ICA Model Order Estimation Using Clustering Method

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Abstract. *In this paper a novel approach for independent component analysis (ICA) model order estimation of movement electroencephalogram (EEG) signals is described. The application is targeted to the brain-computer interface (BCI) EEG preprocessing. The previous work has shown that it is possible to decompose EEG into movement-related and non-movement-related independent components (ICs). The selection of only movement related ICs might lead to BCI EEG classification score increasing. The real number of the independent sources in the brain is an important parameter of the preprocessing step. Previously, we used principal component analysis (PCA) for estimation of the number of the independent sources. However, PCA estimates only the number of uncorrelated and not independent components ignoring the higher-order signal statistics. In this work, we use another approach – selection of highly correlated ICs from several ICA runs. The ICA model order estimation is done at significance level $\alpha = 0.05$ and the model order is less or more dependent on ICA algorithm and its parameters.*

Keywords

EEG classification, brain computer interface, blind source separation, independent component analysis, ICA model order, clustering.

1. Introduction

Our previous works ([1] and [2] among others) were targeted on the movement classification from electroencephalogram (EEG) signals. The aim was to develop a simple movement classification method of EEG signal based on hidden Markov models (HMM) classifier. The developed method has been further improved; one of the improvements we are working on is the amendment of the EEG preprocessing. Our work is focused on the implementation of a technique allowing getting a better signal-to-noise ratio (SNR) than the commonly used Laplacian filtering. Independent component analysis (ICA) represents one possible approach to reach this goal. Although the application of the ICA has been a fast expanding research area and many scientific teams have been engaged in investigation of its contribution to biosignal processing, the important question of the ICA model order selection is still open [3].

A widely used approach to estimate the number of independent sources is based on the usage of principal component analysis (PCA). However, PCA estimates only the number of uncorrelated and not independent components ignoring the higher-order signal statistics. Despite this fact, PCA is commonly used in many works. For example, in work [4], PCA is used for dimension reduction of original 122-channel magnetoencephalography (MEG) data to the dataset containing only the first 20 principal components (PCs). Work [5], which describes EEG data decomposition, uses PCA in order to estimate ICA model order. The ICA model order of 59-channel EEG is estimated at 95% confidence interval and the ICA model order varies in the range of 33-37 depending on EEG data type. Work [6] uses PCA as a preprocessing tool for ICA, and in this way PCA reduces 52-channel EEG to 15 PCs. On the other hand, work [7] describes PCA and ICA methods and evaluates the PCA method as an unsuitable one for ICA model order estimation.

The authors of work [8] perform ICA decomposition several times with different initialization and each computed independent component (IC) is represented by a single equivalent current dipole (ECD). Further, they suppose that only ICs which are independent of algorithm initialization are task-relevant ones.

In the previous works [9], [10] we described a slightly different method for estimation of the number of ICs which is based on selection of highly correlated ICs from several ICA runs. In this work, we describe an improved version based on the previous one which also exploits the results of several ICA runs, and these results are proceeded by a clustering method.

2. Blind Source Separation

Blind source separation (BSS) is a method which aims at recovering unobserved source signals from their mixture or transformation. The observations are typically obtained by means of a set of sensors, where each sensor receives a different mixture of the source signals. It is assumed that no information is available about the mixing transformation and the source signals are not observed. The formulation of such a problem cannot be completely general since it would not be solvable. Therefore, there are several models of the mixing transformation which somehow restrict the generality of the task. There are three basic

models used in the field of BSS: an instantaneous linear mixing model, a convolutional mixing model, and a noisy model. Each of these models is used for a specific application [11].

A direct application of the linear BSS model can be found in biomedical engineering [4], [12] since the measured EEG or MEG signals fit the linear model [13], [14]. Thus, we will deal with the linear model which can be described as follows:

$$\mathbf{X} = \mathbf{AS} \tag{1}$$

where $\mathbf{X} \in m \times N$ is an observation matrix containing observed signals in rows, matrix $\mathbf{S} \in n \times N$ contains unknown source signals (hidden components), unknown matrix $\mathbf{A} \in m \times n$ is called mixing matrix, N is the number of available samples, n is the number of sources and m is the number of sensors. The goal of BSS is to estimate both unknowns from the observations $\mathbf{X}$ and in principle it is done by inverting a mixing process:

$$\mathbf{Y} = \hat{\mathbf{S}} = \mathbf{WX} \tag{2}$$

where $\mathbf{W} \approx \mathbf{A}^{-1}$ is called separating or demixing matrix and matrix $\mathbf{Y}$ contains estimated ICs in rows. The general BSS problem requires $\mathbf{A}$ to be an $m \times n$ matrix, with $m \geq n$ (i.e. there are at least as many mixtures as original sources). From the theoretical point of view, an equal number of sources and sensors ($n = m$) is of the greatest importance.

2.1 Independent Component Analysis

A powerful method to perform BSS is independent component analysis (ICA) whose fundamental assumption is that the sources are mutually independent. ICA algorithm formulations are based on a wide variety of principles, including mutual information, maximum likelihood, higher-order statistics (HOS), and others [11].

Despite such a wide variety, all ICA algorithms are very similar. Most of ICA methods try to estimate the mixing matrix $\mathbf{A}$, or its inverse $\mathbf{W}$, by optimizing an appropriate cost-function which measures the degree of statistical independence among the estimated ICs, or the deviation from a Gaussian distribution (using the central limit theorem, a mixture of independent non-Gaussian sources becomes more Gaussian). As a consequence, this highlights a potential limitation of ICA when it is used for biomedical signal processing. ICA using this technique can only resolve independent sources which have non-Gaussian distributions (or at most only one source having a Gaussian distribution).

It is difficult to imagine that we are estimating the original source signals without knowing the parameters of the mixing process. In fact, it is not possible to uniquely estimate the original source signals without any a priori knowledge. However, one can estimate them up to certain indeterminacies (sign, scaling, and permutation) [11].

3. ICA Model Order Estimation

There is a lot of existing ICA algorithms; we chose a well known algorithm FastICA [15] for the processing owing to its good properties: fast convergence and numeric robustness. The second one which we used for our research is EFICA algorithm [16] which is an improved version of FastICA.

Before ICA application, EEG signals were centered (mean value suppression) and whitened by PCA without any dimension reduction for the reasons mentioned in section 1. Let us assume that we have EEG recorded from m scalp electrodes and after PCA we still have m channels but whitened ones.

The proposed algorithm for the estimation of ICA model order is based on repeated EEG decomposition by the given ICA algorithm with random ICA initial conditions (measure of ICA stability) and processing of ICA results by a clustering method. We exploit the fact that the obtained ICs can be divided into two classes: those independent of the initial conditions of the ICA algorithm (macroscopic brain sources) and those dependent on the initial conditions of the ICA algorithm (microscopic brain sources, noise). From this point of view, only ICs representing macroscopic brain sources can be relevant and task related.

3.1 EEG Database Properties

At first we summarize basic properties of the used EEG database which are needed for an evaluation of the proposed algorithm for ICA model order estimation.

The research was done with the database originally recorded for physiology study [17]. Database contains EEG recordings of 7 subjects performing two kinds of movements: distal right index finger flexion and proximal right shoulder elevation [1], [17]. EEG was recorded using 59 scalp electrodes. Recorded raw EEG was examined visually later on. Artifacts were suppressed and EEG was segmented into 10sec length epochs with the movement localized in the 5th second. The EEG used by our study (ICA processed) was not filtered by any surface filter (Laplacian among others) prior to ICA decomposition in order not to negatively influence the numerical stability of the IC estimation. The data contains 27 realizations of movement, each of them with 5,000 samples.

3.2 Measure of ICA Stability

Since each ICA algorithm is an iterative one it needs an initialization (the first estimation of demixing matrix) for its run and the results of the given ICA algorithm are less or more dependent on its initialization. From this point of view, it is necessary to determine how much the given algorithm is dependent on its initialization or how stable results it provides.

For this analysis the EEG decomposition is repeated N_R times with the demixing matrix randomly initialized prior to IC decomposition in order to determine whether the used ICA algorithm converges to the same results for various initialization.

To determine whether the estimated ICs are stable for all different initializations the correlation of ICs can be used. Each estimated IC is computed as follows:

$$\mathbf{y}_k = \sum_{i=1}^{m} w_{ki} \mathbf{x}_i \qquad (3)$$

where $\mathbf{y}_k$ is the k-th estimated IC (the k-th row of matrix $\mathbf{Y}$), w_{ki} is the ki-th element of matrix $\mathbf{W}$ and $\mathbf{x}_i$ is the i-th observed signal　　(the i-th row of matrix $\mathbf{X}$); thus each IC is described by a corresponding row $\mathbf{w}_k$ of matrix $\mathbf{W}$. Since we need to know only whether the given IC is estimated equally for all initializations the correlation distance of rows of matrix $\mathbf{W}$ is used for measuring the similarity between ICs.

Let us assume that the number of sources is equal to the number of sensors ($m = n$); thus matrix $\mathbf{W} \in n \times n$. Further, let us assume that $\mathbf{W}^{(k)}$ denotes the demixing matrix for the k-th initialization matrix and $\mathbf{w}_i$ denotes the i-th row of matrix $\mathbf{W}$. Now, we can imagine each row of matrix $\mathbf{W}$ as a point in the n-dimensional space. Rows of matrices $\mathbf{W}^{(k)}$ describing the same IC are similar and they create clusters in this n-dimensional space. Thus the estimation of ICA model order and selection of well estimated ICs is based on ICA result clustering. The fact that rows of matrices $\mathbf{W}^{(k)}$ create clusters in n-dimensional space will be proved as follows: we compute correlation distances among rows of one matrix $\mathbf{W}^{(k)}$ (let us assume $k = 1$). The correlation distance between the r-th and s-th row of one given matrix $\mathbf{W}$ is computed as follows:

$$d_{rs} = 1 - \frac{\sum_{i=1}^{n} (w_{ri} - \overline{w}_r)(w_{si} - \overline{w}_s)}{\sqrt{\sum_{i=1}^{n} (w_{ri} - \overline{w}_r)^2} \sqrt{\sum_{i=1}^{n} (w_{si} - \overline{w}_s)^2}} \qquad (4)$$

where w_{ri} and w_{si} are the ri-th and si-th elements of matrix $\mathbf{W}$, $\overline{w}_r$ and $\overline{w}_s$ are mean values of $\mathbf{w}_r$ and $\mathbf{w}_s$ computed as follows:

$$\overline{w}_k = \frac{1}{n} \sum_{i=1}^{n} w_{ki} . \qquad (5)$$

For our analyzed EEG database containing 59 channels ($n = 59$) $\min(d_{rs}) = 0.34$ and $\max(d_{rs}) = 1.53$ which proves the abundant dissimilarity of rows of demixing matrix $\mathbf{W}^{(k)}$ and possibility to cluster rows in n-dimensional space. The correlation distance between the rows is depicted in Fig. 1.

Because of the ICA indeterminacies we cannot resolve the sign of IC; thus we can obtain the same or very similar IC differing in its sign in repeated ICA decomposition. To avoid this problem we use original ICs and the same ones multiplied by -1 as an input data for clustering.
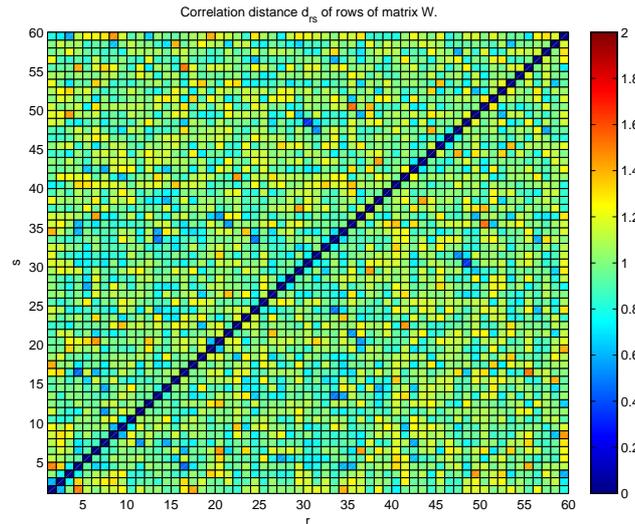

Fig. 1. Correlation distance d_{rs} between rows $\mathbf{w}_r$ and $\mathbf{w}_s$ of one given matrix $\mathbf{W}^{(k)}$.

For N_R times repeated ICA we obtain a dataset containing each IC N_R times with sign $+$ and N_R times with sign $-$. According to (6) we form one final matrix $\mathbf{M}$ containing all matrices $\mathbf{W}^{(k)}$ multiplied by $+1$ and -1.

$$\mathbf{M} = \left(\mathbf{W}^{(1)T} \dots \mathbf{W}^{(N_R)T}, -\mathbf{W}^{(1)T} \dots -\mathbf{W}^{(N_R)T} \right)^T . \qquad (6)$$

The next step is computation of the correlation distance according to (4) between rows $\mathbf{m}_r$ and $\mathbf{m}_s$ of matrix $\mathbf{M}$ ($\mathbf{m}_i$ denotes the i-th row of matrix $\mathbf{M}$) for these indexes: $r = 1 \dots M_r - 1$, $s = r + 1 \dots M_r$, where M_r denotes the number of rows of matrix $\mathbf{M}$. The histogram of correlation distances between rows $\mathbf{m}_r$ and $\mathbf{m}_s$ is depicted in Fig. 2 for subject 4, distal movement, algorithm FastICA. The highest frequency of d_{rs} is in range $\langle 0.5; 1.5 \rangle$ but here are also two local maxims around $d_{rs} = 0$ and $d_{rs} = 2$. These areas ($d_{rs} < 0.1$ and $d_{rs} > 1.9$) represent ICs which are estimated independently of initialization. On the basis of Fig. 2 we suppose that the rows of matrix $\mathbf{M}$ can be easily clus-
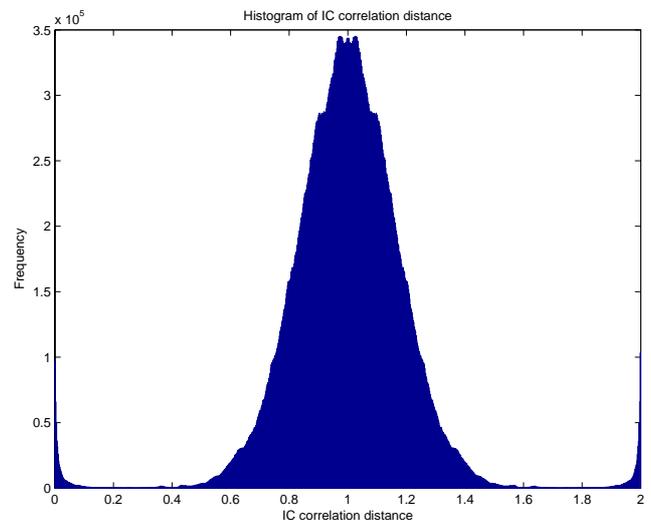

Fig. 2. Histogram of correlation distances between rows $\mathbf{m}_r$ and $\mathbf{m}_s$ of matrix $\mathbf{M}$.

tered in n-dimensional space. If we take any criteria for cluster size we can also estimate the ICA model order. Moreover, with the help of clustering we can eliminate one of ICA indeterminacies – order of ICs.

3.3 Clustering Method

An input data which are used for clustering are correlation distances d_{rs} among rows of matrix **M**. There are a lot of clustering algorithms and methods, for example k-means algorithm, hierarchical clustering, self organizing maps, or self organizing trees. Since we do not know how many clusters are needed we cannot use k-means algorithm (it requires a number of clusters). We use hierarchical clustering with an input condition for forming clusters – cluster size or more precisely correlation distance among elements in a cluster. Clusters are formed according to link criteria (link method). Basic link methods are: single, complete, and average. We chose average method which can be described as follows:

$$d(r,s) = \frac{1}{n_r n_s} \sum_{i=1}^{n_r} \sum_{j=1}^{n_s} \text{dist}(x_{ri}, x_{sj}) \qquad (7)$$

where function dist() denotes computation according to (4), x_{ri} is the i-th element of cluster r and similarly x_{sj} is the j-th element of cluster s, n_r and n_s are numbers of elements in cluster r and s. For selected link method we determined threshold value $d_{avr} = 0.1$ which ensures high correlation (similarity among rows $\mathbf{m}_{i\cdot}$ higher than 90%). With this constrains for forming clusters data obtained form N_R runs of ICA were clustered.

There are 254 clusters for subject 4 and distal movement, each of these clusters contains a different number of elements. The sizes of clusters are depicted in Fig. 3. The clusters containing only a small number of elements (less than 10) were created in consequence of ICA instability; they do not represent relevant ICs. On the other hand, there
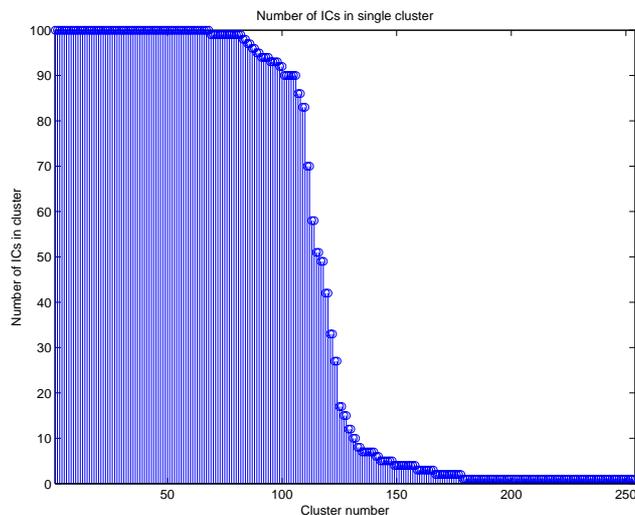
are many clusters containing N_R elements ($N_R = 100$) in Fig. 3; these clusters represent ICs found in each runs. There are 68 clusters for subject 4 and distal movement. Since a half of clusters contains the same elements with opposite sign, the real number of IC is 34. With this approach we assume occurrence of these ICs in all analyzed matrices (100% occurrence). We put this criterion aside and in the following text we will concern ourselves with clusters containing ICs estimated at significance level $\alpha = 0.05$. In other words, we looked for clusters containing at least 95 elements (this holds for $N_R = 100$). There are 90 clusters including at least 95 elements for subject 4 and distal movement, and 98 clusters for subject 4 and proximal movement – 45 and 49 stable ICs. These partial results are summarized in Tab. 1.

	dist	prox
$N_R = 100$	68	86
$N_R = 99$	14	4
$N_R = 98$	2	2
$N_R = 97$	2	6
$N_R = 96$	2	0
$N_R = 95$	2	0
$\sum_{N_R=95}^{100}$	90	98

Tab. 1. Number of clusters which contain N_R elements, subject 4, distal and proximal movements.

The next step after clustering is elimination of duplicate clusters which contain rows of matrix **M** multiplied by −1. At first we compute average element (centroid) in n-dimensional space for each cluster according to the following term:

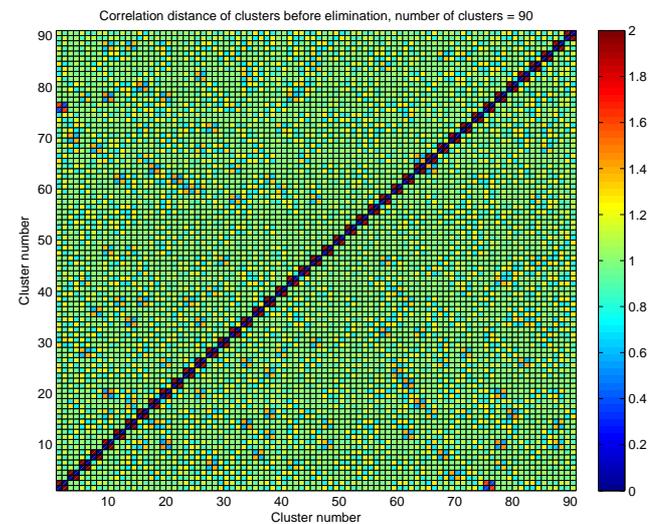$$\overline{\mathbf{x}}^{(c)} = \frac{1}{N_c} \sum_{i=1}^{N_c} \mathbf{x}_i^{(c)} \qquad (8)$$

Fig. 3. Size of clusters – number of similar rows of matrix **M** in numbered cluster, sorted downwardly.

Fig. 4. Correlation distance among elements $\overline{\mathbf{x}}_i^{(c)}$, subject 4, distal movement.

algorithm	nonlinearity	Subject													
		1d	1p	2d	2p	3d	3p	4d	4p	5d	5p	6d	6p	7d	7p
FastICA deflation	gauss	9	7	7	10	9	4	6	13	8	8	12	8	8	5
	pow3	6	13	14	6	16	15	5	23	17	15	22	7	13	8
	skew	28	25	26	21	29	27	17	32	28	24	34	20	23	20
	tanh	22	17	16	15	26	20	16	23	11	21	27	24	17	14
FastICA symmetric	gauss	33	33	41	45	36	37	40	42	42	39	38	34	30	35
	pow3	39	35	48	44	47	43	44	44	39	49	44	45	48	43
	skew	40	37	51	44	44	38	39	41	38	39	44	43	48	44
	tanh	46	34	45	49	44	43	45	49	41	39	49	42	42	40
EFICA symmetric	gauss	37	42	41	45	41	38	41	47	45	40	38	39	33	38
	pow3	45	41	50	44	46	44	45	45	40	48	44	46	48	45
	rati	39	35	44	45	44	40	48	49	45	41	43	41	34	35
	tanh	44	40	46	50	45	42	51	50	44	38	52	43	39	40
PCA – 95% confident int.		34	35	31	31	28	31	35	37	29	29	29	28	35	33

Tab. 2. ICA model order estimation for various ICA algorithms – FastICA and EFICA. For comparison there is model order estimation by PCA for 95% confident interval in table. Subject #d stands for distal movement and #p stands for proximal movement.

where $\mathbf{x}_i^{(c)}$ is the i-th element in cluster c, N_c is the number of elements in cluster c, and $\overline{\mathbf{x}}_i^{(c)}$ is average element (centroid) in cluster c. Among elements $\overline{\mathbf{x}}_i^{(c)}$ we again computed correlation distance according to (3); this is shown in Fig. 4 and it is obvious that there are duplicate elements. For elimination of duplicate elements, we can use the fact that correlation distance between two elements differing in sign is 2. Thus from each pair of clusters we choose only one and among residual clusters we again compute correlation distance to prove that we discarded the correct ones. The number of residual clusters is equal to the number of stable ICs found in all analyzed matrices; this number is 45 for subject 4 and distal movement and 49 for proximal movement. The correlation distance of residual centroids is in interval ⟨0.6, 1.4⟩ which also proves sufficient dissimilarity of rows $\mathbf{m}_i$ forming different ICs.

4. Results

The basic properties of the used EEG database have been already summarized above and the results obtained by described method will be given in this chapter.

4.1 EEG Decomposition Results

The proposed algorithm for estimation ICA model order was tested mainly with algorithm FastICA. We also used another algorithm, EFICA which is an improved version of the FastICA algorithm (it contains a test of saddle points and improves convergence). The FastICA algorithm was used in both approaches – deflation and symmetric [15]. The FastICA algorithm was also tested with all available nonlinearities: gauss, tanh, pow3, and skew [15]. The EFICA algorithm [16] was tested only in symmetric approach (it does not contain deflation approach). Non-

linearities of the EFICA algorithm which we used are the following: gauss, rati, pow3, and skew [16]. The results for the mentioned algorithms and their nonlinearities are summarized in Tab. 2.

The FastICA algorithm with deflation approach provided the worst results – we can see how the number of stable ICs is varying across subjects. This statement holds for all nonlinearities in this approach and we can see that the maximum number of stable ICs is twice or even three times higher than minimum number of stable ICs for given nonlinearity. The similar results are provided in work [5]. From this point of view, the FastICA algorithm with deflation approach is not suitable for decomposition (results are very dependent on algorithm initialization).

The number of ICs independent of initialization is higher for the FastICA algorithm with symmetric approach. We can see that the number of stable ICs is very similar for each subject and nonlinearity. Nonlinearity tanh seems to be the best one and only slightly better than the other ones.

Further improvement can be achieved by using the EFICA algorithm. The number of stable ICs is higher by 1 to 3 for all nonlinearities which are common for the FastICA and EFICA and almost all subjects. These results prove the fact that the EFICA is improved version of the FastICA.

For comparison there are also results obtained by PCA in Tab. 2. The ICA model order of 59-channel EEG is estimated at 95% confidence interval [5]. However, PCA estimates only the number of uncorrelated and not independent components ignoring the higher-order signal statistics.

Finally, we tried to estimate the accuracy of estimation of ICs. For this task we computed the correlation distance between centroid and all elements in the given cluster. From these distances the mean value and
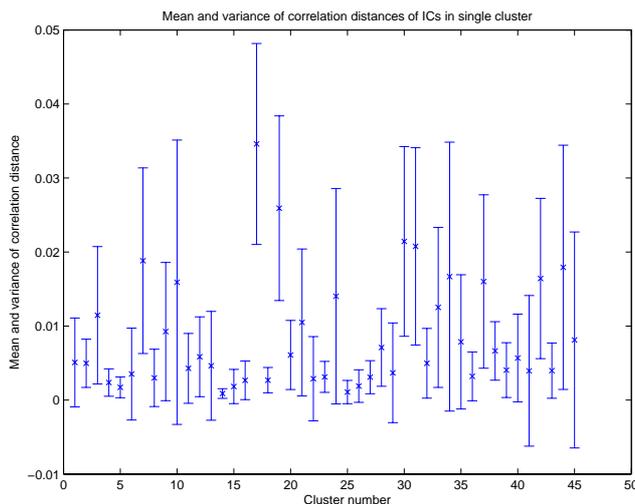
Fig. 5. Estimation accuracy of each IC in the given cluster. Algorithm FastICA (symmetric, tanh), subject 4 and distal movement.

variance were computed and these statistics are depicted in Fig. 5.

In Fig. 5 it may be seen that the mean value and variance of the correlation distance is smaller than 0.01 in most cases (correlation distance is normalized which means that it is in $\langle 0; 1 \rangle$). Moreover, for proximal movement we obtained a smaller mean value and variance of the correlation distance, and also the number of stable ICs is slightly higher for proximal movement than for distal movement. This finding probably originates in the fact that larger part of the sensorimotor area is activated during proximal movement than during distal movement [17] and ICA can utilize it.

5. Conclusion

We estimated ICA model order by means of the stability test of the ICA algorithm (FastICA and EFICA) from movement EEG. According to the previous works we expected a symmetric approach to provide more stable results. Our test was based on repeated EEG decomposition and subsequent correlation and clustering of estimated ICs.

The number of stable ICs (ICA model order) was determined with the help of correlation distance and clustering method. It was shown that the rows of a demixing matrix **W** are sufficiently different and similar rows in demixing matrices create clusters in *n*-dimensional space. We used hierarchical clustering and link method average for cluster forming with different size. EEG decomposition was repeated 100 times and we looked for the cluster with at least 95 elements and average correlation distance $d_{rs} = 0.1$. For these parameters we found the numbers of stable ICs, which are summarized in Tab. 2.

We proved that the symmetric approach provides more stable results than the deflation one. The most stable results were obtained with the EFICA algorithm and tanh or pow3 nonlinearity, see Tab. 2.

At this time we cannot determine which ICs are movement-related and which are not (the found stable ICs involve both). For further analysis it is necessary to determine which ICs are movement-related.

Acknowledgments

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Pavel SOVKA – see Radioengineering, vol. 7, no. 4, December 1998.

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