previously, each subject performed four runs under each task. The first three of these runs are used for the training set while the fourth would be used for the test set.

To determine which classifier should be used for the final product, several different models were explored. These models were naive Bayes, logistic regression, k-nearest neighbors, DecisionTree Classifier, and RandomForestClassifier. Each of these models are then evaluated and compared with a baseline SVM model, which was generated using the 'LIBSVM' software (a library for support vector machines). To evaluate the performance of each model, a confusion matrix was generated, displaying the number of true positives, true negatives, false positives and false negatives. In order for the classifier to have the most optimal performance, the number of true positives and true negatives would be maximized, and the number of false positives and false negatives should be minimized. The train and test accuracies for each model were also calculated, showing how well the model performs on the data it was trained on, along with how well the model performs on unseen data. Precision and recall metrics were also used to evaluate the models. n unseen data. Precision and recall metrics were also used to evaluate the models. Precision refers to how accurate a model is when it predicts a given class, for example if the precision for the 'color wheel' task is 0.85, that means that 85% of the time that the model predicts 'color wheel', it's correct. Recall on the other hand refers to how many instances the model correctly identified. For example, if the recall for the 'colorwheel' task is 0.75, that means the model correctly identifies 75% of all true 'colorwheel' cases.

3 Results

4 Discussion

5 Conclusion

6 Contributions

Judel - started a paper draft with bullet points, wrote the Abstract and Methods section. Performed ⅓ of first-level analysis, and explored naive bayes models, worked with TA to help resolve DSMLP storage issues

Jennifer - wrote the Introduction, the Dataset Description, and the first-level analysis section in the Methods. Performed ⅓ of the first-level analysis, and explored SVM models, worked with TA Gabriel on data preprocessing.

Sahana - worked on the Methods section, performed ⅓ of first-level analysis, worked on feature vector generation, trained several different baseline models, experimented with different methods for training logistic regression.

7 Appendix

References

Abraham, Alexandre, Fabian Pedregosa, Michael Eickenberg, Philippe Gervais, Andreas Mueller, Jean Kossaifi, Alexandre Gramfort, Bertrand Thirion, and Gael Varoquaux. 2014. "Machine learning for neuroimaging with scikit-learn." *Frontiers in Neuroinformatics* 8. [Link]

Aglieri, Virginia, Bastien Cagna, Lionel Velly, Sylvain Takerkart, and Pascal Belin. 2021.

"FMRI-based identity classification accuracy in left temporal and frontal regions predicts speaker recognition performance." *Scientific Reports* 11. [Link]

Avants, B.B., C.L. Epstein, M. Grossman, and J.C. Gee. 2008. "Symmetric diffeomorphic image registration with cross-correlation: Evaluating automated labeling of elderly and neurodegenerative brain." *Medical Image Analysis* 12 (1): 26–41. [Link]

Behzadi, Yashar, Khaled Restom, Joy Liau, and Thomas T. Liu. 2007. "A component based noise correction method (CompCor) for BOLD and perfusion based fMRI." *NeuroImage* 37 (1): 90–101. [Link]

Ciric, R., William H. Thompson, R. Lorenz, M. Goncalves, E. MacNicol, C. J. Markiewicz, Y. O. Halchenko, S. S. Ghosh, K. J. Gorgolewski, R. A. Poldrack, and O. Esteban. 2022. "TemplateFlow: FAIR-sharing of multi-scale, multi-species brain models." *Nature Methods* 19: 1568–1571. [Link]

Esteban, Oscar, Ross Blair, Christopher J. Markiewicz, Shoshana L. Berleant, Craig Moodie, Feilong Ma, Ayse Ilkay Isik, Asier Erramuzpe, Mathias Kent, James D. and-Goncalves, Elizabeth DuPre, Kevin R. Sitek, Daniel E. P. Gomez, Daniel J. Lurie, Zhifang Ye, Russell A. Poldrack, and Krzysztof J. Gorgolewski. 2018. "fMRIPrep." *Software*. [Link]

Esteban, Oscar, Christopher Markiewicz, Ross W Blair, Craig Moodie, Ayse Ilkay Isik, Asier Erramuzpe Aliaga, James Kent, Mathias Goncalves, Elizabeth DuPre, Madeleine Snyder, Hiroyuki Oya, Satrajit Ghosh, Jessey Wright, Joke Durnez, Russell Poldrack, and Krzysztof Jacek Gorgolewski. 2019. "fMRIPrep: a robust preprocessing pipeline for functional MRI." *Nature Methods* 16: 111–116. [Link]

Evans, AC, AL Janke, DL Collins, and S Baillet. 2012. "Brain templates and atlases." *NeuroImage* 62 (2): 911–922. [Link]

Fonov, VS, AC Evans, RC McKinstry, CR Almli, and DL Collins. 2009. "Unbiased nonlinear average age-appropriate brain templates from birth to adulthood." *NeuroImage* 47, Supplement 1, p. S102. [Link]

Gorgolewski, K., C. D. Burns, C. Madison, D. Clark, Y. O. Halchenko, M. L. Waskom, and S. Ghosh. 2011. "Nipype: a flexible, lightweight and extensible neuroimaging data processing framework in Python." *Frontiers in Neuroinformatics* 5, p. 13. [Link]

**Gorgolewski, Krzysztof J., Oscar Esteban, Christopher J. Markiewicz, Erik Ziegler, David Gage Ellis, Michael Philipp Notter, Dorota Jarecka, Hans Johnson, Christopher Burns, Alexandre Manhães-Savio, Carlo Hamalainen, Benjamin Yvernault, Taylor Salo, Kesshi Jordan, Mathias Goncalves, Michael Waskom, Daniel Clark, Jason Wong, Fred Loney, Marc Modat, Blake E Dewey, Cindee Madison, Matteo Visconti di Oleggio Castello, Michael G. Clark, Michael Dayan, Dav Clark, Anisha Keshavan, Basile Pinsard, Alexandre Gramfort, Shoshana Berleant, Dylan M. Nielson, Salma Bougacha, Gael Varoquaux, Ben Cipollini, Ross Markello, Ariel Rokem, Brendan Moloney, Yaroslav O. Halchenko, Demian Wassermann, Michael Hanke, Christian Horea, Jakub Kaczmarzyk, Gilles de Hollander, Elizabeth DuPre, Ashley Gillman, David Mordom, Colin Buchanan, Rosalia Tungaraza, Wolfgang M. Pauli, Shariq

Iqbal, Sharad Sikka, Matteo Mancini, Yannick Schwartz, Ian B. Malone, Mathieu Dubois, Caroline Frohlich, David Welch, Jessica Forbes, James Kent, Aimi Watanabe, Chad Cumba, Julia M. Huntenburg, Erik Kastman, B. Nolan Nichols, Arman Eshaghi, Daniel Ginsburg, Alexander Schaefer, Benjamin Acland, Steven Giavasis, Jens Kleesiek, Drew Erickson, René Küttner, Christian Haselgrove, Carlos Correa, Ali Ghayoor, Franz Liem, Jarrod Millman, Daniel Haehn, Jeff Lai, Dale Zhou, Ross Blair, Tristan Glatard, Mandy Renfro, Siqi Liu, Ari E. Kahn, Fernando Pérez-García, William Triplett, Leonie Lampe, Jörg Stadler, Xiang-Zhen Kong, Michael Hallquist, Andrey Chetverikov, John Salvatore, Anne Park, Russell Poldrack, R. Cameron Craddock, Souheil Inati, Oliver Hinds, Gavin Cooper, L. Nathan Perkins, Ana Marina, Aaron Mattfeld, Maxime Noel, Lukas Snoek, K Matsubara, Brian Cheung, Simon Rothmei, Sebastian Urchs, Joke Durnez, Fred Mertz, Daniel Geisler, Andrew Floren, Stephan Gerhard, Paul Sharp, Miguel Molina-Romero, Alejandro Weinstein, William Broderick, Victor Saase, Sami Kristian Andberg, Robbert Harms, Kai Schlamp, Jaime Arias, Dimitri Papadopoulos Orfanos, Claire Tarbert, Arielle Tambini, Alejandro De La Vega, Thomas Nickson, Matthew Brett, Marcel Falkiewicz, Kornelius Podranski, Janosch Linkersdörfer, Guillaume Flandin, Eduard Ort, Dmitry Shachnev, Daniel McNamee, Andrew Davison, Jan Varada, Isaac Schwabacher, John Pellman, Martin Perez-Guevara, Ranjeet Khanuja, Nicolas Pannetier, Conor McDermottroe, and Satrajit Ghosh. 2018. "Nipype." *Software*. [Link]

Greve, Douglas N, and Bruce Fischl. 2009. "Accurate and robust brain image alignment using boundary-based registration." *NeuroImage* 48 (1): 63–72. [Link]

van 't Hof, Sophie R, Lukas Van Oudenhove, Erick Janssen, Sanja Klein, Marianne C Reddan, Philip A Kragel, Rudolf Stark, and Tor D Wager. 2021. "The brain activation-based sexual image classifier (BASIC): a sensitive and specific fMRI activity pattern for sexual image processing." *Cerebral Cortex* 32 (14): 3014–3030. [Link]

Jenkinson, Mark, Peter Bannister, Michael Brady, and Stephen Smith. 2002. "Improved Optimization for the Robust and Accurate Linear Registration and Motion Correction of Brain Images." *NeuroImage* 17 (2): 825–841. [Link]

Jenkinson, Mark, and Stephen Smith. 2001. "A global optimisation method for robust affine registration of brain images." *Medical Image Analysis* 5 (2): 143–156. [Link]

Kiyonaga, Anastasia, Jason Scimeca, and Mark D'Esposito. 2018. "Dissociating the causal roles of frontal and parietal cortex in working memory capacity [Registered Report Stage 1 - Protocol]." *Springer Nature*. [Link]

Mahmoudi, Abdelhak, Sylvain Takerkart, Fakhita Regragui, Driss Boussaoud, and Andrea Brovelli. 2012. "Multivoxel Pattern Analysis for fMRI Data: A Review." *Computational and Mathematical Methods in Medicine* 2012 (1), p. 961257. [Link]

Patriat, Rémi, Richard C. Reynolds, and Rasmus M. Birn. 2017. "An improved model of motion-related signal changes in fMRI." *NeuroImage* 144, Part A: 74–82. [Link]

Pereira, Francisco, Tom Mitchell, and Matthew Botvinick. 2009. "Machine learning classifiers and fMRI: A tutorial overview." *NeuroImage* 45 (1, Supplement 1): S199–S209.

[Link]

Power, Jonathan D., Anish Mitra, Timothy O. Laumann, Abraham Z. Snyder, Bradley L. Schlaggar, and Steven E. Petersen. 2014. "Methods to detect, characterize, and remove motion artifact in resting state fMRI." *NeuroImage* 84 (Supplement C): 320–341. [Link]

Satterthwaite, Theodore D., Mark A. Elliott, Raphael T. Gerraty, Kosha Ruparel, James Loughead, Monica E. Calkins, Simon B. Eickhoff, Hakon Hakonarson, Ruben C. Gur, Raquel E. Gur, and Daniel H. Wolf. 2013. "An improved framework for confound regression and filtering for control of motion artifact in the preprocessing of resting-state functional connectivity data." *NeuroImage* 64 (1): 240–256. [Link]

Tustison, N. J., B. B. Avants, P. A. Cook, Y. Zheng, A. Egan, P. A. Yushkevich, and J. C. Gee. 2010. "N4ITK: Improved N3 Bias Correction." *IEEE Transactions on Medical Imaging* 29 (6): 1310–1320. [Link]

Zhang, Y., M. Brady, and S. Smith. 2001. "Segmentation of brain MR images through a hidden Markov random field model and the expectation-maximization algorithm." *IEEE Transactions on Medical Imaging* 20 (1): 45–57. [Link]

Appendices

A.1 Quarter 2 Project Proposal

Broad Problem Statement

Functional MRI (fMRI) allows researchers to map patterns of brain activity to specific thoughts or experiences, offering valuable insights into how the brain encodes and processes information. Working memory is the brain's ability to temporarily store and manipulate information while doing a task, and it is crucial for tasks such as reasoning, decision-making, and learning. One leading theory, the sensorimotor recruitment theory, proposes that working memory relies on the same brain regions responsible for perceiving the information. For example, visual details would be stored in the visual cortex, while abstract information would be maintained in high-level brain regions in the front.

To test whether this theory applies universally across task types, we propose developing a model to classify specific working memory tasks based on fMRI activity. By furthering our understanding of how and where the brain stores information, this work could provide groundbreaking insights into Working Memory and contribute to the growing potential of neuroscience to further understand the relationship between brain activity and function. For future work, the model can be used to further understand whether the sensorimotor recruitment theory is applicable to all working memory tasks that have brain imaging.

Narrow Problem Statement

Previous neuroimaging studies on visual Working Memory maintenance sensitivity to task type do not always target the same regions to analyze (for instance, looking into Early Visual Cortex versus intraparietal cortex for low-level, fine detail processing). Moreover, even when studies focus on specific regions (i.e. intraparietal for low-level and prefrontal for high-level), the exact areas are not clearly defined and can vary or overlap across studies. Thus, by delineating an exact voxel cluster of significance, we aim to deploy a computational model that can predict the visual Working Memory task type (high visual detail or abstract semantic) given a fMRI brain imaging.

In our Quarter 1 project, we mainly focused on locating those clusters for one given task (Change Detection, a task that uses more abstract, semantic demands). We want to expand on simply locating a certain brain region associated with some task for a single subject, and train a supervised neural network model to identify whether we can predict task type based on BOLD signals in fMRI data. We plan to run the first level analysis on multiple subject data (as we did in Quarter 1) to get the weights for within-subject variability, then run our neural network on extracted features. We also plan on using the first three runs of each experiment as training data, and the last run for test data. As the two tasks in this experiment are fairly similar, we wonder if their neural circuitry can be discerned and classified. If the model performance is high, this may suggest that there are fundamentally different mechanisms and neural circuits. However, if the model performance is not better than chance, this suggests that the two tasks use similar circuitry and may lead to more discussion on whether fine-detail tasks versus abstract tasks inherently involve similar circuitry, but have different feedforward and feedback mechanisms.

Statement of primary output

For our quarter two project, we plan on creating a classification model that takes in brain imaging data (fMRI) and uses it to predict what task was done in order to produce that data. With this, we plan on being able to establish a strong relationship between the fMRI data and the task. To strongly show this, an ideal form of output would be one that easily supports visualization and interactivity. Therefore, we will create a website to represent our project. On the website, the user will be able to directly interact with our model, by controlling what data to use and classify. Being able to interact with a model, rather than simply reading about its results will strengthen the relation shown between fMRI data and its corresponding task classification.

A.2 fMRI Prep Boilerplate

Results included in this manuscript come from preprocessing performed using *fMRIPrep* 24.1.1 (Esteban et al. (2019); Esteban et al. (2018); RRID:SCR_016216), which is based on *Nipype* 1.8.6 (Gorgolewski et al. (2011); Gorgolewski et al. (2018); RRID:SCR_002502).

Anatomical data preprocessing A total of 1 T1-weighted (T1w) images were found within the input BIDS dataset. The T1w image was corrected for intensity non-uniformity (INU) with `N4BiasFieldCorrection` (Tustison et al. 2010), distributed with ANTs 2.5.3 (Avants et al. 2008, RRID:SCR_004757), and used as T1w-reference throughout the workflow. The T1w-reference was then skull-stripped with a *Nipype* implementation of the `antsBrainExtraction.sh` workflow (from ANTs), using OASIS30ANTs as target template. Brain tissue segmentation of cerebrospinal fluid (CSF), white-matter (WM) and gray-matter (GM) was performed on the brain-extracted T1w using `fast` (FSL (version unknown), RRID:SCR_002823, Zhang, Brady and Smith 2001). Volume-based spatial normalization to two standard spaces (MNI152NLin6Asym, MNI152NLin2009cAsym) was performed through nonlinear registration with `antsRegistration` (ANTs 2.5.3), using brain-extracted versions of both T1w reference and the T1w template. The following templates were were selected for spatial normalization and accessed with *TemplateFlow* (24.2.0, Ciric et al. 2022): *FSL's MNI ICBM 152 non-linear 6th Generation Asymmetric Average Brain Stereotaxic Registration Model* [Evans et al. (2012), RRID:SCR_002823; TemplateFlow ID: MNI152NLin6Asym], *ICBM 152 Nonlinear Asymmetrical template version 2009c* [Fonov et al. (2009), RRID:SCR_008796; TemplateFlow ID: MNI152NLin2009cAsym].

Functional data preprocessing For each of the 1 BOLD runs found per subject (across all tasks and sessions), the following preprocessing was performed. First, a reference volume was generated, using a custom methodology of *fMRIPrep*, for use in head motion correction. Head-motion parameters with respect to the BOLD reference (transformation matrices, and six corresponding rotation and translation parameters) are estimated before any spatiotemporal filtering using `mcflirt` (FSL , Jenkinson et al. 2002). The BOLD reference was then co-registered to the T1w reference using `mri_coreg` (FreeSurfer) followed by `flirt` (FSL , Jenkinson and Smith 2001) with the boundary-based registration (Greve and Fischl 2009) cost-function. Co-registration was configured with six degrees of freedom. Several confounding time-series were calculated based on the *preprocessed BOLD*: framewise displacement (FD), DVARS and three region-wise global signals. FD was computed using two formulations following Power (absolute sum of relative motions, Power et al. (2014)) and Jenkinson (relative root mean square displacement between affines, Jenkinson et al. (2002)). FD and DVARS are calculated for each functional run, both using their implementations in *Nipype* (following the definitions by Power et al. 2014). The three global signals are extracted within the CSF, the WM, and the whole-brain masks. Additionally, a set of physiological regressors were extracted to allow for component-based noise correction (*CompCor*, Behzadi et al. 2007). Principal components are estimated after high-pass filtering the *preprocessed BOLD* time-series (using a discrete cosine filter with 128s cut-off) for the two *CompCor* variants: temporal (tCompCor) and anatomical (aCompCor). tCompCor components are then calculated from the top 2% variable voxels within the brain mask. For aCompCor, three probabilistic masks (CSF, WM and combined CSF+WM) are generated in anatomical space. The implementation differs from that of Behzadi et al. in that instead of eroding the masks by 2 pixels on BOLD space, a mask of pixels that likely contain a volume fraction of GM is subtracted from the aCompCor masks. This mask is obtained by thresholding the corresponding partial volume map at 0.05, and it ensures components are not extracted from voxels containing a minimal fraction of GM. Finally, these masks are resampled into BOLD space and binarized by thresholding at 0.99 (as in the original implementation). Components are also calculated separately within the WM and CSF masks. For each CompCor decomposition, the k components with the largest singular values are retained, such that the retained components' time series are sufficient to explain 50 percent of variance across the nuisance mask (CSF, WM, combined, or temporal). The remaining components are dropped from consideration. The head-motion estimates calculated in the correction step were also placed within the corresponding confounds file. The confound time series derived from head motion estimates and global signals were expanded with the inclusion of temporal derivatives and quadratic terms for each (Satterthwaite et al. 2013). Frames that exceeded a threshold of 0.5 mm FD or 1.5 standardized DVARS were annotated as motion outliers. Additional nuisance timeseries are calculated by means of principal components analysis of the signal found within a thin band (*crown*) of voxels around the edge of the brain, as proposed by (Patriat, Reynolds and Birn 2017). All resamplings can be performed with *a single interpolation step* by composing all the pertinent transformations (i.e. head-motion transform matrices, susceptibility distortion correction when available, and co-registrations to anatomical and output spaces). Gridded (volumetric) resamplings were performed using `nitransforms`, configured with cubic B-spline interpolation.

Many internal operations of *fMRIPrep* use *Nilearn* 0.10.4 (Abraham et al. 2014, RRID:SCR_001362), mostly within the functional processing workflow. For more details of the pipeline, see the section corresponding to workflows in *fMRIPrep*'s documentation.

A.2.1 Copyright Waiver