Algorithm-Agnostic Explainability for Unsupervised Clustering

Algorithm-Agnostic Explainability

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Supervised machine learning explainability has greatly expanded in recent years. However, the field of unsupervised clustering explainability has lagged behind. Here, we, to the best of our knowledge, demonstrate for the first time how model-agnostic methods for supervised machine learning explainability can be adapted to provide algorithm-agnostic unsupervised clustering explainability. We present two novel algorithm-agnostic explainability methods – global permutation percent change (G2PC) feature importance and local perturbation percent change (L2PC) feature importance - that can provide insight into many clustering methods on a "global" level by identifying the relative importance of features to a clustering algorithm and on a "local" level by identifying the relative importance of features to the clustering of individual samples. We demonstrate the utility of the methods for explaining five popular clustering algorithms on low-dimensional, ground-truth synthetic datasets and on high-dimensional functional network connectivity (FNC) data extracted from a resting state functional magnetic resonance imaging (rs-fMRI) dataset of 151 subjects with schizophrenia (SZ) and 160 healthy controls (HC). Our proposed explainability methods robustly identify the relative importance of features across multiple clustering methods and could facilitate new insights into many applications. We hope that this study will greatly accelerate the development of the field of clustering explainability.

 $\textit{CCS CONCEPTS} \bullet \textit{Computing methodologies} \rightarrow \textit{Machine learning} \rightarrow \textit{Learning paradigms} \rightarrow \textit{Unsupervised learning} \rightarrow \textit{cluster analysis}$

Additional Keywords and Phrases: clustering	, explainable AI,	, resting-state	IMKI, schize	ophrenia
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1 INTRODUCTION

In recent years, there has been an explosion of research into methods for explaining supervised learning approaches. However, there has been relatively little research into methods for explaining unsupervised clustering approaches, and there is a need for more approaches to be developed. Explainability methods from the domain of supervised machine learning offer one potential avenue for improving clustering explainability.

Explainability methods for supervised learning fall into two categories - model-specific and model-agnostic methods. Model-specific methods are only applicable to a specific class of models. For example, layer-wise relevance propagation (LRP) is a model-specific method applicable to deep learning classifiers [1], and Gini or impurity-based feature importance is a model-specific method applicable to decision tree-based methods [26]. In contrast, model-agnostic methods are applicable to a much larger variety of supervised models. Examples of popular model-agnostic methods include LIME [33], SHAP [28], permutation feature importance [16], PD plots [18], and ICE plots [20]. Note that both of these classes of explainability methods are distinct from interpretable machine learning methods in which models are inherently interpretable, like logistic regression with elastic net regularization [42] or decision trees.

Approaches analogous to model-specific explainability methods and interpretable machine learning methods have been developed for clustering. There are interpretable clustering approaches [3,5–7,17,27]. Some approaches have properties of both model-specific explainability methods and interpretable machine learning methods [19], and some are feature selection methods that are analogous to the model-specific explainability methods of the supervised machine learning domain [9].

However, to the best knowledge of the authors, the potential of model-agnostic explainability methods still remains untapped within the space of interpretable and explainable clustering methods. Model-agnostic explainability methods, if slightly adapted, have tremendous potential to be directly transferred from the domain of explainable supervised learning to explainable unsupervised clustering and to greatly accelerate the development of the field of interpretable and explainable clustering. We call this adapted class of explainability methods, "algorithm-agnostic". Many clustering methods that are not inherently interpretable have unique characteristics that are distinct from those of tree-based

clustering methods. Algorithm-agnostic methods would make those clustering methods more explainable.

While there are multiple taxonomies of clustering methods [15,32], for the purposes of this study, we consider how modelagnostic explainability methods can be applied to five types of clustering methods: (1) partition-based [21], (2) density-based [35], (3) model-based [2], (4) hierarchical [22], and (5) fuzzy [34] methods. Clustering has been applied in many domains [4,30,39]. In this work, we validate our approaches within the field of computational neuroscience for resting state functional magnetic resonance imaging (rs-fMRI) functional network connectivity (FNC) analysis. Clustering approaches have been applied to FNC data to gain insight into a variety of brain disorders and mechanisms [36-38,41]. However, the high dimensionality of the data makes understanding clusters extremely challenging, and as a result, most studies only examine a small number of domains and train a supervised machine learning classifier after clustering to gain insight into the identified clusters.

Here, we seek to demonstrate how model-agnostic explainability methods can be generalized to the domain of clustering explainability by adapting permutation feature importance [16]. We present two novel methods for algorithmagnostic clustering explainability: Global Permutation Percent Change (G2PC) feature importance and Local Perturbation Percent Change (L2PC) feature importance. G2PC can be used to obtain "global" insight into the relative importance of features to a clustering, and L2PC can be used to obtain "local" insight into the importance of features to the clustering of an individual sample. We demonstrate the utility of these approaches for the previously mentioned five categories of clustering methods on low-dimensional synthetic data and further demonstrate how they can provide insight into highdimensional rs-fMRI FNC data from the Functional Imaging Biomedical Informatics Research Network (FBIRN) dataset including 151 subjects with schizophrenia and 160 controls [14].

2 METHODS

Here we describe (1) our proposed clustering explainability methods and (2) the experiments by which we determine the utility of our proposed clustering explainability methods.

2.1 Explainability Methods for Clustering

We first discuss permutation feature importance, a model agnostic explainability method, from which G2PC and L2PC were derived. We then discuss G2PC and L2PC.

Table 1: Synthetic Dataset Distributions

Feature -	Synthetic Dataset 1		Synthetic Dataset 2				
	Class 1	Class 2	Class 1	Class 2	Class 3	Class 4	
1	11±1	3±1	3±0.5	11±0.5	19±0.5	27±0.5	
2	9±1	3±1	3±0.5	9±0.5	15±0.5	21±0.5	
3	7±1	3±1	3±0.5	7±0.5	11±0.5	15±0.5	
4	5±1	3±1	3±2	5±2	7±2	9±2	
5	3±1	3±1	3±2	4±2	5±2	6±2	

2.1.1 Permutation Feature Importance

Permutation feature importance is a well-known modelagnostic explainability method that is typically applied within the context of supervised machine learning algorithms. It was originally developed within the context of random forests [10] and has since been expanded to be compatible with a variety of machine learning classifiers [16]. It involves a straightforward procedure for estimating the importance of each feature. (1) A model performance metric is calculated on a particular set of data for an existing classifier. (2) The data from one feature is permuted across all samples. (3) The permuted data is fed to the preexisting classifier, and the performance metric is again calculated. (4) The ratio of the performance before and after permutation is calculated and reflects the overall importance of that feature to the model. (5) Steps 2 through 4 are repeated multiple times for the same feature to obtain a distribution of feature importance values, and (6) steps 2 through 5 are repeated for each feature. Afterwards, the calculated importance values can be compared across features.

2.1.2 Global Permutation Percent Change (G2PC) Feature Importance

Permutation feature importance approach can be generalized to provide an estimate of feature importance for clustering algorithms. G2PC feature importance is highly similar to the standard permutation feature importance applied to supervised machine learning models. However, there are several key distinctions. Rather than calculating the ratio of the change in performance before and after permutation, G2PC calculates the percentage of all N samples that change from

ALGORITHM 1: G2PC 1: function permute_group(X_2 , j, groups) 2: $p \leftarrow permute(0 \text{ to } N \cdot 1)$ 3: X_2 [:, groups = j] $\leftarrow X_2$ [p, groups = j] 4: return X_2 1: procedure G2PC(mdl, X, Y, groups) 2: for all j of J groups do 3: for all k of K repeats do 4: $X_2 \leftarrow copy(X)$ 5: $X_2 \leftarrow permute_group(X_2, j, groups)$ 6: $Y_2 \leftarrow predict(X_2, mdl)$ 7: $Pct_Chg[j, k] \leftarrow sum(Y \neq Y_2)/N$ > Results

their original pre-permutation clusters to a different post-permutation cluster. The percentage of samples that switch clusters following the permutation of a particular feature reflects the importance of that feature to the clustering. We also added an optional grouping component to G2PC that allows related features to be permuted simultaneously. The determination of groups is dependent upon domain knowledge. If there are no known groups, each feature can be assigned to its own group. Algorithm 1 describes the method in greater detail. The *Groups* parameter is an array that contains an identifying group number for each feature. The *mdl* parameter is an object that contains the information necessary to assign a new sample to the preexisting clusters. Parameters *X* and *Y* are the original data and cluster assignments, respectively.

2.1.3 Local Perturbation Percent Change (L2PC) Feature Importance

L2PC feature importance is an extension of G2PC. Rather than permuting across all samples and measuring the overall clustering percent change, L2PC perturbs each of F features from an individual sample M times using values randomly selected from the same feature of other samples in the dataset and calculates the percentage of times that the sample changes clusters following perturbation. It performs this operation for a predefined number of repeats (K) for each sample. The perturbation percent change values obtained from each repeat could be used to obtain the statistical significance of each feature by comparing the values to a null hypothesis of zero perturbation percent change. As the percent change increases, the importance of a feature for the clustering of the individual

ALGORITHM 2: L2PC 1: **function** permute_group(X2, X, M, j, groups) 2: p ← permute(0 to N - 1) 3: $X_2[:, groups = j] \leftarrow X[p < M - 1, groups = j]$ 4: return X2 1: procedure L2PC(mdl, X, Y, groups) 2: for all n of N samples do for all j of I groups do for all k of K repeats do 5: $X_2 \leftarrow copy(X[n,:])$ MxF $X_2 \leftarrow permute_group(X_2, X, M, j, groups)$ $Y_2 \leftarrow predict(X_2, mdl)$ $Pct_Chg[n, j, k] \leftarrow sum(Y[n] \neq Y_2)/M$ Results

sample increases. While L2PC is principally a method for obtaining a measure of feature importance for each sample individually, L2PC can, like other local methods [1], be applied to each sample to provide a global measure of feature importance, and the mean of the resulting distribution of perturbation percent change values across subjects can provide a global measure of feature importance. The application of L2PC as a global measure of feature importance is much more computationally intensive than G2PC. The computational complexity is not a concern when examining feature importance for a small number of samples. Using L2PC as a global metric in high dimensions could be made more tenable via the use of a smaller number of repeats or perturbations per repeat. Additionally, the approach could easily be parallelized to greatly increase the speed of computation. We added an optional grouping component to L2PC that allows related features to be perturbed simultaneously. The determination of groups is dependent upon domain knowledge. If there are no known groups, each feature can be assigned to its own group. Algorithm 2 describes the method in greater detail.

2.1.4 Additional Notes on G2PC and L2PC

It should be noted that one aspect of both G2PC and L2PC is the assignment of new samples to existing clusters. Some might argue that the assignment of new samples to existing clusters violates the intended purpose of clustering methods. Regardless, it is still possible to effectively assign new samples to existing clusters without the use of a supervised classifier. For k-means, samples can be assigned to the cluster of the nearest cluster center. For GMMs, the locations of a new sample within the existing cluster probability density functions can be obtained, and the sample can be assigned to the cluster with the highest probability. For fuzzy c-means, new samples can be assigned to existing clusters by retraining a new clustering model with fixed cluster centers and parameters identical to those of the original clustering. K-means, Gaussian mixture models, and fuzzy c-means clustering have functions for predicting the assignment of new samples in scikit-learn and scikit-fuzzy. For DBScan, new samples can be assigned to the cluster of a core sample that is within the predefined ε distance, and new samples can be assigned to clusters derived from agglomerative clustering by placing them in the cluster of the nearest sample.

2.2 Description of Experiments

We evaluated the performance of the two explainability methods through a series of 3 experiments. The first two experiments involved the use of low-dimensional, synthetic, ground-truth data, and the last experiment involved the application of the methods to functional network connectivity values extracted from the FBIRN rs-fMRI dataset [14]. Five popular clustering methods were applied to each dataset, and both introduced explainability methods were applied to evaluate the relative importance of each feature to the clustering.

2.2.1 Synthetic Datasets

We generated two synthetic datasets with different numbers of clusters and random distributions.

2.2.1.1 Synthetic Dataset 1

Synthetic Dataset 1 consisted of 5 features with two 50-sample clusters. The features – numbered 1 through 5 - each consisted of random variables generated from two separate normal distributions that formed two clusters. As the feature number increased (i.e. from feature 1 to feature 5), the difference between the means (μ) of the two random variable normal distributions within each feature decreased, meaning that the overall expected importance of the features decreased. The standard deviation (σ) of the random variables was consistent across both clusters and all 5 features. Table 1 shows the mean and σ of the random variables. For testing G2PC, 100 sets of randomly distributed data were generated, and 1 set of randomly distributed data was generated for testing L2PC.

2.2.1.2 Synthetic Dataset 2

Synthetic Dataset 2 consisted of five features with four 50sample clusters. It provided an opportunity to examine the behavior of the explainability methods in a context involving more than two clusters. The features - numbered 1, 2, 3, 4, and 5 - each consisted of random variables generated from four separate normal distributions that formed four clusters. As the feature number increased, the difference between the u of each of the random variables within the features decreased. Additionally, the variance of the first three features was decreased below unit variance, and the variance of the last two features was increased above unit variance. It was expected that feature importance would decrease from Feature 1 to Feature 5 and that Features 4 and 5 would be significantly less important than Features 1 through 3. Table 1 shows the mean and SD of the random variable distributions of each feature. For testing G2PC, 100 sets of randomly distributed data were generated, and 1 set of randomly distributed data was generated for testing L2PC.

2.2.2 FBIRN rs-fMRI Dataset

This study used rs-fMRI and clinical data from the FBIRN dataset [14]. The dataset contains 151 schizophrenia (SZ) subjects and 160 healthy controls (HC) that were collected from seven sites, including the University of California, Irvine; the University of California, Los Angeles; the University of California, San Francisco; Duke University/the University of North Carolina at Chapel Hill; the University of New Mexico; the University of Iowa; and the University of Minnesota collected neuroimaging data. The dataset can be made available upon a reasonable request emailed to the corresponding author and contingent upon IRB approval.

Six 3T Siemens and one 3T General Electric scanner with the same protocol were used to collect the imaging data. T2*weighted functional images were collected using AC-PC aligned echo-planar imaging sequence with TE=30ms, TR=2s, flip angle = 77°, slice gap=1 mm, voxel size= $3.4 \times 3.4 \times 4$ mm³, and 162 frames, and 5:24 min. All participants were instructed to close their eyes during the rs-fMRI data collection. Neuroimaging data were preprocessed using statistical parametric mapping (SPM12, https://www.fil.ion.ucl.ac.uk/spm/) in the MATLAB 2019 environment. We used rigid body motion correction to account for subject head movement. Next, the imaging data underwent spatial normalization to an echo-planar imaging (EPI) template in standard Montreal Neurological Institute (MNI) space and was resampled to 3x3x3 mm³. Finally, we used a Gaussian kernel to smooth the fMRI images using a full width at half maximum (FWHM) of 6mm. The Neuromark automatic independent component analysis pipeline within the group ICA of fMRI toolbox GIFT (http://trendscenter.org/software/gift) was used to extract 53 independent components (ICs) [12]. We put the ICs in seven domains, including subcortical network (SCN), auditory network (ADN), sensorimotor network (SMN), visual network (VSN), cognitive control network (CCN), defaultmode network (DMN), and cerebellar network (CBN). Lastly, we used Pearson correlation between each IC time-series pair estimate each subject's static functional network connectivity (FNC). This resulted in 1378 whole-brain correlation values (i.e. features) for each subject.

2.2.3 Clustering Methods

We utilized algorithms from 5 different categories of clustering methods: (1) k-means clustering, a partitioning method, (2) DBScan, a density-based method, (3) a Gaussian mixture model (GMM), a model-based method, (4) agglomerative clustering (AGC), a hierarchical clustering method, and (5) fuzzy c-means clustering, a fuzzy clustering method. The GMM, AGC, k-means, and DBScan were

implemented in scikit-learn [31], and fuzzy c-means was implemented in scikit-fuzzy (https://github.com/scikit-fuzzy).

2.2.4 Experiment Parameters for Clustering and Explainability Methods

For the synthetic datasets, the known, ground-truth number of clusters was provided to the k-means, GMM, AGC, and fuzzy c-means algorithms. For the rs-fMRI FNC analysis, the number of clusters for each algorithm was optimized via the silhouette method. For each DBScan analysis, the ϵ distance parameter was optimized using the silhouette method, and the minimum number of points parameter was equal to 4. For fuzzy c-means in all of the analyses, m=2, error = 0.005, and maximum number of iterations = 1000. When calculating the percent change in clustering, the cluster of each sample was assigned to the class with the highest predicted likelihood.

The number of repeats (K) parameter was set to 100 for the G2PC and L2PC analyses on all datasets, and the number of perturbations per repeat (M) was set to 30 for L2PC for all datasets. We performed G2PC and L2PC on the FBIRN data, both with grouping based upon the established FNC domains and without grouping. Both synthetic datasets were z-scored on a feature-wise basis. Python code for all experiments can be found on GitHub (link removed for double-blind review). Note that Figures 2 and 3 were generated separately in MATLAB with the results output by the Python scripts.

3 RESULTS

Here we detail the results for both the synthetic data and rs-fMRI FNC experiments.

3.1 Synthetic Datasets

In Synthetic Dataset 1, importance generally decreased from features 1 to 5 in alignment with expectations for all clustering and both explainability methods. It should be noted, however, that the sensitivity of each of the clustering methods to perturbation varied widely both on a feature-to-feature basis and on an overall percent change basis. For G2PC, features 4 and 5, which were supposed to be minimally important, were generally categorized as having little to no effect upon the clustering. Additionally, features 1-3 generally had descending importance estimates. However, GMMs with G2PC seemed to mainly emphasize one feature (i.e. feature 1) in their clustering, contrary to the other methods that placed more importance upon features 2 and 3. Also, some methods seemed much more sensitive to perturbation than others. The mean percent change for feature 1 of both the GMM and DBScan was around 30%,

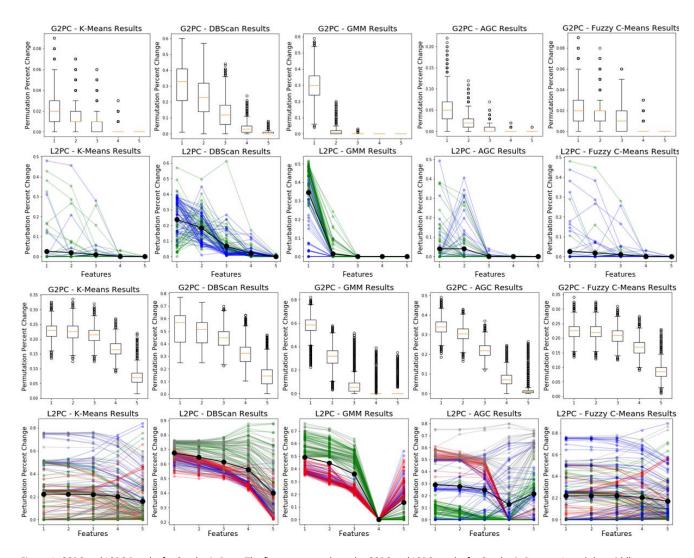


Figure 1: G2PC and L2PC Results for Synthetic Data. The first two rows show the G2PC and L2PC results for Synthetic Dataset 1, and the middle two rows show the G2PC and L2PC results for Synthetic Dataset 2. Each column shows the results for a different clustering algorithm. Note that as expected, the permutation and perturbation percent change values, in general, decrease from left to right, indicating a relative decrease in feature importance. The x-axis of each plot indicates the 5 synthetic data features.

while for feature 1 of k-means, AGC, and fuzzy c-means, the median importance was around 2% to 5%. Similar findings occurred for L2PC with Synthetic Dataset 1. As can be seen in the black line on Figure 1, the mean feature importance across all samples and repeats was very similar to the median values of the G2PC results. For k-means, AGC, and fuzzy c-means, only a few samples were sensitive to perturbation. However, in the GMM and DBScan, a majority of the samples were sensitive to perturbation. It can be seen for some of the clustering methods like fuzzy c-means, AGC, k-means, and the GMM that there were differences in the sensitivity of samples to perturbation on a per-cluster basis.

For Synthetic Dataset 2, the G2PC and mean L2PC results looked as expected. The results are shown in Figure 1. The first

three features were generally ranked as much more important than the last two features, which accounted for both the difference in the means and variance of the random variables from which the synthetic data was generated, and importance generally decreased from features 1 to 3 and 4 to 5, which accounted for the differences in the means of the random variables of each cluster. It is interesting that the GMM and AGC had a sharp increase in mean L2PC importance from feature 4 to 5, while the other three cluster methods had the expected decrease. Additionally, the samples in some clusters of the GMM and AGC L2PC results were highly distinct. For the GMM, the red and grey clusters had higher importance for features 1 to 3 and lower importance for features 4 and 5 than the red and blue clusters. For features 1 to 3 of AGC, the red and grey clusters

had high importance, the blue cluster had moderate importance, and the green cluster had low importance.

3.2 FBIRN rs-fMRI Data

All clustering methods, except for DBScan which only found noise points, identified 2 clusters as optimal. The identification of two clusters was consistent with the underlying SZ and HC groups. K-means had an accuracy, sensitivity, and specificity of 63.99%, 78.81%, and 52.98%, respectively. Fuzzy c-means had better clusters with an accuracy, sensitivity, and specificity of 68.81%, 74.17%, and 67.55%, respectively.

When performing clustering with G2PC and L2PC for the FBIRN data, we initially found that perturbation did not have a widespread effect upon the clustering when perturbing each of the 1378 whole-brain correlation values individually. However, when we perturbed the whole-brain correlation values within each domain simultaneously, we obtained feature importance results for k-means and fuzzy c-means that can be seen in Figure 2. Panels A and B are box plots of the G2PC importance values for each of the 100 repeats, and for the sake of easy visualization, panels C and D reflect the mean perturbation percent change across all repeats and perturbation instances for each sample, where the green samples and the blue samples are those belonging to the SZ dominant cluster and the HC

dominant cluster, respectively. Figure 3 shows the values of the mean FNC for the SZ dominant cluster minus the mean FNC for the HC dominant cluster. The domains surrounded by white boxes were those identified by G2PC and L2PC as most important. The figure used the magma colormap [8].

The feature importance results were highly consistent across both clustering methods and both explainability methods. Top domains identified by k-means with G2PC and L2PC included the cross-correlation between the ADN and CCN (ADN/CCN), the SCN/VSN, the CCN/DMN, and the SMN/DMN. Top domains identified by fuzzy c-means with G2PC and L2PC included the ADN/CCN, the CCN/DMN, the SCN/VSN, ADN, and SMN/VSN. For k-means, relative to the HC dominant group, the SZ dominant group had higher ADN/CCN FNC for around half of the domain, much higher levels of SCN/VSN FNC, a mixture of moderately higher to lower levels of CCN/DMN FNC, and a mixture of higher to lower SMN/DMN connectivity. For fuzzy cmeans, relative to the HC dominant group, the SZ dominant group had ADN/CCN FNC values that were higher for around half of the domain, a mixture of higher to lower CCN/DMN FNC values, much higher SCN/VSN FNC values, slightly lower ADN FNC values, and much smaller SMN/VSN FNC values.

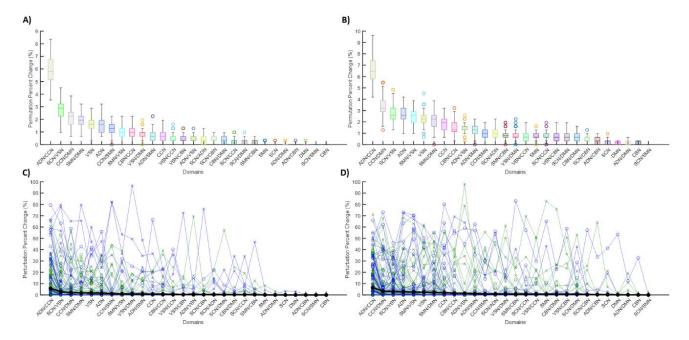


Figure 2: FBIRN G2PC and L2PC Results. Panels A and B show the G2PC results for k-means and fuzzy c-means clustering, respectively, and Panels C and D show the L2PC results for k-means and fuzzy c-means clustering respectively. On the x-axis of each panel are the domains in order of most important to least important based upon their mean value, and on the y-axis is the perturbation or permutation percent change value. G2PC shows the relative importance of each of the features to the clustering. In panels C and D, the samples belonging to the SZ and HC dominant clusters are green and blue, respectively. The values marked with an "o" or an "x" indicate the samples that were correctly or incorrectly clustered, respectively. The black line on Panels C and D reflects the mean L2PC values across all subjects and provides a measure of global feature importance.

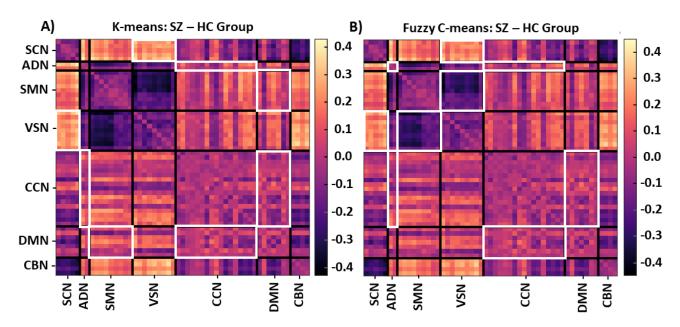


Figure 3: FNC Clustering Results. Panel A shows the result of the mean FNC of the SZ dominant k-means cluster minus the HC dominant cluster, and Panel B shows the result of the mean FNC of the SZ dominant fuzzy c-means cluster minus the HC dominant cluster. The colormaps to the right of each matrix show the magnitude of its values. The black grid denotes the boundaries of FNC domains, and the white rectangles indicate the domains that were identified as most important for the clustering.

Both G2PC and L2PC indicated that a minority of samples were sensitive to perturbation, and L2PC demonstrated that many of those samples were very sensitive to perturbation, indicating that they may have been closer to the boundaries of their clusters. For fuzzy c-means, more samples belonging to the SZ dominant cluster rather than the HC dominant cluster seemed sensitive to perturbation. Most of the HC samples that were sensitive to perturbation seemed to have been correctly assigned to the HC dominant cluster, while most of the subjects in the SZ dominant cluster that were sensitive to perturbation seemed to actually be HC subjects. For k-means, some samples in the HC dominant cluster that were actually SZ subjects seemed to be extremely sensitive to perturbation, while other samples belonging to the SZ dominant cluster that were actually HC subjects were sensitive to perturbation at smaller levels.

4 DISCUSSION

Here we propose that model-agnostic methods for supervised machine learning explainability can be adapted for use in clustering explainability. We further demonstrate two novel approaches for clustering explainability: G2PC feature importance and L2PC feature importance. G2PC provides a global measure of the relative importance of features to the clustering, and L2PC provides a local measure of which features are important to the clustering of an individual sample.

We applied both G2PC and L2PC to clusters generated by five popular clustering algorithms from low-dimensional synthetic data and demonstrated that they were able to work with each clustering algorithm to identify the features that were expected to be most important. There were some instances with GMMs in which several of the features that were expected to be of importance to the clustering of the synthetic data seemed to be unimportant after analysis with G2PC and L2PC. G2PC and L2PC allowed the importance of each feature to different clustering algorithms to be compared via a single percent change metric that could later be used to provide greater insight into the similarities and differences of clustering algorithms. While G2PC and L2PC worked well for lowdimensional data across all of the clustering methods with which we paired them, they were not as generalizable to high dimensional data as we would have hoped.

To generalize G2PC and L2PC to neuroimaging analysis, we applied all 5 clustering methods with G2PC and L2PC to the high-dimensional FBIRN dataset to identify key FNC features differentiating the SZ dominant cluster and the HC dominant cluster. However, very few of the individual features seemed to have an effect upon the clustering. This is not entirely surprising given the high dimensionality of the data and that Euclidean distance was utilized. We implemented a grouping component that allowed related features to be perturbed or permuted simultaneously, and we obtained feature importance

results for both k-means and fuzzy c-means clustering that were highly consistent, supporting the reliability of the feature importance results for those clustering algorithms in high dimensions.

The grouping component of G2PC and L2PC is ideal for high dimensional datasets with features that can be divided into groups based upon domain knowledge. Additionally, a known weakness of perturbation and permutation methods is that they can generate samples that are outside the space of the typical data distribution and thus produce unreliable results when a high degree of correlation exists between some features. The grouping parameter can help address this problem when highly correlated features are grouped together during analysis.

Our results for the FBIRN FNC analysis agreed with and extended existing literature. Five cross-network domain sets -ADN/CCN, SCN/VSN, CCN/DMN, SMN/DMN - and 1 network -ADN - were selected as most important. This is consistent with a previous study that showed that schizophrenia causes widespread dysconnectivity across throughout the brain [24]. Additionally, our results showed a disrupted (i.e., both increase and decrease) pattern in different brain networks. For example, we found VSN/SMN FNC is lower in SZ subjects than in HC ones. A previous study reported a decrease in SZ subjects' SMN/VSN FNC versus HC ones [11]. That potentially could explain the impairment of sensory information processing in SZ subjects. Multisensory information processing is a prerequisite for selfawareness. It has been proven that matching visual perception and proprioceptive signals from SMN are necessary for selfconsciousness perseverance [13], which is impaired in SZ subjects [29]. Therefore, the disconnection among SZ sensory networks could potentially explain the underlying mechanisms of self-awareness deficit in SZ subjects.

We also found a decrease in ADN connectivity in SZ subjects, which aligns with a previous study [23]. This piece of evidence might explain the link between hearing loss at an early age and the later development of schizophrenia [25]. Interestingly, we found an increase in the ADN/CCN FNC in SZ subjects. Increased ADN/CCN FNC could serve as a compensatory mechanism and suggests a prospective study. We also found an increase in the FNC between VSN/SCN. A previous study showed increased FNC between the thalamus as a part of SCN and occipital cortices/postcentral gyri as part of VSN in SZ subjects compared with that of HC subjects [40].

Throughout each of our experiments, we utilized similar G2PC and L2PC settings. Different parameter settings would likely produce slightly different G2PC and L2PC results, and it might be helpful for future studies to examine the effects of the

parameter settings. We hypothesize that as K for G2PC and L2PC is increased, the feature importance results will likely become more reliable. For L2PC, a decreased M would likely result in higher variance across repeats. However, the need for more reliable L2PC results must be balanced with the need for less computational intensity. The ideal M is also likely affected by the total number of samples in the dataset.

Additionally, in our clustering analyses, we used Euclidean distance, which can be less than ideal for highly dimensional data. Future studies could investigate the effects of other distance metrics and how they would enable G2PC and L2PC to be more broadly applied to other clustering algorithms.

It is likely that other model-agnostic explainability methods from the domain of supervised machine learning explainability could also be generalized to enable explainability for clustering methods. Permutation feature importance differentiates itself from many other model-agnostic explainability methods in that it can be applied to classifiers that output a hard classification. In contrast, an important requirement for many model-agnostic explainability methods is that a classifier predict a class probability, rather than a binary class label. Given this requirement, it is likely that soft-clustering methods like GMMs and fuzzy c-means would be ideal for compatibility with the majority of model-agnostic explainability methods. It is also feasible that G2PC could be used as a feature selection method to obtain optimal clustering.

5 CONCLUSION

In this study, we proposed, to the best of our knowledge, for the first time that model-agnostic explainability methods from the domain of supervised machine learning explainability can be adapted for algorithm-agnostic clustering explainability. We introduced two new explainability methods and demonstrated on low-dimensional, ground-truth synthetic data that they can be paired with multiple clustering algorithms to identify the features most important to differentiating identified clusters. We further demonstrated the utility of the methods for highdimensional datasets by analyzing rs-fMRI FNC data and identifying cross-domain connectivity associated schizophrenia. It is our hope that this paper will (1) stimulate rapid growth in the domain of clustering explainability via an infusion of algorithm-agnostic methods from the domain of supervised machine learning explainability and (2) enable data scientists across a variety of fields to gain more insight into the variety of clustering algorithms that they employ.

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