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Graph Theory Analysis of Microstates in Attention-Deficit Hyperactivity Disorder

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Abstract: Attention-Deficit Hyperactivity Disorder (ADHD) is one of the most common disorders of childhood and youth. The diagnosis of ADHD remains essentially clinical, based on history and questionnaires for symptom assessment, therefore, a biomarker can be of great value to reduce the inherent uncertainty of clinical diagnosis. In recent years, several studies have been carried out to assess the usefulness of neurophysiological (electroencephalography - EEG) and functional image data to assist in the process of diagnosing ADHD. Previous researches have revealed evidences that microstates are selectively affected by ADHD, indicating that their analysis may be a useful tool in methods of automatic disease identification. In this paper is proposed a new methodology for the detection of ADHD using EEG microstate analysis and graph theory. The proposed method allows modeling and interpreting each microstate as a complex network, which permits to identify the effect of ADHD on some characteristics of the built networks. In addition, it provides useful information to identify ADHD and subtypes patients with an accuracy around 99%, indicating that the proposed method is promising.

Resumo: O Transtorno de Déficit de Atenção e Hiperatividade (TDAH) é um dos distúrbios mais comuns da infância e adolescência. O diagnóstico de TDAH permanece essencialmente clínico, com base no histórico do paciente e nos questionários para avaliação dos sintomas. Dessa forma, encontrar um biomarcador pode ser apropriado para reduzir as incertezas inerentes ao diagnóstico clínico. Nos últimos anos, diversos estudos foram realizados para avaliar a utilidade dos dados de EEG (eletroencefalografia) e de imagem funcional no diagnóstico do TDAH. Tais estudos revelaram evidências de que os microestados são afetados seletivamente pelo TDAH, indicando que sua análise pode ser uma ferramenta promissora na identificação automática da doença. Neste artigo é proposta uma nova metodologia para a detecção de TDAH utilizando a análise de microestados do EEG e a teoria de grafos. O método proposto permite modelar e interpretar cada microestado como uma rede complexa, permitindo identificar o efeito do TDAH em algumas características das redes construídas. Além disso, fornece informações úteis para identificar pacientes com TDAH (e subtipos) com uma acurácia em torno de 99%, indicando que o método proposto é promissor.

Keywords: EEG-Microstates; ADHD; Signal Processing; Graph Theory; Classification.
Palavras-chaves: Microestados do EEG; TDAH; Processamento de Sinais; Teoria de Grafos; Classificação.

1. INTRODUCTION

Attention-Deficit Hyperactivity Disorder (ADHD) is a neuropsychiatric disorder that affects approximately 3-6% of children, making it one of the most common disorders of childhood and youth (Thomas et al., 2015). The main symptoms refer to inattention, hyperactivity and impulsivity. ADHD is divided into subtypes according DSM-5: predominantly innatentive (ADD), predominantly hyperactive/impulsive (ADHD-H) and combined (ADHD-C) (Association et al., 2013). Patients with ADHD have significant attention problems, but only patients of the ADHD-C subtype are additionally affected by impulsivity and hyperactivity (Ahmadi et al., 2014). The diagnosis of ADHD remains essentially clinical, based on history and questionnaires for symptom assessment. Neuropsychological tests are also used, however due to heteregeneous cognitive profiles in patients with ADHD these do not provide a fully diagnostic, but a supportive function. Other underlying diseases can also lead to symptoms seen in ADHD patients, for example, other psychiatric conditions, vision and hearing problems, abnormalities in thyroid function, etc. (Ahmadi et al., 2014; Ghanizadeh, 2011), complicating the diagnosis. Therefore, a biomarker can be of great value to reduce the inherent uncertainty of clinical diagnosis (Dubreuil-Vall et al., 2020; Vahid et al., 2019). In recent

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years, several studies have been carried out to assess the usefulness of neurophysiological (electroencephalography - EEG) and functional image data to assist in the process of diagnosing ADHD (Vahid et al., 2019; Dubreuil-Vall et al., 2020).

The EEG activity can be described by a limited number of topographies (maps) of the scalp that remain stable for a certain period of time before switching rapidly to a different topography that remains stable again (Lehmann et al., 1987; Pascual-Marqui, 2002). These discrete intervals of topographic stability are referred as microstates, highlighting the idea that the scalp potential field reflects the momentary state of global neural activity and that variations in the topography of this field indicate changes in the overall coordination of neural activity over time (Pascual-Marqui et al., 1995; Lehmann, 2010). Previous researches have revealed evidences that specific sets of ERP (event-related potentials)-microstates are selectively affected by ADHD, indicating that their analysis may be a useful tool in methods of automatic disease identification (Brandeis et al., 2002; Albrecht et al., 2015). However, the study of microstates and ADHD is still a poorly explored field and requires greater contributions (Albrecht et al., 2015).

This paper proposes a new methodology for the analysis of microstates and automatic patients identification with ADHD. The proposed analysis is based on the graph theory to modeling each topographic map as a complex network. Thus, the global and local properties can be evaluated in order to select characteristics that better describe ADHD. The results show that the proposed methodology is effective in the automatic identification of patients with ADHD.

The remainder of this paper is organized as follows. In Section 2 we presented the proposed methodology, involving the description of the EEG database, the techniques used for the analysis of microstates and the experimental setup. In Section 3, we present the experimental results. Our conclusions and suggestions for future work are presented in Section 4.

2. MATERIALS AND METHODS

2.1 Database Description and Preprocessing

The public database (Vahid et al., 2019) used in this work consists of a set of EEG signals of 144 children classified into three groups: 44 (15 females, age: 11.3 ± 2.2) healthy individuals; 52 individuals (10 females, age: 10.9 ± 2.4) with ADD according to ICD-10 and 48 individuals (12 females, age: 10.6 ± 1.9) with the combined subtype ADHD-C. The patients revealed no other severe or acute psychiatric co-morbities (Vahid et al., 2019). The EEG records were acquired at a sampling frequency equal to 500 Hz and they were collected with pairs of symmetrical electrodes (60 channels) located according to the international 10-20 system. The measures were obtained using the BrainAmp system with band-pass filter 0.5–20 Hz, impedances < 5 kΩ. The electrodes P9, P10, P11 and P12 were removed from the data set due to their high electrode impendances, remaining 56 channels. The reference electrode was positioned at Fpz (Vahid et al., 2019). Pulse artifacts and horizontal and vertical eye movements were removed using independent component analysis (ICA) and the data was stimulus-locked and segmented; finally, an automated artifact rejection procedure was applied to exclude any remaining trials containing artifacts. All individuals performed a time estimation task. During the task, participants were required to estimate a time of 1200 ms following visual stimulus and they were asked to press a button whenever they thought that this time had elapsed (Vahid et al., 2019). The duration of the EEG signals of each patient varies according to their precision in the time estimation task, so that the duration ranging from 1.2 to 3.3 minutes. In this work, the EEG signal of each patient is treated as an instance, i.e., the database contains a total of 144 instances (only an instance for each patient).

2.2 Microstates Analysis

To perform the data study, a method called microstate analysis (Lehmann et al., 1987) was used. In this method, the EEG multichannel register is converted in a series of microstates, each one characterized by a single topography of electrical potentials that remain stable for a certain period of time (60 to 120 ms), before switching rapidly to a different topography. As this technique simultaneously considers the recorded signals of all areas in the cortex, it is possible to evaluate the function of brain network as a whole, whose alterations are related to various neuropsychiatric disorders (Pascual-Marqui et al., 1995; Michel et al., 2009; Khanna et al., 2014).

The extraction of microstates from EEG signal starts calculating the Global Field Power (GFP), which quantifies the overall potential variance across the set of electrodes, according to Equation 1.

$$GFP(t) = \sqrt{(\sum_{i}^{N}(V_i(t) - V_{mean}(t))^2)/N} \qquad (1)$$

Where $V_i(t)$ is the potential of the electrode i on the instant of time t, N is the total number of electrodes and $V_{mean}(t)$ is the potential mean of all electrodes on the instant of time t.

From the GFP signal, the EEG topographic maps are obtained in the time points of maximum GFP that there is a greatest signal noise ratio, and therefore more likely to observe the microstates. Finally, an algorithm called modified k-means is used to cluster these maps according to their topographic similarities metric, called GEV (Global Explained Variance) (Pascual-Marqui et al., 1995). Figure 1 shows the process to obtain the microstates.

2.3 Graph Theory applied to Microstate Analysis

Graph theory is a widely used tool in the analysis of Functional Connectivity Networks, that are defined as the temporal correlation among the activity of different neural assemblies, in terms of significant dependencies between distinct brain regions (de Vico Fallani et al., 2014). Therefore, brain networks can be modeled mathematically using graph theory, in which each node is represented by an electrode and the edges are defined by temporal correlations

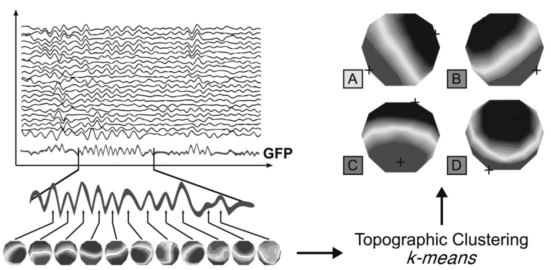

Figure 1. Microstates segmentation process (Khanna et al., 2015).

between such electrodes. Using this concept, in this work, the microstates are modeled in a similar way, i.e., each microstate is modeled as a complex network, in which each node of the network represents an electrode and the edges represent the correlations between them. As can be seen in Figure 1, the EEG signals are represented by a sequence of microstates. As the microstates time series has scale-free property, i.e., similar topographies can be observed at different time scale (M. Michel and Koenig, 2017), in this work, each microstate is represented by a time series by concatenating the time instants where the microstate occurred. From these four time series (in this work, we use four microstates), the correlation matrix is calculated to represent each microstate as a complex network. Thus, each microstate was modeled as a weighted undirected graph of 56 nodes using Pearson's correlation according to the Equation 2,

$$r_{ij} = \frac{cov(V_i, V_j)}{\sqrt{var(V_i)var(V_j)}} \tag{2}$$

where $cov(V_i, V_j)$ is the covariance between the potential V of the nodes i and j, and $var(V_i)$ is the potential variance of the node i. In this work, the correlation is calculated over the time interval of each microstate. Therefore, different from the functional connectivity networks, the EEG signals are sampled according to the microstates labeling. The Correlation Matrix (CM) with dimension 56×56 is $CM_{ij} = r_{ij} = w_{ij}$, and w_{ij} is a weighted element of CM. Then, the adjacency matrix is obtained by thresholding the CM matrix. The threshold used in this work for the connection density was of $TH = 60\%$, to omit spurious links (Telesford et al., 2011). In this case, the nodes and edges are constructed by fixing the connection density, resulting in a weighted connectivity matrix.

Although in the literature, unweighted connectivity networks obtained from binarization are well common on the study of brain networks, weighted network analysis can provide more specific information about the relationship between node pairs (Telesford et al., 2011). A threshold is used in order to eliminate the links that representing spurious connections, noises, and indirect connections in the correlation matrices. In this work was used a fixed value of the connection density, this method results in a different absolute threshold for each network. A measurement of the connection density was usually defined as the ratio of the total number of existing edges K to the maximum possible number of edges $N(N-1)/2$. Then, the differences between the groups of topological metrics were further calculated by fixing the sparsity of networks. In this study, each microstate's correlation matrix was transformed into a set of corresponding weighted matrices with edge density equal to 60% (number of actual edges divided by the total possible number of edges). Finally, all of the wheighted matrices were quantitatively analyzed using graph theory tools (Zhang et al., 2018).

2.4 Global and Local Properties

Exploring different network properties can provide valuable insight into the internal function of microstates networks, and these data may be useful to identify patients with ADHD. The most commonly used graph metrics are described in two main groups: global (that describe the characteristics of the entire network) and local (that describe how vertices and edges integrate into the network) properties. The global metrics evaluated in this work were: clustering, path length, global efficiency, modularity, assortativity and small-worldness. The local metrics evaluated were: degree, strength, local efficiency and degree centrality. All metrics evaluated in this work were calculated using the Brain Connectivity Toolbox (Rubinov and Sporns, 2010) and all respective equations can be found at supplementary matterial of Rubinov and Sporns (2010).

Global measures are primarily aimed at revealing segregation and integration of information flows within the network, small-worldness (that displays an optimal balance between network segregation and integration) and network resilience against failure (Fallani et al., 2010).

Next, the equations used to calculate the most relevant metrics (identified in this work) are described as follows. For all equations described below, consider: N is the set of all nodes in the network, and n is the number of nodes and l is the number of links. The link (i, j) are associated with connection weight w_{ij}.

The small-worldness is the indice that quantifies the balance between segregation and integration, and is dedicated to graphs in which most nodes are not neighbors but they can be reached by any other node with possibly the shortest path length. This property was measured using Equation 3 (Fallani et al., 2010).

$$S^W = \frac{C^W / C^W_{rand}}{L^W / L^W_{rand}} \tag{3}$$

where S^W is the small-worldness indice of the weighted network W, C^W and C^W_{rand} are the clustering coefficients, L^W and L^W_{rand} are the characteristic path lengths of the respective tested network in a random network.

The most relevant local property in the analysis of microstates using graph theory on machine learning classification task of ADHD was local efficiency (between two vertices), that is defined as the inverse of the shortest distance between the vertices. Eventually, local efficiency provides an indication of how effectively information is integrated between the immediate neighbors of a given network node. This measure quantifies a network's resistance to failure on a neighborhood scale and was calculated using Equation 4 (Fallani et al., 2010).

$$E_{loc}^{W} = \frac{1}{n} \sum_{i \epsilon N} \frac{\sum_{j,h \epsilon N, j \neq i} (w_{ij} w_{ih} [d_{jh}^{W}(N_i)]^{-1})^{1/3}}{k_i(k_i - 1)} \quad (4)$$

where E_{loc}^{W} is the local efficiency, d_{jh}^{W} is the shortest path between j and h, that contains neighbors of i and k_i is the degree of i.

2.5 Classification

After calculating the local and global metrics of microstates networks, the boxplot graph was used to assess which metrics are able to separate data into two groups: healthy control and ADHD. After this step the kNN (k-Nearest Neighbor), MLP (Multilayer Perceptron) and SVM (Support Vector Machine) classifiers were used. The classification task was performed in two parts: in the first part, the metrics indicated by the boxplot that best characterize the data were evaluated. In the second part of the experiments, all global and local metrics were evaluated in the classification task. Finally, the results of this two parts were compared. In addition to the two-class problem, the experiments were also carried out to assess the efficiency of three classes separation, i.e. to perform the identification of ADHD subtypes.

The classifier parameters were optimized using bayesian optimization. The optimized hyperparameters were: for kNN the nearest neighbors (1 to 21), for MLP the number of hidden neurons (1 to 50) and for SVM with gaussian kernel the Box Constraint (0.001 to 100) and the Kernel Scale (0.001 to 100). The experiments were carried out using 3-fold cross validation. One fold was used to train and one fold was used to validate hyperparameters with Bayesian optimization. After finding the best hyperparameters, the classifier was trained with the two folds and tested with the remaining fold. This procedure is repeated until all folds are used as a test. For more robust results, the 3-fold cross-validation was repeated 30 times. The data of the experiments were standardized to have zero mean and unitary standard deviation. For evaluating the proposed method, the metric accuracy was used, according to Equation 5 (Baratloo et al., 2015).

$$Accuracy = \frac{NC}{NP} \times 100\% \quad (5)$$

where NC is the number of patients correctly classified and NP is the total number of patients.

3. RESULTS AND DISCUSSION

Previous works involving the study of microstates in ADHD have been carried out with the aim of finding relevant features in their topologies capable of distinguish individuals with ADHD and healthy ones, as well assessing the efficiency of medication in the treatment of symptoms (Zillessen et al., 2001; Meier et al., 2012). In this work, four microstates of EEG signals were evaluated using graph theory, to identify healthy and ADHD individuals. Figure 2 shows the four microstate class prototype topographies obtained according to the optimal value of GEV for the database. The Matlab software and EEG Microstates

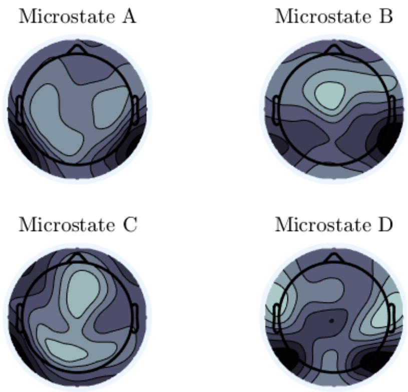

Figure 2. The topographies of the four microstate classes from the clustering algorithm. Note that only map's topography is important, whereas polarity is disregarded in the spontaneous EEG clustering algorithm.

Toolbox (Poulsen et al., 2018) were used to perform the microstates segmentation process.

After modeling the microstates networks as graphs, global and local metrics were extracted and evaluated as described in Sections 2.3 and 2.4. Figure 3 shows the metrics that were visually the most relevant in characterizing healthy and ADHD individuals.

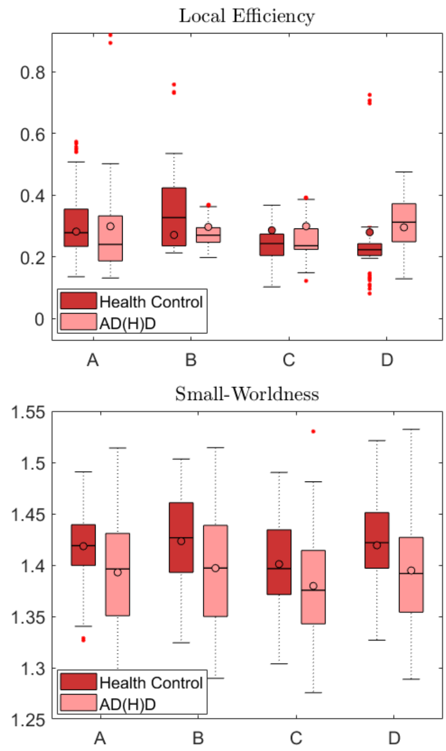

Figure 3. Selected metrics that better characterize the database, where the x-axis represents the microstates and the y-axis is the metrics values.

As seen in Figure 3, the topological architecture of the microstate networks of patients with ADHD tend to have lower values of small-worldness. Small-worldness is a property of some networks in which most nodes are not neighbors of each other but can be reached from every other node by a small number of steps. It was observed that the microstate networks of healthy individuals are more efficiently wired, showing high small-worldness, and are more clustered and hierarchically organized. Previous works using fMRI (Functional Magnetic Ressonance Imaging) studies evaluated brain functional connectivity and found similar results, this means that the topological architecture of the studied microstates tend to show similarities with the topology of functional connectivity networks (Wang et al., 2009).

According to Figure 3 for local efficiency measures, only microstates B and D showed significant differences. The topologies of microstates B (D) of patients with ADHD tend to present small (high) local efficiency, that can be understood as a measure of the fault tolerance of the network, indicating how well each subgraph exchanges information when a node is eliminated.

These measures were used to train kNN, MLP and SVM model, as described in Section 2.5, in order to classify healthy controls and ADHD patients, i.e., two class problem. The means and standard deviations of the results are shown in Table 1. As can be noted, all results were above 95% and the best classification result was obtained using the kNN classifier that obtained mean accuracy of 95.51% and standard deviation of 2.99.

Table 1. Classification results using selected metrics (normal and ADHD individuals).

Cassifier	**Mean accuracy (%)**	**Std.**
kNN	95.51	2.99
MLP	95.12	3.20
SVM	95.46	2.66

Next, the ability of such measures to distinguish between ADHD subtypes was assessed. Previous works have suggested that the EEG of interval timing processes differ between ADHD subtypes. The reason is that interval timing task depends on specific neurotransmitters and region brain network mechanisms, which have been shown to be altered in patients with ADHD (Hwang et al., 2010; Smith et al., 2013; Bluschke et al., 2018). Thus, in order to assess these selected characteristics to distinguish between ADHD subtypes, Table 2 shows the classification results (means and standard deviations) for the three-class problem (healthy, ADD and ADHD-C individuals). As can be observed, the best result was for SVM which obtained mean accuracy of 92.82% and standard deviation of 3.42.

Table 2. Classification results using selected metrics (healthy, ADD and ADHD-C individuals).

Cassifier	**Mean accuracy (%)**	**Std.**
kNN	88.66	4.49
MLP	92.48	3.24
SVM	92.82	3.42

In addition to the characteristics selected visually by analyzing boxplot graphics, the classification process was also evaluated using all global and local metrics, presented in Section 2.4. Using all metrics, the learning models were more successful in the classification task. In other words, the combination of all metrics extracted from the microstate networks proved to be more efficient in the classification task than using only small worldness and local efficiency measures. The classification results for the problems of two and three classes can be seen in Table 3. Thus, the global and local metrics extracted from the microstate networks proved to be promising both in the identification of patients with ADHD, presenting an average accuracy of 100% using SVM, as well in the identification of ADHD subtypes, with an average accuracy of 99.19% and standart deviation of 1.42 using MLP.

Table 3. Classification results using all metrics.

	2-class Problem		**3-class Problem**	
Classifier	Mean Acc.(%)	Std.	Mean Acc.(%)	Std.
kNN	99.93	0.38	98.24	1.71
MLP	99.93	0.37	99.19	1.42
SVM	100	0.00	99.07	1.25

Previous studies have reported that changes in ERP-microstates may be potential biomarkers in the diagnosis of ADHD (Brandeis et al., 2002; Albrecht et al., 2015) and studies related to other brain diseases evaluated the characteristics of the microstates using statistical properties such as Frequency of Occurrence, Duration Time, and Transition Probabilities (Khanna et al., 2015; M. Michel and Koenig, 2017). Each property can be interpreted based on the underlying neural activities. Then, the frequency of occurrence represents the tendency of microstates to be active, the average duration represents the temporal stability of each microstate, while the transition probabilities extract the asymptotic behavior of transitions between microstates (Khanna et al., 2015). We used such features of the microstates to perform the same experiment of Table 3, however, the classifiers were not successful in the classification, as showed in Table 4, being the mean accuracy obtained by SVM of 68.80% (two-class problem) and mean accuracy obtained by SVM and kNN of 33.13% (three-class problem). The Frequency of Occurrence, Duration Time, and Transition Probabilities from microstates were calculated using the Microstate EEGlab Toolbox (Poulsen et al., 2018).

Table 4. Classification results using classic microstates features.

	2-class Problem		**3-class Problem**	
Classifier	Mean Acc.(%)	Std.	Mean Acc.(%)	Std.
kNN	65.94	4.86	33.13	6.02
MLP	57.55	6.59	32.57	6.06
SVM	68.80	2.65	33.13	4.55

The most recent works involving the use of machine learning to identify ADHD use deep learning techniques with EEG signals (Vahid et al., 2019; Dubreuil-Vall et al., 2020).The work of Vahid et al. (2019) was the first study showing that deep learning methods applied to EEG data are capable to dissociate between patients with ADHD and healthy controls with accuracy up to 86%. In their work was used EEGNet model as a deep learning architecture. That model was previously examinaded in regards to ERP (Event-Related Potentials) such as the P300, visual-evocked and sensory motor rhythms (SMR).

Using the same database as Vahid et al. (2019), this work proposes a different methodology of analysis using techniques of graph theory to modeling and extract features of microstates networks. The advantages of the proposed method in relation Vahid et al. (2019) is also making a good separation between the subtypes of ADHD and the ability to obtain greater accuracy with less computational effort, since the proposed technique produced good results without the need to apply deep learning models, which require greater time and computational capacity.

4. CONCLUSION

In this paper was proposed a method that combines EEG microstates with graph theory in order to identify ADHD individuals. This method allows to model and interpret each microstate as a complex network. In addition, the model asses the distintion of the ADHD subtypes and the automatic classification resulted in an average accuracy of 99% with metrics extracted from microstate networks. This result indicates that the method is promising in the detection of ADHD and subtypes.

In future work, other brain diseases can be analyzed and, possibly, detected using the proposed method, e.g., diseases that have similar symptoms and that are often difficult to differentiate early. Different statistical models can also be proposed in the analysis of the relationship between pairs of EEG electrodes in order to obtain other models of microstate networks. Moreover, different metrics can be evaluated to increase the reliability of the proposed method.

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