Abstract—Graph Signal Processing (GSP) is a promising method to analyze high-dimensional neuroimaging datasets while taking into account both the spatial and functional dependencies between brain signals. In the present work, we apply GSP with dimensionality reduction techniques to decode brain activity from real and simulated fMRI datasets. We introduce seven graphs obtained from a) geometric structure and/or b) functional connectivity between brain areas at rest and compare them when performing dimension reduction for classification. We show that mixed graphs using both a) and b) offer the best performance. We also show that graph sampling methods works better than classical dimension reduction methods including Principal Component Analysis (PCA) and Independent Component Analysis (ICA).

Index Terms—Neuroimaging, fMRI, Graph Signal Processing, Classification, Dimensionality Reduction

I. INTRODUCTION

Analyzing neuroimaging data is a major challenge due to several intrinsic limitations of neuroimaging datasets. For instance, neuroimaging data have a large number of dimensions (e.g. several hundred thousand voxels every two seconds in MRI recordings) and only a few observations per subject. In addition, imaging methods are by themselves sensitive to various noise sources originating from physiological artifacts (e.g. heart beats, eye of head movements), intrinsic differences in the population (inter or intra subject variability), or the imaging techniques themselves (e.g. magnetic field bias in MRI).

While many discoveries in neuroscience have been made using massively univariate statistics or signal processing techniques such as time-series or time-frequency analysis, there has been a recent paradigm shift towards the application of multivariate analysis and machine learning to “decode” brain functions [1]. The relevance of considering multivariate dependencies in brain signals is further justified by the rapidly growing literature on the application of network science and graph theory for studying brain connectivity [2]. Surprisingly, few analysis methods take into account both the multivariate aspect and connectivity features of the brain, such as structural connectivity (white matter tracts), functional connectivity (i.e. statistical dependencies between signals over time) or simply geometrical relationships between observations.

A promising avenue to address this important gap resides in Graph Signal Processing (GSP) [3]. GSP is an emerging subfield of signal processing whose objective is to take into account the underlying graphical structure of multivariate data, in order to generalize common signal processing techniques (such as filtering, deconvolution, denoising, or time-frequency analysis) to irregular graph/network domains. GSP is built on the idea that the eigenvectors of the graph Laplacian are analogous to Fourier modes, and can thus be used to provide a spectral representation of signals defined on a graph, through the so-called Graph Fourier Transform operator (GFT). In this paper, we evaluate the application of GSP for the analysis of neuroimaging data. More specifically, we assess whether GSP can lead to more accurate supervised classification, as well as whether GSP can be used for dimensionality reduction. Instead of considering each observation independently, GSP can incorporate geometrical and statistical dependencies between observations.

Methods for GSP are still under active research, with applications such as the analysis of temperature sensor data [4] or epidemiology [5]. Also, GSP-based methods have recently been applied to neuroimaging using fMRI data [6] and EEG/MEG data [7], [8], [9]. Huang and collaborators [6] have applied graph frequency analysis to fMRI data in order to observe how brain activity changes during a learning task. Graph frequency analysis allows to study spatial variation of the signal, with low graph frequencies representing smooth and regular variations across brain network, whereas high graph frequencies represent important spatial variations, described by the authors as randomness. After decomposing fMRI data into graph frequency bands, Huang et al. observed that during learning, low graph frequencies correlate with the learning rate at the start of the training, while higher frequencies correlate with participants’ familiarity with the task.

Other studies have applied GSP techniques to EEG/MEG signals, for instance for noise suppression [8], dimensionality reduction [7], [8], [10] and classification [7], [10]. The authors of the latter article compared classification accuracy when
building graphs using different connectivity measures, and showed that projecting the data into the eigenspace associated with graph strongest eigenvalues to reduce dimensions leads to better classification results than Principal component analysis (PCA) and linear discriminant analysis (LDA) [7]. In a second study [10], they also showed that GSP dimensionality reduction techniques leads to more interpretable classifier weights. While these studies provide promising results suggesting a positive impact of GSP to neuroimaging data analysis, an important drawback is the lack of geometrical information in the construction of the graph edges.

In the present paper, we aim to evaluate whether GSP can positively impact classification and dimensionality reduction in functional MRI (fMRI) datasets. First, we propose to study the influence of different types of graphs on brain signal classification, taking into account either geometrical or statistical dependencies between voxels, or both. Second, we use Graph Fourier Transform to decompose brain signals on the graph fourier components. Finally, we compare several methods for dimensionality reduction of the decomposed signals (namely, graph sampling or statistical selection), and compare the performance of these methods to state-of-the-art reduction techniques such as PCA and ICA. We perform our experiments on two datasets, a simulated fMRI dataset and a real open source fMRI dataset [11].

II. METHODS

A. Graph Signal Processing

Throughout this paper, we consider a weighted graph $\mathcal{G}$ over a set $\mathcal{V}$ of vertices indexed from 1 to $N$ ($\mathcal{V} = \{v_1, \ldots, v_N\}$). The graph adjacency matrix is denoted $W$ such that $W_{ij} \in \mathbb{R}^+$ encodes a similarity between vertices $v_i$ and $v_j$. We consider symmetric (\forall i,j : W_{ij} = W_{ji}) graphs. In the following sections, we introduce several graphs constructed from geometrical and/or statistical properties of the fMRI signals.

Being symmetric and real-valued, $W$ can be decomposed as $W = F\Lambda F^\top$, where $F$ is an orthonormal matrix, $F^\top$ is its transposed matrix, and $\Lambda$ is the diagonal matrix of eigenvalues, in descending order. Note that equivalently, some authors introduce $F$ on the Laplacian matrix $L = F(I-\Lambda)F^\top$, where $I$ is the identity matrix of size $N$.

A signal over $\mathcal{G}$ is a vector $x \in \mathbb{R}^N$ interpreted as scalars observed on each vertex. Its Graph Fourier Transform (GFT) is given by $\hat{x} = F^\top x$. The first coordinates of $\hat{x}$, associated with the lower eigenvalues in $\Lambda$, are called low frequencies (LF) and its last are called high frequencies (HF).

As far as our application case is concerned, vertices correspond to regions of interest in the brain. We denote by $X$ a matrix of all measures obtained during rest periods (containing $M$ columns and $N$ lines) obtained from all subjects. These measures are distinct from the one we aim to classify, and serve as a baseline that incorporate average statistical dependencies which are used to build the graphs. We denote by $X_m \in \mathbb{R}^N$ the $m$-th observation and by $X^i \in \mathbb{R}^M$ the $i$-th line of $X$ corresponding to all measures at vertex $v_i$.

B. fMRI dataset

We use an open source fMRI dataset from Haxby et al. 2001 [11]. This dataset consists of fMRI scans of 6 subjects during a visual stimulation experiment. For each subject, 1452 volumes of size $40 \times 64 \times 64$ (voxel size $3.5 \times 3.75 \times 3.75$ mm) were recorded every 2.5 seconds. The experiment is a block design with 12 sessions in which 8 types of stimuli (human faces, houses, cats, chairs, scissors, shoes, bottles and scrambled images) were presented during blocks of 24 seconds separated by 12 seconds of rest. Further details on the experiment are described in [11]. Volumes were normalized in MNI space. We restrict our analysis to two contrasts: Face vs House and Cat vs Face.

C. Simulated fMRI data

We simulate fMRI datasets of size $53 \times 63 \times 46 \times 421$ (corresponding to 3 mm$^3$ isotropic voxels, and a volume repetition time of 2 seconds) with NeuRosim [12], an R-software package. The activation of 6 areas are simulated depending on two conditions. The areas are modeled as spheres whose center corresponded to the MNI coordinates of brain areas known to be involved in visual processing. We use a baseline obtained from the Haxby dataset (the averaged data from the rest conditions of subject 2). The experimental design is a block design with 12 blocks of 22 seconds per condition, separated by 10 seconds of rest. A one minute rest period is also included at half the experiment. The haemodynamic response is simulated using the Balloon model with the parameters described in [13]. We simulate noise as a mixture of Rician system noise, temporal noise of order 1, spatial noise, low-frequency drift, physiological noise (due to heart and respiration rates) and task-related noise, as described in [12].

A total of 90 “subjects” are simulated by randomly varying the coordinates of the spheres, the activation magnitude of each area, and the signal-to-noise ratio (from 1.4 to 4.8). We calculate 20 simulations for each “subject”, resulting in 1800 simulations in total. We discarded 4 simulated “subjects” because their classification performances between the two conditions was at chance level (below 55% of accuracy using a SVM classifier as described in the next section).

D. Data preprocessing

Both fMRI datasets are analyzed with nilearn and scikit-learn [14]. All data is normalized in MNI space and parcellated into 444 symmetrical regions of interest using the BASC atlas [15]. We compute the coordinates of the baricenters of the ROIs to obtain geometrical relationships between ROIs. The fMRI data are high-pass filtered at 0.01Hz, and no spatial smoothing is applied. The data used for classification is the raw BOLD signal of the 444 regions: for Haxby, 9 volumes in each block are used in the analysis resulting in 108 volumes per condition. For the simulated data, the first volume of each block is removed to account for the delayed haemodynamic response, therefore 10 volumes in each block are used, resulting in 120 volumes per condition.
E. Graph construction

We consider seven different graphs for each subject/simulation. Two graphs model the geometric structure of the brain (Full and Geometric) by computing a Gaussian kernel (with empirically determined parameters) of the Euclidean distance between the barycenters of the 444 brain areas. The Full graph is fully connected and the Geometric only connects close brain areas (distance inferior to a radius, empirically determined), the weights of edges between distant brain areas being set to 0. Three other graphs model the functional connectivity at rest between the brain areas, using different connectivity measures: absolute values for Correlation and Covariance, and the Kalofolias method to infer the graph Laplacian matrix $L = I - W$, assuming smoothness of the observed graph signals. Finally, two other graphs are built, modeling both the structure and connectivity of the brain: the Semilocal graph connects only close brain areas (as the Geometric graph) but its weights correspond to the covariance measures sum up the graphs we consider, where $d$ is a product of distance and connectivity. The following equations sum up the graphs we consider, where $d(v_i, v_j)$ denotes the Euclidean distance between vertices $v_i$ and $v_j$ according to their spatial coordinates, $\sigma, \alpha, \beta$ and $\theta$ are empirically determined parameters, $X$ is the matrix of all measurements and $Y$ is an optimization parameter with same dimensions as $X$, and $L$ denotes the set of Laplacians of graphs (positive diagonal and nonpositive nondiagonal elements):

**Geometric graphs:**

- **Full:** $W_{i,j} = \exp\left(-\frac{d(v_i, v_j)^2}{2\sigma}\right)$
- **Geometric:** $W_{i,j} = \begin{cases} \exp\left(-\frac{d(v_i, v_j)^2}{2\sigma}\right), & \text{if } d(v_i, v_j) < \alpha \\ 0, & \text{otherwise} \end{cases}$

**Functional graphs:**

- **Absolute correlation:** $W_{i,j} = |\text{corr}(X^i, X^j)|$
- **Absolute covariance:** $W_{i,j} = |\text{cov}(X^i, X^j)|$
- **Kalofolias:** $\arg\min_{L \in L, Y} \sum_{m=1}^{M} \|X_m - Y_m\|_2^2 + \beta Y_m^TLY_m$

**Mixed graphs:**

- **Semilocal:** $W_{i,j} = \begin{cases} |\text{cov}(X^i, X^j)|, & \text{if } d(v_i, v_j) < \alpha \\ 0, & \text{otherwise} \end{cases}$
- **Fundis:** $W_{i,j} = \exp\left(-\frac{(1-|\text{corr}(X^i, X^j)|)^2}{2\sigma} - \frac{d(v_i, v_j)^2}{2\sigma}\right)$

We use the Laplacian matrices of these graphs to perform GFT of the acquired signals, but also to reduce dimension using graph sampling methods, as explained in the following paragraphs. All GSP operations were done using the Matlab and Python versions of the GSP toolbox.

F. Dimensionality reduction

We test different methods of dimensionality reduction, in particular we compare graph sampling to other graph-free methods: principal component analysis (PCA), independent component analysis (ICA), and selection of the $K$ best components using analysis of variance (ANOVA).

Graph sampling is a method adapted from [18] to select the nodes where the signal energy is the most concentrated. To do so, we compute the graph weighted coherence for a frequency band of interest ($f_{\text{min}}, f_{\text{max}}$) and extract the $K$ vertices achieving maximum scores. The graph weighted coherence for vertex $v_i$ is defined as $\sum_{k=f_{\text{min}}}^{f_{\text{max}}} F_{ik}^2$. We restrict our analysis to either only low frequencies (LF) (below $N/2$) or high frequencies (HF) (above $N/2$).

We also apply a method to perform graph frequencies sampling [7], where we select $K$ eigenvalues (HF/LF/ANOVA), then project the signals to keep only the corresponding components. We compare the results for $K = 50$ and $K = 200$ components.

G. Classification

Classification is performed to disentangle brain signals originating from different conditions using Support Vector Machine (SVM). To avoid excessive over-fitting and given the block design, cross-validation is performed across different sessions, leaving two sessions out: 16% of the data is used as test data, the remaining as training. Classification is performed on the fMRI data (all data or reduced data: PCA/ICA/ANOVA/Graph Sampling) and on the signal projected in the graph Fourier domain using GFT (All features, or reduced data (HF, LF and ANOVA)). Standardization, Dimension reduction (for PCA, ICA and ANOVA when applied) and SVM are all performed within the cross-validation procedure. We report cross-validated accuracy scores.

For the simulated fMRI data, classification is performed for each simulation. We average the results of 20 simulations per “subject”, resulting in one value for each. The classification of the full brain fMRI data serve as reference, and the difference $\text{Accuracy}_{\text{Method}} - \text{Accuracy}_{\text{AllfMRI}}$ is computed to measure the gain or the loss of accuracy of a reduction method.

H. Statistics

We perform a statistical analysis of accuracy scores across methods in order to estimate the significance of accuracy gains/losses. Non-parametric Friedman tests for repeated measures are computed to identify differences between the conditions and Wilcoxon tests are used as post-hoc tests (Bonferroni adjusted for multiple comparisons). For the simulated dataset, we test if the difficulty level of the classification influence the accuracy by computing a Mann-Whitney U test (corrected for multiple comparisons) on the difference $\text{Accuracy}_{\text{Method}} - \text{Accuracy}_{\text{AllfMRI}}$. For the Haxby dataset, the same statistical tests are performed for exploratory purposes, however they should be interpreted with caution since the sample size is small ($s = 6 + 6$).

III. RESULTS

We first present classification results for the raw data using all 444 areas, to define a reference for further comparisons. For the Haxby dataset, Face vs. House classification achieves on average an accuracy of 88.4% ± 4.4, and Cat vs. Face achieves 69.8% ± 6.8. For the simulated data, accuracy ranges
from 55.9% to 95.9%. In order to compare our results with the Haxby dataset, two groups of simulated “subjects” are determined: Easy (accuracy > 80%) comprised of 40 simulated subjects (average 89.8 % ± 4.0), and Difficult (accuracy between 55% and 80%) comprised of 46 simulated subjects (average 67.0 % ± 6.4).

### A. Graph Fourier transform

First, the effect of projecting the data into the spectral domain using the GFT operator is assessed by comparing the results of the classification of the full data with the classification of the projected signal using all graph frequencies. For the simulated data, no effect of Difficulty effect is significant, therefore all simulated “subjects” are analyzed together. Post-hoc tests show a significant difference between the classification of the raw data and classification with 4 graph types: Geometric (+1.2) (Z = 7.3; p < 0.001), Full (+0.8) (Z = 6.5; p < 0.001), Fundis (+1.1) (Z = 6.2; p < 0.001) and Absolute correlation (+0.4) (Z = 3.5; p < 0.001). No significant effects are obtained for the other graph types.

### B. Dimensionality reduction

Several GSP-based methods for dimensionality reduction have been compared. An effect of Difficulty has been identified on the difference Accuracy_{Full} - Accuracy_{Easy} for all methods. Therefore each difficulty group is reported separately. Classification results for all methods are presented in Table 2.

We observe that for all graph types but the Kalofolias graph and the Full graph, high frequencies are more relevant for the classification than low frequencies (classification is close to chance level in most of the classifications). Moreover, the Semilocal graph stands out from the other graph types and reaches better scores in nearly all methods, especially when selecting 50 dimensions (72.5%, 90.9%). The Semilocal graph was selected for further analysis. When comparing the optimal number of dimension, graph sampling yield the best accuracy when selecting 30 components for the Difficult group and 50 components for the Easy group (see Figure 1).

### C. Comparisons of GSP, PCA, ICA and ANOVA

The performance of Graph Sampling to state-of-the-art reduction techniques such as PCA, ICA and ANOVA are then compared for the simulated and the real fMRI data. The results are presented in Table 3.

**TABLE I**

| Method          | Accuracy |
|-----------------|----------|
| Easy            | 77.7% ± 12.7 |
| Difficult       | 78.4% ± 12.9 |
| Face-House      | 79.9% ± 13.0 |
| Cal-Face        | 78.6% ± 12.5 |

**TABLE II**

| Data            | Accuracy |
|-----------------|----------|
| fMRI            | 77.6% ± 12.8 |
| Covariance      | 77.6% ± 12.8 |
| Kalofolias      | 77.6% ± 12.5 |
| Semilocal       | 77.9% ± 12.7 |
| Fundis          | 78.8% ± 12.8 |

**TABLE III**

| Method          | Simulation | Haxby   |
|-----------------|------------|---------|
| PCA             | 88.8%      | 82.7%   |
| ICA             | 90.7%      | 84.4%   |
| ANOVA           | 92.1%      | 85.5%   |
| Graph sampling  | 90.9%      | 88.2%   | 69.0%   |

For the simulated fMRI data, the classification with Graph Sampling is significantly more accurate in the Difficult group than PCA (Z = 5.9, p < 0.001), ICA (Z = 5.9, p < 0.001) and ANOVA (Z = 5.9, p < 0.001). In the Easy group, classification is significantly more accurate for the ANOVA (PCA: Z = 4.4, p < 0.001; ICA: Z = 5.5, p < 0.001; and Graph Sampling: Z = 3.7, p < 0.001). Classification with Graph Sampling is significantly more accurate than PCA (Z = 5.2, p < 0.001), but not than ICA (Z = 2.0, p = 0.05).

For the Haxby dataset, the classification with graph sampling produces the most accurate results for both conditions. However, those differences do not reach statistical significance (PCA: Z = 2.3, p = 0.022 uncorrected, ICA: Z = 1.5, p = 0.126 uncorrected, ANOVA: Z = 1.5, p = 0.126 uncorrected).

### IV. Conclusion

In this work, we tested the contribution of Graph Signal Processing to brain signal analysis. We constructed graphs that model the geometric and/or the functional dependencies of brain activity on simulated and real fMRI data, and compared classification accuracy for difference choices of graphs and dimensionality reduction techniques. We showed that applying graph sampling to a semilocal graph selected meaningful nodes for classification, without any prior hypothesis on the categories to distinguish, and led to a significant improvement in classification accuracy compared to PCA, ICA and ANOVA, when categories are difficult to distinguish. Taking into account both the geometric structure of the data and functional
TABLE II

| Group   | Graph type | 50  | 200  |
|---------|------------|-----|------|
|         |            | GFT LF | GFT HF | GFT ANOVA | Sampled LF | GFT Sampled HF | GFT LF | GFT HF | GFT ANOVA | Graph Sampled LF | Graph Sampled HF |
| Difficult | Full      | 54.8% | 51.1% | 66.6% | 52.0% | 51.3% | 63.1% | 60.4% | 66.7% | 62.2% | 60.5% |
|          | Geometric | 56.7% | 64.8% | 64.8% | 50.5% | 65.2% | 56.8% | 65.4% | 66.3% | 52.6% | 66.5% |
|          | Correlation | 52.4% | 60.8% | 64.7% | 50.9% | 60.3% | 58.7% | 66.8% | 57.0% | 67.9% |
|          | Covariance | 52.4% | 67.6% | 65.2% | 51.2% | 66.2% | 54.8% | 66.4% | 65.7% | 53.8% | 67.3% |
|          | Kalofolias | 61.6% | 51.9% | 65.9% | 61.6% | 51.9% | 63.6% | 57.0% | 66.0% | 65.1% | 57.0% |
|          | Semiclusal | 51.8% | 69.5% | 65.6% | 50.3% | 72.5% | 54.0% | 66.6% | 66.2% | 51.4% | 68.7% |
|          | Funds      | 54.9% | 64.2% | 65.1% | 49.7% | 62.8% | 55.6% | 66.0% | 66.8% | 50.9% | 68.5% |
| Easy     | Full      | 65.1% | 60.0% | 88.9% | 49.6% | 60.6% | 87.8% | 80.0% | 90.5% | 86.1% | 79.9% |
|          | Geometric | 71.3% | 79.9% | 86.0% | 57.8% | 79.1% | 78.2% | 83.2% | 90.1% | 68.3% | 85.3% |
|          | Correlation | 59.5% | 86.5% | 86.9% | 53.5% | 75.2% | 67.0% | 88.9% | 89.3% | 62.1% | 90.2% |
|          | Covariance | 57.2% | 87.0% | 88.8% | 52.8% | 84.8% | 68.6% | 88.7% | 89.5% | 66.1% | 89.2% |
|          | Kalofolias | 88.2% | 54.2% | 89.4% | 87.5% | 52.6% | 88.9% | 65.3% | 89.2% | 58.0% | 66.7% |
|          | Semiclusal | 61.3% | 87.9% | 88.6% | 52.3% | 90.9% | 64.5% | 88.4% | 89.8% | 60.8% | 90.2% |
|          | Funds      | 67.4% | 77.5% | 86.7% | 52.4% | 71.5% | 73.5% | 71.1% | 90.2% | 62.8% | 89.3% |

connectivity between brain areas at rest improved classification and dimensions reduction of neuroimaging data.

Interestingly, only the high graph frequencies enable to discriminate between conditions. Those frequencies are often associated with noise or “randomness” [6], [8] since they carry highly spatially variable signal. Those results are in agreement with [6], who found that the eigenvectors associated with high frequencies corresponded to more stable activity and dimensions reduction of neuroimaging data.

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To conclude, GSP is a promising method to improve the analysis of neuroimaging signals. Future work should focus on defining appropriate graphs, since it has a strong impact on the performances. Structural connectivity measures could provide additional information for graph construction.

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