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Recovering Wood and McCarthy's ERP-prototypes by means of ERP-specific procrustes-rotation

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HIGHLIGHTS

- Conventional rotation methods fail to recover Wood and McCarthy's prototypes.
- Conventional rotations result in a substantial amount of variance misallocation.
- Two new rotation-methods based on ERP-characteristics are proposed.
- The new rotation-methods need no a priori knowledge on treatment-effects.
- The new rotation-methods: reduce variance misallocation.

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ABSTRACT

Background: The misallocation of treatment-variance on the wrong component has been discussed in the context of temporal principal component analysis of event-related potentials. There is, until now, no rotation-method that can perfectly recover Wood and McCarthy's prototypes without making use of additional information on treatment-effects.
New method: In order to close this gap, two new methods: for component rotation were proposed. After Varimax-prerotation, the first method identifies very small slopes of successive loadings. The corresponding loadings are set to zero in a target-matrix for event-related orthogonal partial Procrustes-(EPP-) rotation. The second method generates Gaussian normal distributions around the peaks of the Varimax-loadings and performs orthogonal Procrustes-rotation towards these Gaussian distributions. Oblique versions of this Gaussian event-related Procrustes- (GEP) rotation and of EPP-rotation are based on Promax-rotation.
Results: A simulation study revealed that the new orthogonal rotations recover Wood and McCarthy's prototypes and eliminate misallocation of treatment-variance. In an additional simulation study with a more pronounced overlap of the prototypes GEP Promax-rotation reduced the variance misallocation slightly more than EPP Promax-rotation.

Comparison with Existing Method(s): Varimax- and conventional Promax-rotations resulted in substantial misallocations of variance in simulation studies when components had temporal overlap. A substantially reduced misallocation of variance occurred with the EPP-, EPP Promax-, GEP-, and GEP Promax-rotations.
Conclusions: Misallocation of variance can be minimized by means of the new rotation methods: Making use of information on the temporal order of the loadings may allow for improvements of the rotation of temporal PCA components.

1. Introduction

Principal components analysis (PCA; Harman, 1976) can be used for the quantification of event-related potentials (ERP) of the electroencephalogram. Many empirical studies have used this method for ERP analysis (e.g., Barry and De Blasio, 2013; Dien et al., 2003; Donchin et al., 1975; Leue et al., 2012; Tenke et al., 2008) and important methodological advice for optimal PCA of ERP is available (Dien, 2012; Dien et al., 2005; Dien et al., 2007; Donchin, 1989; Donchin and Heffley, 1979; Donchin et al., 1977, 1978; Kayser and Tenke, 2003; Kayser and Tenke, 2005). In temporal PCA the time points are the variables whereas the channels of

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each participant are the cases. It is possible to disentangle temporally overlapping electrical brain processes with temporal PCA (Chapman and McCrary, 1995). In spatial PCA the channels are the variables whereas the time points of each participant are the cases. Temporal and spatial PCA use the complete information of the multi-channel ERP for component identification, which is impossible with simple baseline-to-peak measures.

However, an early methodological concern was the misallocation of treatment variance on the wrong ERP component in temporal PCA. Wood and McCarthy (1984) demonstrated in a simulation study based on temporally overlapping, sinusoidal prototypes (with a single peak of each prototype) that treatment effects were misallocated on the wrong PCA component. However, Beauducel and Debener (2003) have shown that the misallocation effects shown by Wood and McCarthy (1984) were overemphasized because of an unrealistically large statistical power. Moreover, Beauducel and Leue (2015) eliminated the misallocation of variance by means of a treatment-based component rotation, which they termed 'effect-rotation'. Variance-misallocation was eliminated in their simulation study when the loading shape of the effect-rotated components was identical to the prototypes of Wood and McCarthy (1984). This demonstrated again the relevance of component rotation for the validity of ERP-PCA results. Component rotation is necessary because an interpretation of the unrotated components is typically very difficult or impossible whereas rotation towards simple structure typically leads to loading matrices that can more clearly be interpreted (Harman, 1976). Dien (2010) noted that the extent to which rotation yields interpretable solutions depends on the extent to which the rotation criteria match the characteristics of the true components. In the context of ERP-components the correspondence between the morphology of the true population components (prototypes) and the criterion for component rotation determines the improvements that are possible through component rotation.

The misallocation effects found by Wood and McCarthy (1984) were related to Varimax-rotation (Kaiser, 1958). Although they overemphasized the misallocation effects due to an unrealistic statistical power (Beauducel and Debener, 2003), a notable difference between the population component loading shape and the Varimax-rotated loading shape occurred in their simulation study. In order to illustrate this difference, the loading parameters reported by Wood and McCarthy (1984) were entered into IBM SPSS (Version 23) software for Varimax-rotation. The number of zero-loadings on component 2 is substantially larger in the prototypes than in the corresponding loadings of the Varimax-rotated component 2 (see Fig. 1A and B). Moreover, some Varimax-loadings on component 3 are smaller than the corresponding loadings of the population component. The coefficient of congruency (Tucker, 1951) of the Varimax-loadings with the prototypes was 1.000 for component 1, 0.984 for component 2, and 0.990 for component 3. This indicates that the Varimax-criterion does not perfectly fit the definitions of Wood and McCarthy's prototypes 2 and 3.

Although Effect-rotation successfully eliminated variance-misallocation, this rotation method uses information from experimental conditions (e.g., target versus non-target) that is external to the loading shape for component definition. This might be interesting, for example, when a specific effect can be expected for the channels of a temporal component. Accordingly, the fronto-parietal shape of a P300 component (Sutton and Ruchkin, 1984) might be used as a criterion for effect-rotation of components. Although effect-rotation might be used for the improvement of component-rotations, there are situations where an *a priori* definition of the components by means of experimental conditions is impossible. Therefore, the aim of the present paper is to explore whether the variance-misallocation found by Wood and McCarthy (1984) can be also eliminated by means of a component rotation that is not based on *a priori* information on experimental conditions. First, the precision in recovering the prototypes by means of different methods of component rotation was investigated. Second, two criteria for component rotation were proposed that allow for an improved rotation of the prototypes. Third, these criteria were implemented in two different methods for component rotation and they were investigated in a simulation study based on Wood and McCarthy's (1984) parameters. Fourth, a simulation study based on correlated prototypes was performed in order to compare the performance of an oblique Promax-based version of the new rotation methods with conventional Promax-rotations. Note that Promax-rotation is typically based on a Varimax-prerotation (Hendrickson and White, 1964). The loadings of the Varimax-solution are raised to a given power (Kappa, typically between 2 and 4) with larger powers for more oblique rotations. The resulting target-matrix is then used for oblique Procrustes-rotation (Hurley and Cattell, 1962). The two rotation-methods proposed here are orthogonal and their oblique versions are based on Promax-rotation (i.e., the Varimax-solution is replaced by the respective other solution).

1.1. *Rotations of Wood and McCarthy's prototypes*

The previous results imply that the problem of variance-misallocation was due to Varimax-rotation. In order to explore whether the impossibility to recover the prototype loadings and the related variance-misallocation was specific to Varimax-rotation, further rotations of the prototypes provided by Wood and McCarthy (1984) were investigated. Since the prototypes and the Varimax-rotated components are both orthogonal, the difference in the loading shape (Fig. 1A and B) cannot be due to the effect of orthogonal rotation of an oblique prototype. However, substantial secondary loadings as they occur on the Varimax-rotated component 2 typically indicate that oblique component rotation would be more appropriate in order to minimize the secondary loadings. Dien (2010) recommended oblique component rotation. According to Dien (2010) the spatial overlap of ERP components should induce inter-correlations between the components of temporal PCA. Moreover, Dien's (2010) simulation study demonstrated that the results from oblique Promax-rotation (Hendrickson and White, 1964) and from oblique Infomax-rotation (Bell and Sejnowski, 1995) were superior to the results from orthogonal Varimax-rotation. Oblique Infomax-rotation performed best for spatial PCA and (oblique) Promax-rotation performed best for temporal PCA. Although Wood and McCarthy's (1984) simulation study implies a temporal PCA, oblique and orthogonal Infomax-rotation, as well as Promax (Kappa = 4)-rotation, and Oblimin (Delta = 0)-rotation of the prototypes were performed with IBM SPSS software (Fig. 1C–F). The orthogonal and oblique Infomax-rotations were performed by means of the method proposed by Jennrich (2001, 2002) with the SPSS Matrix-syntax as it has been proposed by Bernaards and Jennrich (2005).

It turned out that the loadings from orthogonal Infomax-rotation were nearly identical to the Varimax-loadings (Fig. 1B and C). The corresponding coefficients of congruence can be found in Table 1 (for Prototype inter-correlations = 0.00). The loadings of component 2 in the time-window of component 3 (temporal overlap) were reduced by means of oblique rotation (see Fig. 1D–F). The loadings of component 2 in the time-domain of component 3 were nearly zero for oblique Infomax-rotation, indicating that this rotation was most successful in minimizing the temporal overlap of component 2 with component 3. Accordingly, the oblique Infomax loadings of component 2 were perfectly congruent with the respective prototype (Table 1). However, oblique rotations resulted in a substantial correlation between component 2 and 3. The correlation between these components was 0.54 for Promax (Kappa = 4)-rotation, 0.45 for oblique Infomax-rotation, and 0.49 for