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ICA's bug: How ghost ICs emerge from effective rank deficiency caused by EEG electrode interpolation and incorrect re-referencing

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Independent component analysis (ICA) has been widely used for electroencephalography (EEG) analyses. However, ICA performance relies on several crucial assumptions about the data. Here, we focus on the granularity of data rank, i.e., the number of linearly independent EEG channels. When the data are rank-full (i.e., all channels are independent), ICA produces as many independent components (ICs) as the number of input channels (rank-full decomposition). However, when the input data are rank-deficient, as is the case with bridged or interpolated electrodes, ICA produces the same number of ICs as the data rank (forced rank deficiency decomposition), introducing undesired ghost ICs and indicating a bug in ICA. We demonstrated that the ghost ICs have white noise properties, in both time and frequency domains, while maintaining surprisingly typical scalp topographies, and can therefore be easily missed by EEG researchers and affect findings in unknown ways. This problem occurs when the minimum eigenvalue λ_{min} of the input data is smaller than a certain threshold, leading to matrix inversion failure as if the rank-deficient inversion was forced, even if the data rank is cleanly deficient by one. We defined this problem as the effective rank deficiency. Using sound file mixing simulations, we first demonstrated the effective rank deficiency problem and determined that the critical threshold for λ_{min} is 10^{-7} in the given situation. Second, we used empirical EEG data to show how two preprocessing stages, rereferencing to average without including the initial reference and non-linear electrode interpolation, caused this forced rank deficiency problem. Finally, we showed that the effective rank deficiency problem can be solved by using the identified threshold ($\lambda_{min} = 10^{-7}$) and the correct re-referencing procedure described herein. The former ensures the achievement of effective rank-full decomposition by properly reducing the input data rank, and the latter allows avoidance of a widely practiced incorrect re-referencing approach. Based on the current literature, we discuss the ambiguous status of the initial reference electrode when re-referencing. We have made our data and code available to facilitate the implementation of our recommendations by the EEG community.

KEYWORDS

rank deficiency, principle component analysis, independent component analysis, dimension reduction, spherical spline interpolation, re-reference, average reference

Introduction

Independent component analysis (ICA) has been widely used in EEG studies for the purposes of both artifact rejection and signal extraction (Bell and Sejnowski, 1995; Makeig et al., 1996). The ICA model can be described as indicated in the following expression.

$$x = As, \tag{1}$$

where x represents the observed multi-channel EEG signals at scalp electrodes, A is the mixing matrix, and s is the multi-channel timeseries activation of the latent independent components (ICs). ICA solves this problem such that A makes the time-series of ICs temporally maximally independent. The physiological interpretation of the ICA model is that the mixing process with no delay by A corresponds to the volume conduction effect and the temporal independence of s corresponds to the neuroscientific assumption that when groups of neurons are engaged in different processes, the observed electric signals from them should be independent. Thus, temporal independence is identified as functional independence.

ICA relies on several assumptions and requirements to be reliable and accurate. Violating them may lead to inaccurate findings or even processing failure, depending on which assumption is violated. In this technical study, we focused on one of these cases in which ICA produces erroneous results without being detected by the algorithm. We also caution against the widely adopted, incorrect practice of re-referencing EEG data to average, which is a human error that also causes this issue.

Defining the problem: The effective rank deficiency

When we see multi-channel EEG recording as a matrix, the rank of the data refers to the number of linearly independent channels. For example, standard unipolarly referenced 64-ch EEG data have a data rank of 64. When the multi-channel data consist of linearly independent channels, the data are considered rank-full. On the other hand, if a pair of scalp electrodes adjacent to each other are bridged due to an injection of an excessive amount of saline water, for example, these pairs of electrodes are electrically connected and record identical signals redundantly. In this case, two channels have identical data and the data rank is no longer 64; it is reduced to 64-1 = 63. When the number of channels is larger than the number of linearly independent sources, the data are called rank-deficient. Data rank is important in ICA because ICA produces the same number of ICs as the data rank number, not the apparent number of scalp electrodes. When ICA is forced to produce more ICs than the data rank, the process fails and yields ghost ICs, at least in the case of implementation in EEGLAB (Delorme and Makeig, 2004). The ghost IC is akin to ICA's "bug," which we have examined to determine its properties in the time, frequency, and spatial domains.

Whether a pair of channels are linearly dependent or not is a qualitative question that can be answered with yes or no. However, the mathematical meaning of the rank has more granularity, as shown as follows. First, we applied the eigenvalue decomposition to the channel-by-channel covariance matrix of the input EEG data matrix. Next, we obtained the *condition number c* by dividing the largest eigenvalue λ_{max} by the smallest eigenvalue λ_{min} (Strang, 2006).

$$c = \frac{\lambda_{max}}{\lambda_{min}}.$$
 (2)

A very large condition number c indicates that the input data matrix is close to being rank-deficient and singular (i.e., not invertible), if not fully rank-deficient. A geometric explanation for this situation is that a pair of vectors are near parallel but not completely parallel. Since λ_{max} is usually bounded by the range of the measurement, λ_{min} is the dominant factor that determines the scale of c. Based on this observation, we propose the effective rank deficiency, which we define as follows: an input EEG data matrix is effectively rank-deficient if λ_{min} is non-zero, but ICA (and any other operation that involves matrix inversion) results show signs of forced rank-deficient decomposition. The effective threshold of λ_{min} is expected to be dependent on the application, but providing a demonstration under controlled conditions should still be useful for gaining insight regarding this issue. For example, when EEG data have a very small λ_{min} , such as 10^{-8} , and ICA results show at least one ghost IC, then the EEG data are considered effectively rank-deficient. If the same data are differently processed so that λ_{min} is slightly larger, such as 10^{-6} , and ICA results do not show any ghost ICs, then the EEG data are effectively rankfull. We aimed to achieve the following goals in our study: 1) to determine the effective threshold using a simulation study; 2) to confirm the signatures of forced rank-deficient decomposition, namely ghost ICs, using empirical EEG data; and 3) to identify solutions and recommendations for this problem. In the following paragraphs, we discuss two EEG preprocessing stages in which effective rank deficiency can arise.

Case 1: Incorrect re-referencing practice causes effective rank deficiency

In performing standard scalp-EEG preprocessing, there are two stages during which effective rank deficiency can occur. The first stage is re-referencing, which is often performed to the average potential because it is easy to calculate and it minimizes local bias if uniform electrode spacing is applied (Bertrand et al., 1985; Nunez and Srinivasan, 2006). However, the 'problem' arises from an incorrect implementation of average re-referencing, at least as observed in EEGLAB. First, we review the basic facts of EEG rereferencing in the following paragraphs.

It has been common practice to use a unipolar reference (i.e., potentials at multiple scalp locations are measured against a

potential at one, often non-scalp, location) when recording scalp EEG data. The unipolarly referenced data have three key properties (Hu et al., 2019): 1) rank-deficient by 1; 2) no memory effect; and 3) orthogonal projector centering. The first property is the most important and naturally leads to the second property. We focus on the first two properties in the following paragraph.

The first property can be rephrased as follows: the unipolarly referenced scalp EEG data are always rank-deficient by 1 if the initial reference is taken into account. For those who have not yet considered this, the statement may sound counterintuitive and could even be a stumbling stone. Imagine the case of a simple bipolar recording: two electrodes record a one-channel signal as a difference (voltage is by definition a difference between potentials at two locations). This relation of two-electrodes-to-one-signal is the origin of rank deficiency by 1. Because unipolarly referenced recording can be understood as the parallel repetition of bipolar recordings for multiple electrodes while keeping the same reference location, the same rank deficiency by 1 is inherited. This is the EEGcontext explanation to support the need for rank deficiency by 1 to be corrected before re-referencing. If we follow the convention that *n*-channel data refer to the data that contain *n* non-zero, full-rank data channels, we need to ensure n+1 channels by adding an additional zero-filled channel to the rank-full EEG data before re-referencing.

The second property, the "no memory effect," indicates that, as long as we follow the correct re-referencing, we can re-reference to any other location without changing the linear property of the data *if the data are unipolarly referenced*. In other words, one can rereference unipolarly referenced EEG data offline from the original reference location A to the new reference location B, then from B to C, and from C to A, which brings back the original data without any change, regardless of the history of prior re-referencing processes. However, once we re-referenced to the average potential, for example, we would need to re-reference back to a unipolar reference with any chosen electrode for the next re-referencing. Repeating average-referencing after rejecting the initial reference electrode invalidates the data and should be avoided.

Based on these facts, there is no ambiguity about how to rereference the data properly. Unfortunately, the current implementation of the re-referencing process in the past and current versions of EEGLAB (ver. 2022.0 or prior) does not follow this correct practice. Additionally, there are several implementation issues in the related solutions, which further complicate the problem:

- 1. EEGLAB does not account for the initial reference electrode. Therefore, EEGLAB reduces data rank by re-referencing. This violates the first and second properties described previously (Hu et al., 2019).
- 2. Although EEGLAB's implementation of the ICA (*pop_runica*) includes an effective rank deficiency checker, the hard-coded detection of $\lambda_{min} < 10^{-7}$ at the bottom (suggested by SH) does not operate to make the input data effectively rank-full by reducing input data dimensions; instead, it forces ICA into effectively rank-deficient decomposition.
- 3. Even if the data rank is ensured to be cleanly deficient by one [which can be detected by using the *rank* () function] through EEGLAB's re-referencing process, EEGLAB calculates λ_{min} ,

which reintroduces a non-zero small number (typically $<10^{-10}$) *via* numerical error. This non-zero noise forces effectively rank-deficient decomposition.

In this study, we focused on these processes to quantify the margin of the effective rank deficiency. We report the influence of using the initial reference on λ_{min} in applying average reference.

Case 2: Electrode interpolation can cause effective rank deficiency

The second common practice that can produce effective rank deficiency in EEG data is the spatial interpolation of rejected electrodes (considered artifactual) using non-linear methods such as spherical spline (Perrin et al., 1989), which is the default interpolation method implemented by EEGLAB. Although linear interpolation leads to a clean rank deficiency, non-linear methods result in interpolated electrode signals that are not exactly the weighted linear sum of other electrodes, leading to effective rank deficiency. Similar to Case 1, we quantified the effect of the non-linear electrode interpolation on λ_{min} to evaluate the margin of the effective rank deficiency.

The goal of the current study

The study goals included the following: 1) to determine the effective λ_{min} threshold; 2) to confirm the signatures of forced rankdeficient decomposition, namely ghost ICs, using empirical EEG data; and 3) to confirm solutions for this problem. For these goals, we split the study into two parts. The first part was a simulation study using auditory signals to determine the smallest λ_{min} that causes the ghost IC issue. We parametrically manipulated the mixing weights to systematically vary λ_{min} from 10^{-1} to 10^{-12} logarithmically to determine where ICA starts to fail. In other words, the aim of the first part was to perform a torture test for ICA to determine its tolerance to the progressively smaller λ_{min} .

The second part was an investigation of how effective rank deficiency arises from the two EEG preprocessing stages, namely, incorrect re-referencing and electrode interpolation, using empirical EEG data and EEGLAB. Based on the critical threshold of λ_{min} determined in the first part, the goal of the second part was to evaluate λ_{min} obtained from incorrectly re-referenced data, correctly re-referenced data.

Materials and methods

Audio signal mixing simulation

As an homage to the original ICA demonstration performed in the late 1990s by four researchers from the Salk Institute (Terry Sejnowski, Te-Won Lee, Scott Makeig, and Tzyy-Ping Jung), we recorded the following four sentences as independent sound recordings:

"Independent component analysis is a new data tool that is sensitive to higher-order structure in multidimensional data" (JL). "Neural networks that perform information maximization may emulate processes that drive evolution and brain organization" (MM).

"Infomax ICA is proving successful at modeling complex biological time series and imaging data" (TPJ).

These sound demonstrations are available at https://github.com/ MakotoMiyakoshi/Effective-Rank-Deficiency.

In the current study, the audio files were recorded using a condenser microphone Perception 200 (AKG), a USB audio interface E-MU 0404 (Creative), and Thinkpad T42 (IBM) with a sampling rate of 44,100 Hz. Offline, the signals that were shorter than 9.288 s were zero-padded at the end, so they all were of equal length. The signals were z-scored.

The four-channel audio signals were mixed differently to generate four mixed signals. The mixing matrix M that was used is as follows:

$$M = \begin{bmatrix} 1 & 1-\rho & 0.5 & 0.5 \\ 1-\rho & 1 & 0.5 & 0.5 \\ 0.5 & 0.5 & 1 & 0.5 \\ 0.5 & 0.5 & 0.5 & 1 \end{bmatrix},$$

where ρ varied logarithmically from 10⁻¹ to 10⁻¹², which gives the ground truth of the minimum eigenvalue λ_{min} . The mixed signals were imported into EEGLAB 2022 (Delorme and Makeig, 2004) and decomposed using Infomax ICA (Bell and Sejnowski, 1995). The criterion for successful decomposition was to hear a single person's voice when playing the decomposed signals.

In addition to the required conditions relating to the goal of the study, we took advantage of this simulation to perform several confirmatory demonstrations in hope of helping novice ICA users directly experience important properties of ICA by listening to the decomposed signals, including 1) the time-invariant property by shuffling the 1-s time blocks before ICA; 2) undercomplete data decomposition by using four three-source mixings with four channels—see Chapter 13 of the book *Independent Component Analysis* (Hyvärinen et al., 2001); and 3) overcomplete data decomposition by using three four-source mixings with three channels. In addition, the difference between correct and incorrect re-referencing to average is demonstrated to provide an additional example that can be tested by ears. For these demonstrations, the following mixing matrix *M* was used.

$$M = \begin{bmatrix} 1 & 0.9 & 0.8 & 0.8 \\ 0.8 & 1 & 0.7 & 0.9 \\ 0.7 & 0.8 & 1 & 0.9 \\ 0.6 & 0.8 & 0.7 & 1 \end{bmatrix}.$$

Empirical EEG data demonstrations

We designed a demonstration of the two cases of effective rank deficiency caused by 1) incorrect re-referencing and 2) non-linear electrode interpolation using EEGLAB's tutorial dataset (128 Hz sampling, 32 channels, 238.3 s), which was obtained from a previously published study (Makeig et al., 1999). To briefly describe the data, a visual attention experiment was performed,

λ_{min}	Description of the decomposed signals
> 10 ⁻⁶	Normal decomposition obtained
10 ⁻⁷	Two ICs had mixed voices
10 ⁻⁸	One IC had mixed voices, and one IC became white noise
10 ⁻⁹	Complex numbers appeared in the mixing matrix
10^{-10}	Complex numbers appeared in the mixing matrix
10 ⁻¹¹	Two ICs had mixed voices, and one IC became silent
10 ⁻¹²	Yielded only three ICs

TABLE 1 Results from the audio signal mixing simulation.

where stimuli appeared in any of five squares arrayed horizontally above a central fixation cross. In each experimental block, one (target) box was a color that was different from the rest. Whenever a square appeared in the target box, the subject was asked to respond quickly with a right thumb button press. If the stimulus was a circular disk, the subject was asked to ignore it. These data were constructed by concatenating 3-s epochs from one subject, each containing a target square in the attended location ("square" events, left-hemifield locations 1 or 2 only), followed by a button response ("rt" events). The data were stored in continuous data format to illustrate the process of epoch extraction from continuous data. There were 80 trials included in the analysis, regardless of the conditions.

For the case of incorrect average referencing, we compared two re-referencing approaches: one with the addition of the initial reference channel (i.e., a channel with zero-filled data) and the other approach without (current default method). We calculated λ_{min} for each case to determine how much margin they had before causing effective rank deficiency. The additional ICA was performed using the Infomax algorithm implemented in EEGLAB's *runica*() function with default parameters ("extended," 1). The subsequent equivalent dipole fitting was applied to ICs using Fieldtrip library (Oostenveld et al., 2011) and the electric forward model based on the Montreal Neurological Institute (MNI) template (Evans et al., 1993; Collins et al., 1994).

For the case of spherical spline channel interpolation (Perrin et al., 1989) implemented in the default EEGLAB option, we performed leave-one-out cross-validation (LOOCV) to balance the possible effect of spatial selection on the minimum eigenvalue obtained. The final number of channels used was 30, after rejecting two non-EEG channels. Mean values were reported.

The properties of the ghost ICs were evaluated for the case of spherical spline interpolation, in both the frequency (power spectral density, PSD) and time domains (event-related potential, ERP).

Results

Audio signal mixing simulation

Logarithmic variation of λ_{min} from 10^{-1} to 10^{-12} demonstrated that ICA fails when $\lambda_{min} < 10^{-7}$. The results are summarized in Table 1. The source audio signals, their linear mixings, the

TABLE 2 Results from the ICA demonstration using audio signals.

Description of the conditions	Description of the decomposed signals	
Randomly shuffling the 1-s blocks	Normal decomposition obtained	
Undercomplete (three sources and four mixings)	Two ICs mixed; success after PCA dimension reduction to 3	
Overcomplete (four sources and three mixings)	All ICs mixed	

TABLE 3 Results from the empirical EEG demonstration.

Operation	Description of the decomposition	Order of λ_{min}
Control data	Normal decomposition obtained	100
Re-referencing (correct)	Normal decomposition obtained	100
Re-referencing (incorrect)	Ghost IC appeared	10 ⁻¹⁰
Electrode interpolation	Ghost IC appeared	10^{-10}



FIGURE 1

Left, power spectral density (PSD) of all the independent components (ICs) after applying spherical spline electrode interpolation. The PSD plot for the ghost IC is highlighted in red, and those for other ICs are represented in gray. Note that the ghost IC's PSD does not follow the 1/f exponent or the large line noise at 60 Hz that is commonly present in other ICs. Right, ERP, the time-domain representation, of the ghost IC compared with the first-ranked (i.e., it had the largest variance) "Normal" IC. The shaded area indicates one standard error of the mean. The ghost IC was ranked as the last IC (i.e., it had the smallest variance), and the averaged potential did not show any ERP modulation. The ghost IC showed surprisingly normal spatial distribution with below-average (3.6% vs. mean 20.2%, SD 12.0) residual variance from the equivalent dipole fitting, and it largely overlapped with the "Normal" IC.

decomposed signals obtained, and the demonstrating summary movies are available at https://github.com/MakotoMiyakoshi/ Effective-Rank-Deficiency/.

The results from the ICA demonstration are summarized in Table 2. Note that the condition of random shuffling of the 1-s blocks should not impact ICA performance because all the time frames are shuffled differently to minimize learning bias at the

beginning of each iteration of the gradient descent process. Also, note that, due to the lack of an effective countermeasure for the rank-deficient input data, the decomposition under the undercomplete condition failed. It was necessary to manually specify the correct rank number by using the "pca" option, which performs dimension reduction by rejecting principal components, as many as required, by counting the ones with the smallest eigenvalues. These results from the case of undercomplete ICA replicated the predictions made by the classic study on the nature of ICA (Hyvärinen et al., 2001). We will discuss the recommended solution for the case of EEG preprocessing in which data are known to be rank-deficient. The source audio signals, their linear mixings, and the decomposed signals obtained are available at https://github.com/MakotoMiyakoshi/Effective-Rank-Deficiency/.

Empirical EEG data demonstrations: Ghost ICs are ICA's bug

For the case of re-referencing, the correct method, i.e., including the initial reference when re-referencing and then discarding the initial reference channel, resulted in a successful rank-full decomposition. Meanwhile, the incorrect method, i.e., without including the initial reference ICA, failed to decompose the signals. ICA failed for the case of non-linear electrode interpolation using spherical spline interpolation. These results are summarized in Table 3.

The spatial, temporal, and frequency properties of the ghost IC obtained are illustrated in Figure 1. The frequency domain analyses confirmed that the ghost IC did not follow the patterns of other ICs and showed unreasonable independence. The ghost IC's flat PSD resembled white noise. In the time domain analysis, the ghost IC did not show visible ERP modulation. The ghost IC was ranked as the last IC among others, indicating it had the smallest variance. Visual inspection of the scalp topography of the ghost IC indicated surprisingly normal spatial distribution. The subsequent equivalent current dipole fitting produced a very good result, and the residual error was as small as the most dominant IC (i.e., the first-ranked IC after variance sorting; 3.5% vs. 3.6%, respectively). The scalp topography of the ghost IC showed overlap with the most dominant IC. This suggests the ghost IC's dependence on the most dominant IC and the formation of a subspace.

Discussion

What is the bug, after all?

The main problem we were motivated to address in this study is that even if the input data are confirmed to be rank-full (e.g., using MATLAB's rank () function), under the condition where the minimum eigenvalue λ_{min} is smaller than 10⁻⁷, the effective rank is no longer full from the viewpoint of ICA, which causes rank deficiency. Such decomposition produces ghost ICs, which forces the ICA to produce a number of components that is larger than the effective rank; hence, the "bug". We investigated the two major causes of this issue in the scenario of standard EEG preprocessing, namely an incorrect average reference calculation and the non-linear spherical spline interpolation for electrode interpolation. To avoid this issue, we propose two solutions: 1) apply the correct average referencing, and 2) calculate the effective data rank that is used for PCA dimension reduction in applying ICA.

The first goal of the study: To determine the practical threshold of λ_{min}

Although the effective threshold is expected to be dependent on each application, with the given conditions and tools that are described in this study, we determined that the critical threshold of λ_{min} exists between 10^{-6} and 10^{-7} . This means that whenever we perform ICA, we should check whether the criterion $\lambda_{min} > 10^{-6}$ is met to prevent ghost ICs from appearing. For better validation of this critical threshold, more empirical tests are required. We hope user information and feedback on this point are systematically accumulated to improve the accuracy of this estimate.

The second goal of the study: To confirm the signature of forced decomposition of rank-deficient data

In this study, we established a reproducible procedure to generate ghost ICs. We confirmed the properties of the ghost ICs as follows: 1) power spectral density (PSD) does not follow the pattern that all other ICs follow, such as the 1/f exponent, the alpha peak, or even the large 60-Hz line noise peak. The PSD of the ghost IC was rather flat, which indicates a resemblance to white noise; 2) the ghost IC did not show the temporal structure of the event-related potential, which is shown, as expected, by other ICs. This observation is in line with the PSD finding that the data appear similar to white noise; 3) counterintuitively, the scalp topography of the ghost IC had a normal appearance. The subsequent equivalent dipole fitting showed a good result, and the residual variance was below average. We speculated that the ghost IC may appear as an imperfect or broken subspace of the most dominant IC. If this is the case, it suggests that a ghost IC should be paired with a dominant IC with a largely overlapping scalp topography. Overall, the ghost IC showed clearly distinguishable properties in the time-frequency domain, which is a useful clue for suspect detection. Meanwhile, the presence of ghost ICs can be easily missed upon visual inspection of the IC scalp topographies.

The third goal of the study: To confirm the solution

The effective rank deficiency caused by EEGLAB's rereferencing is a human error as there is no theoretical reason for data rank to become deficient during this operation. Although we wait for EEGLAB's update and correction, we provide a modified function "reref.m" that can be used to overwrite the relevant code as a temporary patch to address the issue; the patch code can be downloaded at https://github.com/MakotoMiyakoshi/Effective-Rank-Deficiency. On the other hand, to address the effective rank deficiency introduced by non-linear electrode interpolation, the best solution is to explicitly input the effective rank for ICA, i.e., the number of eigenvalues larger than 10⁻⁶. Using the MATLAB command line, it can be calculated as follows:

dataRank = sum(eig(cov(double(EEG.data'))) > 1E - 7).

Then, enter the obtained number as input for the "pca" option for runica.m or "pcakeep" for runamica.m. Meanwhile, we suggest changing the default behavior of the rank checker implemented in pop_runica () so that when it detects $\lambda_{min} < 10^{-7}$, the algorithm uses the number of the effective rank by using the "pca" option to prevent ghost ICs from appearing.

Is using PCA before ICA always bad?

One study made a claim that applying the principal component analysis (PCA) before applying ICA for the sake of dimension reduction requires caution because abusing PCA for excessive dimension reduction deteriorates the quality of ICA (Artoni et al., 2018). This conclusion itself is not surprising based on the definition of lossy compression, i.e., greater dimension reduction at the cost of greater information loss. However, our confirmatory demonstrations using sound files showed that undercomplete ICA (i.e., number of sources < number of mixings) failed, and specifying the correct data rank by using PCA dimension reduction to manually set the rank-full decomposition helped ICA yield the sources correctly. The failure in the undercomplete decomposition and the use of PCA dimension reduction to make it effectively rank-full or reduce non-signal-subspace redundancy are predicted by the classical study on ICA, per Chapter 13 of the book by Hyvärinen et al. (2001). Thus, the study by Artoni and colleagues should not be taken as a message that using PCA before ICA is unconditionally bad. Rather, our view is that their study focused on the upper bound (i.e., abuse) of the use of PCA in preprocessing, while the study by Hyvärinen and colleagues focused on the lower bound (i.e., shortage) of the use of PCA. We recommend that PCA dimension reduction should be used whenever effective rank deficiency is detected. One important point Artoni and colleagues clarified, in our opinion, is that obtaining 95% of the variance after PCA reduction could be still considered aggressive, whereas Hyvärinen and colleagues casually hinted at 90% as a general idea. Because the scalp-recorded EEG data are heavily correlated due to volume conduction, the variance distribution across PCs is severely skewed. For the case of applying ICA to realistic scalp EEG recordings, it is an overcomplete decomposition (i.e., more sources than electrodes) as long as the data signal-to-noise ratio is reasonably high. Thus, for the standard EEG data decomposition, the recommended practice is to use PCA only for rank adjustment and to avoid possible overfitting (i.e., data length is too short for the number of electrodes). The EEGLAB developers have been suggesting a heuristic criterion, indicating that the input data length should be greater than (number of electrodes)² x 20 (Makeig and Onton, 2011), given a 256 Hz sampling rate or lower. If the input data length is shorter than this criterion, the use of PCA is recommended to avoid overlearning. Unfortunately, the current implementation of the data rank checker in EEGLAB is suboptimal because it is unable to reduce the data rank using PCA to allow effective rank-full decomposition. We propose that the number of λ larger than 10^{-6} should be routinely calculated to enable rank-guided ICA for improvement.

Ambiguous status of the initial reference in the literature when re-referencing

The difference between "correct" and "incorrect" re-referencing could be trivial if the matrix inversion is not calculated; hence, the rank of data does not matter. Otherwise, the widely used spherical spline channel interpolation (Perrin et al., 1989; Kang et al., 2015) would have been considered an issue. However, as the use of a linear spatial filter including ICA became popular, the impact of the problem caused by effective rank deficiency also became nonnegligible.

The literature on EEG research shows that one of the earliest studies on the use of average reference is a one-page article with a large schematic illustration that clearly shows the "rank-deficient by 1" property (Offner, 1950). Another early study clearly indicated that the initial reference is included when rereferencing the unipolarly referenced EEG to the average potential (Osselton, 1965). Thereafter, however, the status of the initial reference electrode when re-referencing became ambiguous. Whether the initial reference should be included or not is not discussed in a later theoretical study (Bertrand et al., 1985). Similarly, whether n in p.35 (Dien, 1998), N in Eqs 7.8-7.10 (Nunez and Srinivasan, 2006), and m in Eq. 3 (Dong et al., 2017) include the initial reference electrode or not remains ambiguous. We contacted these authors and confirmed that they included the initial reference when re-referenced data were calculated (Dezhong Yao, Joseph Dien, Ramesh Srinivasan, and Paul Nunez, personal communications). We summarized the problem that relates to the confusion about average referencing in Figure 2. There are actually 2×2 ways to calculate average-referenced data, depending on whether the initial reference is included in calculating the average and whether it is recovered after subtraction. However, there is only one incorrect method, which is method "A", as this approach does not include the initial reference electrode in any way. As a result, after re-referencing, the data rank is deficient by 1, indicating a loss of information. The other three methods, "B," "C," and "D", do not cause this rank deficiency, and the original information and data, in a linear sense, are preserved. In this sense, these three methods are all valid. Interestingly, in our personal communications, four researchers indicated that "D" was the correct method, while two researchers indicated that method "B" was correct. Note that the differences between "B" and "D" are only scalar and minor (for an n-channel system, the denominator is $\frac{1}{n}$ for "B" and $\frac{1}{n+1}$ for "D" and "C"). Unfortunately, some of the popular EEG analysis toolboxes, such as EEGLAB (Delorme and Makeig, 2004) and Fieldtrip (Oostenveld et al., 2011), take an approach that follows method "A". This may be due to the lack of a clear description of this point in the previous literature. We suggest that the authors of these toolboxes adopt a correct re-referencing method to prevent the problems of effective rank deficiency and ghost ICs from arising in the downstream process. Meanwhile, some other applications, such as EP Toolkit (Dien, 2010), support correct re-referencing, thereby eliminating the potential issue of "ghost PCs" in later PCA decomposition.

Definitions

A channel shows bipolar recording data derived from a pair of electrodes.

A unipolar-referenced EEG dataset has <u>N data channels</u> with <u>rank N</u> derived from <u>N + 1 electrodes</u>. The (N + 1)th electrode is the <u>initial reference</u>.

The (N + 1)th channel refers to the reference electrode's self connection, which is by definition <u>0</u>.

Problem

When I re-reference the data to the average potentials,

Answe	er list Results	
	I calculate the average potentials from ${N \atop N+1}$ channels	m and I subtract it from ${N \\ N+1}$ channels.

A: $\{N, N\}$ B: $\{N, N + 1\}$ C: $\{N + 1, N\}$ D: $\{N + 1, N + 1\}$ A: N-channel data with rank (N - 1). B: (N + 1)-channel data with rank N. C: N-channel data with rank N. D: (N + 1)-channel data with rank N.

FIGURE 2

Summary description of the problem, which relates to confusion about average referencing. There are 2×2 ways to calculate the average reference. Note that rank deficiency occurs only when using method A. For the case of method B, one may discard any one channel, except the initial reference, to retain the data rank *N* and make the averaged reference data rank-full. We found that there is debate regarding the correctness of methods B, C, and D; however, in the linear sense, they are all the same since they maintain the same rank between the points before and after the average referencing. The difference between subtracting the average potentials of the *N* and *N* + 1 channels only relates to scalar differences.

Future study

A potential future study on the issue of effective rank-deficient ICA includes an investigation of the validity of other ICs when a ghost IC appears. Because of the multivariate nature of ICA, obtaining one invalid IC could undermine the quality of all other ICs. However, as demonstrated in this study, a ghost IC may be paired with a certain normal IC as a pseudo-subspace, and the impact on other ICs may be limited. We attempted to address this in our study but encountered an issue with the reproducibility of the ICA. Using the same tutorial data, we confirmed that using the options "extended," 1, "Irate," 1e-5, and "maxsteps," 2000 allowed reproducible results in IC scalp topographies and their variancesorted orders across 10 runs. However, we decided not to include this test in the current report for practical purposes; when we find a ghost IC in our results, the whole batch of datasets processed using the same code should be re-processed anyway, for the sake of perfection. In that sense, investigating the validity of other ICs in the presence of a ghost IC is not very meaningful.

Conclusion

To conclude, effective rank deficiency occurs in electrode interpolation because the spherical spline interpolation is a nonlinear method; however, it should not be a concern in rereferencing if re-referencing is applied correctly by including the initial reference. We propose a simple effective rank deficiency checker, which should be used to perform the effective rank-full decomposition as it reduces the data dimension using PCA dimension reduction whenever it detects effective rank deficiency. For future steps, it is advised that, when preprocessing EEG data, the proposed effective rank is explicitly calculated before using any solution involving matrix inversions.

Data availability statement

Publicly available datasets were analyzed in this study. The data can be found at https://github.com/MakotoMiyakoshi/Effective-Rank-Deficiency.

Author contributions

SH contributed to the original concept and the final solution indicated in the conclusion. HK and MM contributed to the conception and design of the study. JL, SC, and MM collected data and performed initial analysis. HK and MM analyzed the final data and generated figures and tables. MM contributed to contacting authors of previous studies. All authors contributed to the manuscript revision, and read and approved the submitted version.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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