OPTIMIZING PRINCIPAL COMPONENTS ANALYSIS OF EVENT-RELATED POTENTIALS: MATRIX TYPE, FACTOR LOADING WEIGHTING, EXTRACTION, AND ROTATIONS

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Abstract

Objective: Given conflicting recommendations in the literature, this report seeks to present a standard protocol for applying principal components analysis (PCA) to event-related potential (ERP) datasets.

Methods: The effects of a covariance versus a correlation matrix, Kaiser normalization vs. covariance loadings, truncated versus unrestricted solutions, and Varimax versus Promax rotations were tested on 100 simulation datasets. Also, whether the effects of these parameters are mediated by component size was examined.

Results: Parameters were evaluated according to time course reconstruction, source localization results, and misallocation of ANOVA effects. Correlation matrices resulted in dramatic misallocation of variance. The Promax rotation yielded much more accurate results than Varimax rotation. Covariance loadings were inferior to Kaiser Normalization and unweighted loadings.

Conclusions: Based on the current simulation of two components, the evidence supports the use of a covariance matrix, Kaiser normalization, and Promax rotation. When these parameters are used, unrestricted solutions did not materially improve the results. We argue against their use. Results also suggest that optimized PCA procedures can measurably improve source localization results.

Significance: Continued development of PCA procedures can improve the results when PCA is applied to ERP datasets.

Keywords: Event-related Potentials, Principal Components Analysis, Source Localization

Optimizing Principal Components Analysis Of Event-Related Potentials: Matrix Type, Factor Loading Weighting, Extraction, And Rotations

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Event-related potentials are the electrophysiological signals recorded from the scalp surface that are time-locked to an event of interest, such as the presentation of a word. The waveform recorded at a site on the head, typically over the course of a second, represents a complex superposition of different overlapping potentials, termed components. Such recordings can stymie visual inspection, especially when obtained with a high-density montage containing over a hundred recording sites. The complex superpositions involved can also complicate source localization efforts when trying to co-register with fMRI datasets.

A common approach for decomposing an ERP dataset into its constituent components is principal components analysis or PCA (Dien & Frishkoff, in press; Donchin, 1966; Glaser & Ruchkin, 1976; Möcks & Verleger, 1991). This method summarizes the relationships between the variables (such as recordings at each time point) as latent variables that ideally correspond to the individual components. While PCA latent variables are normally termed "components," to avoid confusion with ERP "components" this report will use the term "factors." We suggest this is a reasonable convention since "factor analysis" is used as a general term for principal component analysis (which normally uses the term "component") and principle axes factoring (which normally uses the term "factor"). We also suggest this is a reasonable convention since these two major types of factor analysis are essentially identical in the context of ERPs where the communalities are essentially at unity (during the initial factoring of the relationship matrix), so replacing the diagonal with the communalities does not materially change the relationship matrix (cf. Gorsuch, 1983). We also suggest this is reasonable because "factor analysis" is used as a generic term for both types of analysis. The term "components" will therefore be used to refer to coherent patterns of covariance in ERP data that can be usefully replicated and interpreted (Donchin, Ritter, & McCallum, 1978).

Principal Components Analysis

Although the ideal result of a PCA is to achieve a one-to-one relationship between the factors and ERP components, the unrotated factors are most likely combinations of ERP components. The reason for this is that the initial extraction criterion of maximizing variance for each successive factor can often be best met by including variance from multiple components. The rotation procedure seeks to establish a simpler relationship between the factors and the components that is more likely to correspond to constructs of interest (Gorsuch, 1983). In this simulation study, we operationally define simplicity as the extent to which a single factor corresponds to a single simulated component.

In order to do so, the eigenvectors are converted to factor loadings, a term that can refer to either the factor pattern matrix or the factor structure matrix. The factor pattern matrix is the beta weights for generating the variables from the factor scores (for the case where both the variables and the factor scores are standardized). The factor structure matrix is the correlations between the variables and the factors. For an orthogonal rotation (see below) the factor pattern matrix and the factor structure matrix are identical.

Most PCAs are conducted using the Varimax rotation (Kaiser, 1955), although others are available. In this approach, pairs of factors are rotated in the two-dimensional space formed by their two axes such as to maximize the sum of the variances of the squared loadings. The factors are systematically rotated in pairs until changes are negligible. This procedure has the effect that factor loadings tend to be as extreme as possible (either zero or high), a quality shared by other members of the Orthomax family of rotations (Gorsuch, 1983; Mulaik, 1972). This is an appropriate criterion for ERP datasets (especially for a temporal PCA) since most

ERP components (with the exception of DC shifts) tend to be restricted to a discrete set of time points.

Most implementations of Varimax utilize a later modification termed "Normal Varimax" (Kaiser, 1958), although some statistics packages like BMDP allow this to be turned off (Dixon, 1992, p. 357). In this procedure, prior to rotation, the factor loadings are reweighted by the communalities, the portion of the variance accounted for by each variable. This is done by dividing each factor loading by the communality. After rotation, the weighting process is reversed.

It is also possible to use covariances instead of correlations during the rotation step (as the factor loadings). This is essentially an alternative to the Kaiser normalization in that it represents a different way of weighting the factor loadings. Kayser and Tenke (2003) proposed applying this procedure to ERPs, terming them unstandardized solutions. We found this terminology to be somewhat confusing since there are several ways a solution may be standardized (such as the factor scores) and will therefore refer to such a procedure as using covariance loadings, as opposed to the usual procedure in which the loadings are correlations (Tabachnick & Fidell, 1989, p. 599).

A final, optional step is implemented by the Promax rotation (Hendrickson & White, 1964). In this step, a Procrustes algorithm is utilized to relax the orthogonality restriction by individually rotating each individual factor (in the factor pattern matrix) to a simpler solution (defined as larger high loadings and smaller low loadings) without regard to the other factors. Such a solution may be reasonably expected to better approximate the real underlying structure of the ERP component to the extent that it really is characterized by being temporally delimited (high for some time points and essentially zero for the others). Of course, factors may remain orthogonal, depending on the data. The amount of relaxation is determined by a parameter called Kappa.

The Issues

The impetus for ERP papers on PCA is that PCA was developed by statisticians primarily with psychometric data in mind and hence is optimized for questionnaire data rather than ERP data. There is therefore a need to evaluate what the most effective parameters are for ERP datasets. The present paper will evaluate potential choices for the relationship matrix, factor loading weighting, unrestricted solutions, and rotation.

1. Relationship Matrix. In the ERP literature reviews have recommended the covariance matrix (Curry, Cooper, McCallum, Pocock, Papakostopoulos, Skidmore, & Newton, 1983; Donchin & Heffley, 1979; Möcks & Verleger, 1991) but have also suggested the choice does not make a difference (Chapman & McCrary, 1995; van Boxtel, 1998). Studies continue to be published with both correlation (Liu & Perfetti, 2003) and covariance (Papo, P.-M., Hugueville, & Caverni, 2003) matrices. Comparisons with real data do suggest this choice makes a difference (Curry et al., 1983; Dien, Spencer, & Donchin, 2003b; Kayser & Tenke, 2003) but cannot say which is more accurate without inarguable knowledge of the underlying ERP components, which is not yet possible. Simulation studies have the strength of having known correct answers but are limited by their realism. An initial study using simulations (as well as real data) supports the use of covariance matrices (Kayser & Tenke, 2003). This report provides an even more realistic simulation study of this issue.

The sum-of-squares-cross-products (SSCP) matrix will not be addressed due to complexities outside the scope of these simulations. For average reference datasets, such as the present, the SSCP is essentially identical to the covariance matrix for temporal PCA because the average reference sets the mean for every time point to zero. For other reference schemes, the effect of the SSCP depends on reference site activity. To the extent that there is activity at the reference site, the inverse of the activity will be superimposed on the other recording sites, resulting in a non-zero mean. Mean correction (covariance and correlation matrices) will normally remove this mean (desirable) as well as shared activity that does not sum to zero (not desirable). For a mean mastoid reference, a SSCP matrix can result in a factor with the shape of the dataset means (Curry et al., 1983). For more information on the ramifications of reference choice, see (Dien, 1998b). For spatial PCA, the SSCP will also be identical to the covariance matrix to the extent that the head's surface is evenly and comprehensively sampled since the integral of the potential fields over a spherical surface will sum to zero. The SSCP will differ from the covariance matrix to an extent that will be dependent on the particular montage used relative to the orientation of the ERP components. Given the unpredictable effects that these parameters can have on the SSCP results, it is not recommended.

2. Factor loading weighting.

Another important parameter is choice of factor loading weighting during rotations. In a conventional truncated solution the majority of the factors are dropped with the result that some of the variance of each variable has been discarded (presumably noise variance). Some variables will be affected more by this process than others (presumably variables with a lower signal-to-noise ratio). Such variables will have lower communalities (the amount of the variance accounted for by the factor solution) and will hence have less influence on the rotation process.

In Kaiser normalization the loadings of each variable are divided by the square root of their communalities to ensure that each variable has equal influence on the rotation process (their communalities are normalized to all equal one for the duration of the rotation). Kaiser (1958) advocated the use of this procedure in his original formulation of the Varimax on the grounds that it counteracts the tendency for larger factors to dominate the rotation process. This has become such an integral part of the Varimax rotation that it is the default in statistics packages such as BMDP (Dixon, 1992, p. 357). The graphical user interface of SPSS does not give the option to turn Kaiser normalization off (SPSS, 2001), although it is possible through the command syntax interface. JMP does not even give the option to turn it off (SAS Institute, 2002).

Examining the effects of Kaiser normalization on ERP analyses is worthwhile since Kaiser based his recommendation on datasets in which the variables tended to have comparable amounts of signal. In ERP data, one would expect this procedure to also amplify the effect of the noise inherent in the inactive time points (which normally have very low communalities during rotation since the factors representing most of their noise have been dropped at the retention stage).

Software packages such as BMDP also offer the option of using covariance loadings rather than correlation loadings. Covariance loadings are factor loadings in which the loadings are multiplied by the variable variances in order to give more influence to the more active variables. This is essentially the opposite effect of the Kaiser normalization. An argument has been made for using this weighting scheme with ERP datasets (Kayser & Tenke, 2003). These two weighting schemes are mutually incompatible[1], so a three-way comparison between unweighted, Kaiser Normalization, and covariance loadings is needed. This report provides such a comparison for ERP datasets for the first time.

3. Unrestricted Solutions. Another issue is whether to truncate factor solutions prior to rotation, as is the norm or to use an unrestricted (or untruncated) solution. Kayser and Tenke (2003) argue that all factors should be retained in the final solution on the grounds that underextraction (retaining too few factors) degrades solution quality (Fava & Velicer, 1992, 1996; J. M. Wood, Tataryn, & Gorsuch, 1996).While this is a reasonable concern, there are also good arguments against this procedure. The chief problem is multiple comparison problems. A chief motivation for high-density ERP researchers to use PCA is to control multiple comparison problems. The procedure recommended by Kayser and Tenke (2003) could easily result in several hundred factors, and it is not clear what researchers are to do when presented with this situation. Obviously, investigators cannot choose a factor at random for formal analysis; however, a choice must necessarily be made as to which ones to formally analyze. Regardless of whether the choice is made on the basis of a visual inspection of the

waveforms or using a formal statistical test, it still constitutes an opportunity to capitalize on chance variations and hence a Type I error rate hazard. Consider a 128-channel dataset with two conditions and a one-second epoch digitized at 250 Hz. In the course of normal analysis, there are 128 channels times perhaps eight general time windows resulting in 1,024 possible comparisons. At an alpha of .05, this virtually guarantees 51 significant spurious results. Lack of independence between the channels means the situation is not actually quite so dire (the true dimensionality is likely less than 128) but it remains that such datasets are full of potential effects that do not replicate and are likely to be false positives. The most effective strategy is to use a priori knowledge about ERP components to identify real components such as the P300 but many components are not yet characterized. While multiple comparison procedures such as the Bonferroni are available they drastically reduce statistical power (in this case reducing the alpha threshold to 0.00005 for the Bonferroni).

PCA will help control the multiple comparison problem only for truncated solutions. A typical 12-factor temporal PCA solution reduces the number of comparisons from 1,024 to just 12 if one restricts the ANOVA to a single channel or uses a two-step PCA to generate a spatial factor from the temporal PCA results. As noted elsewhere (Dien, 1998a; Spencer, Dien, & Donchin, 1999, 2001), a straight temporal PCA will conflate different ERP components with similar time courses so a two-step PCA (temporo-spatial or spatio-temporal) is preferable. In a temporo-spatial PCA with 12 temporal factors followed by 5 spatial factors the total number of factors is 60 which still suffers multiple comparison problems but is a vast improvement over 1,024 potential comparisons. Furthermore, if one has a priori grounds for restricting analyses to a particular time window (such as the N400 window) then this can reduce the analysis to just five potential comparisons. If one also has a priori knowledge about scalp topography, one may be able to restrict the analysis to a single factor.

In contrast, an unrestricted temporal PCA would yield 250 factors (in the absence of collinearity, which is generally the case for ERP datasets). A temporo-spatial PCA with 5 spatial factors would balloon the number of factors to 1,250 leaving one with an unresolved multiple comparison dilemma. Even if one restricts analysis to a single window of interest (such as the N400 window), with so many temporal factors dozens will fall within this window; likewise with scalp topographies. We do not believe it is defensible to examine all these factors without some sort of control for multiple comparisons.

The question of whether to truncate also raises more fundamental issues of analysis philosophy. Consider, for example, the N400 component. This component is largely temporally invariant with a peak at about 400 ms. At an individual level, however, there will be variations in the exact time course even in the averaged waveform. In a truncated PCA, a single factor will generally capture the central tendency of the individual N400s since the initial factors of the unrotated solution are designed to capture the maximum possible variance; the variance corresponding to the sometimes subtle individual variations will be represented in the smaller factors that are dropped. In an unrestricted solution, on the other hand, it is entirely possible that each individual subject's version of the N400 will have a separate factor. Whether this is good or not depends on whether one is pursuing an analysis of the group central tendency or a more case study approach.

Kayser and Tenke (2003) acknowledge that overextraction can cause problems too (Fava & Velicer, 1992, 1996) but conclude that it is "a less serious problem" on the basis of another study (J. M. Wood et al., 1996) and their own data. Wood et al. (1996), however, point out that overextraction is still a serious problem and "recommended that researchers use reliable methods to estimate the number of factors before extraction" (p. 361). The following passage describes some of the drawbacks of overextraction:

> The effects of overextraction, followed by rotation, are less well documented but equally important. Comrey (1978) describes some of the dangers, such as minor factors being built up at the expense of major factors and/or the creation of factors with only one high loading and a few low

> loadings. These are factors that are both uninterpretable and unlikely to replicate (Velicer & Jackson, 1990 p. 432).

The present report will contrast the quality of the results produced by a conventional truncated solution against an unrestricted solution. If a limited number of factors can accurately reproduce the simulated components, this result would provide evidence that the multiple comparisons problem posed by unrestricted solutions is not necessary.

Ultimately, the question of factor restriction (or truncation as it is also termed) involves weighing two contrasting imperatives of science. The first imperative is the need to use informed expertise to flexibly interpret data using knowledge of prior experiments, theoretical expectations, and well-trained observation. While the value of expertise is indisputable, the experience of the introspectionists such as Titchener and Wundt at the turn of the twentieth century demonstrated the limits of such an approach. When one relies solely on expertise one is vulnerable to the situation wherein two equally eminent experts come to differing conclusions. Further compounding the problem is that the process of arriving at an expert judgment is often not readily documented, leading to an inability for other labs to replicate the decision-making. Using expertise to choose which factor of hundreds is meaningful is very much an exercise in expertise with all its strengths and weaknesses.

The contrasting imperative is systematic objectivity, which is the need to develop a procedure that can mechanically yield an objective judgment. The value of such an approach is that such a system can be explicitly documented and hence replicated and improved upon. Furthermore, the bases for discrepant judgments of two such systems can be readily contrasted for reconciling discrepancies. There is also no concern about subjective biases or expectancies contaminating the judgment process. The drawback of such an objective system is that it will tend to be mechanical, inflexible, and limited. The use of the Scree test to control the multiple comparison problem is an example of a relatively objective system to constrain the drawbacks of the former approach while not seeking to replace it. Ultimately expertise is absolutely essential to the data analysis process but it needs to be constrained by an objective system to minimize the amount of decision-making to the point where the decisions that are made can be documented and justified.

4. Rotation. The final parameter is rotation choice. The first author has elsewhere argued that an oblique rotation like Promax (Hendrickson & White, 1964) yields better results than the standard Varimax rotation. Extraction of simulated components was markedly more accurate with a simulated dataset (Dien, 1998a). In a further test, a PCA of the P300 in a real dataset compared the source solutions from a Varimax and a Promax rotation. Since the TPJ is the only area that is consistently shown to be activated in fMRI and PET oddball paradigms (Dien, 1998a) and lesions in this region abolish the P300 (Knight, Scabini, Woods, & Clayworth, 1989), this is a likely source for the P300. The Promax yielded a P300 factor that localized to the TPJ. Since other researchers continue to express reservations about the Promax rotation (cf. Kayser & Tenke, 2003), this report will further test the efficacy of the Promax rotation.

There is a particularly strong argument for oblique rotations in ERP analyses because in a temporal PCA the effect of scalp topography is to introduce correlation between the components (the degree to which the components co-occur in the observations is partly determined by the extent to which they are represented in the same channels). For example, two superficial components with sources with phi values 30 degrees apart can result in a correlation of .76 from spatial variance alone. For further discussion of how spatial topographies produce correlations even between unrelated components in temporal PCA, see (Dien, 1998a).

Simulation Analyses

When considering simulation studies, one must consider their strengths and weaknesses. Simulations by their nature will never be as realistic as real data. The trade-off is between realism and control. The issue is analogous to that faced by all experiments. The rigorously controlled experimental designs we use to study language, for example, rarely bear much resemblance to real reading situations; nonetheless, we find them to be of real value because they represent simplified and tightly controlled situations that make it possible to obtain reliable and interpretable results. In much the same fashion, the strength of simulations is that they make it possible to form a controlled and simplified environment in which one can make conclusions. Furthermore, the problem with real data for this sort of study is that one does not know the “real” answer.

On the other hand, an unrealistic simulation is of no use no matter how controlled it might be. The present simulations not only meet the standards set by previously published simulation studies, it improves upon them. In contrast to earlier studies that included simulation analyses of these issues (Dien, 1998a; Kayser & Tenke, 2003), the present dataset utilizes real background EEG noise, a more realistic head topography, and subject variance. The use of background EEG is especially important since the noise utilized in both studies were not auto-correlated across the variables, unlike real EEG noise, making this a much more realistic challenge for the PCA algorithm. Furthermore, the dataset includes more than one source of coherent variance in that the two simulated components have amplitudes that vary independently, making it possible for them to be distinguished by the PCA.

Nonetheless, one must keep the inherently artificial nature of simulations in mind when evaluating the results. For example, the present simulation datasets contain only two simulated components. Although a real dataset has more than two ERP components, adding more components can introduce complex interactions that would make it difficult to evaluate the effects of the manipulations. Additionally, the presence of the background EEG ensures that the overall dimensionality of the dataset is high and more comparable to that of a real ERP dataset (at least an ERP dataset with two components). Furthermore, the waveforms and scalp topographies do not vary between conditions or between subjects. Although such variations could be added, there is something of a chicken-and-an-egg situation with respect to making such variations realistic. An effective PCA technique would be needed to determine the exact nature of such variations separate from superimposed noise but a fully realistic simulation test of PCA effectiveness would need such information to be constructed. Finally, the simulated components are not real components nor are they meant to be. Instead they are meant to be representative of some of the full spectrum of possibilities. Constructing fully realistic simulated components would again require information that is not currently available and is a goal that this current work is meant to help advance towards.

The choice of how to evaluate the simulations is a critical concern. For an ERP researcher, the three chief characteristics of interest of the PCA solutions are the reconstruction of the time course, the reconstruction of the spatial topography, and the allocation of condition effects. Rather than use a global measure of factor accuracy that agglomerates all three aspects of the solution into a single measure, this report measures each aspect separately. In this way, ERP researchers can determine what effect the different manipulations have on the particular aspect of most interest to their own research (for example, scalp topography for source localization or misallocation of variance for an experimentalist). These three measures together measure the full variance represented in the dataset (temporal, spatial, condition, and subject).

<u>1) Waveform time course.</u> Fit was measured as the correlation between the two waveforms, using the time points as the observations. The correlation measure was used because it is familiar to most readers and because it standardizes the two variables, removing the effects of amplitude. Amplitude was removed because otherwise the effects on spatial topography and condition effects would necessarily be confounded with the time course measure. Furthermore, the raw factor loadings cannot be directly examined without rescaling because the actual factor reconstructions are a joint function of the factor loadings and the factor scores multiplied together. For example, a given feature in the data could be reconstructed by the PCA as either the product of a set of small factor loadings multiplied by a large factor score or a set of large factor loadings multiplied by a small factor score.

Examining the amplitude of the factor loadings in the absence of the factor score information would be meaningless. By using the correlation measure, only the shape of the waveform is evaluated, without concern for the effects of the factor scores, which are in turn evaluated by the other two measures.

2) Spatial topography. In order to evaluate success at reconstructing spatial topography in a concise manner, dipole localization was adopted as a simple summary measure. Since dipole localization is directly dependent on scalp topography, success at reconstructing the original dipole location can be construed as success at reconstructing the scalp topography. Furthermore, source localization is the primary analysis where accurate scalp topography is required so this measure has direct relevance for the utility of these parameters for ERP research. The residual variance (RV) provides a measure of fit between the factor topographies and the original components. An additional goal of these analysis is to help evaluate the helpfulness of PCA as a preprocessing step when co-registering ERP data with fMRI data. For this purpose, data is provided on the degree of localization error in Talairach space. Since fMRI data contains only location information, not orientation information, only location information is provided.

3) Misallocation of condition effects. Ever since the publication of the influential demonstration by Wood and McCarthy (1984) that PCA can misallocate condition effects to the wrong factor, misallocation of variance has been a primary concern of ERP researchers. For this reason, this has been chosen as the third measure of solution accuracy. Not only does it examine the remaining variance (condition and subject) not examined by the prior two measures but also it has direct import regarding the utility of the PCA procedures for ERP datasets.

PCAs of ERPs can be conducted with a number of data arrangements including temporal PCA with time points as the variables, spatial PCA with channels as the variables (Dien, 1998a; Ruchkin, Villegas, & John, 1964), and two-step PCA with a combination of the two

(Dien et al., 2003b; Spencer et al., 1999, 2001). To keep the present comparisons simple, only the most common arrangement, temporal PCA, will be utilized. This does mean that the present results are specific to this approach and it is possible that a different approach would yield different results.

For the simulation study, all twelve combinations of the parameters of interest will be compared: correlation versus covariance matrix, no weighting versus Kaiser normalization vs. covariance weighting, and Varimax versus Promax rotations. In addition, all simulations will be examined with and without unrestricted solutions (all factors retained) to evaluate this issue. Another point of especial interest is whether a given manipulation has a greater effect on the smaller or the larger component. It is possible that the optimal combination of parameters might depend on whether the component of interest is a smaller or larger component; for example, as noted earlier the Kaiser normalization procedure is explicitly intended to favor the smaller components. In order to address confounds present in these comparisons (latency, topography, and condition effect), a second study examines three further variations of the simulation dataset to determine if any of the differences between the Component 1 and the Component 2 accuracies are mediated by component size.

Methods

For the current simulation study, the true number of signal components is known so a fixed number of factors will be chosen based on a simple Scree test. In any case, even if the number of factors retained was too small, this underextraction would affect all the conditions and would therefore not produce a confound in the comparisons. In order to ensure that this is the case, unrestricted solutions with all 65 factors were also analyzed and presented for the first study.

The focus of the following simulation datasets is to evaluate the specific principles necessary to evaluate the present procedures. The test datasets were constructed to represent a simple average with twenty subjects, two conditions (small and large Component 1), 125 time points, and 65 channels. 100 simulation datasets were constructed and were used for all four simulation tests. All simulation datasets and the elements used to construct them are available upon request.

Two identical overlapping components were introduced for examination, a sharply peaked Component 1 and a broader Component 2 (which are not meant to represent any particular real components since doing so would entail addressing issues outside the focus of this work). These components were constructed from a half-sine wave covering ten and thirty time points respectively (for details, see Dien, 1998a). The two components start at samples 39 and 41 respectively. The peak amplitude of each of the two components was independently varied from 2 to 4 microvolts for each set of 65 channels times 125 time points. Subject variance (correlation between the two component amplitudes) was simulated by setting the amplitude of the Component 2 to be the mean of the Component 1 amplitude and of an independent 2 to 4 microvolts value. The peak amplitude of the Component 2 at the focal channel in the small and large Component 1 cells had a mean (standard deviation in parentheses) of 1.72 μv (.34) and 1.71 μv (.34) respectively. A condition effect was introduced by multiplying the Component 1 by a factor of .9 for the small Component 1 cell and 1.1 for the large Component 1 cell. The peak amplitude of the Component 1 at the focal channel had a mean of 2.2 μv (.30) in the small Component 1 cell and 2.6 μv (.39) in the large Component 1 cell. This level of effect was intended to yield F-values comparable to published P300 studies since it has been shown that unrealistically large condition effects can exaggerate the degree of misallocation variance effects (Beauducel & Debener, 2003). Table 2 provides the Monte Carlo estimates of Type I and Type II error rates (and thus the statistical power in the present dataset) since Type I error is, by definition, the proportion of false positives and Type II error is, by definition, the proportion of false negatives (cf. Davidson, 1972; Keselman, Keselman, & Lix, 1995).

The scalp topographies of the components were generated using Patrick Berg's Dipole Simulator program version 2.1.0.5 (available for download from http://www.megis.com/udbesa.htm). The Component 1 corresponds to a single surface dipole pointed at Cz. The Component 2 corresponds to a single surface dipole pointed at Pz (Such a midline equivalent dipole could be produced by two bilateral sources closely spaced on either side of the midline. Such sources are too close to model with separate dipoles without producing artifactual dipole interactions. For this reason, BESA has a parameter for keeping dipoles from approaching each other too closely. For examples of two real ERP components that are best modeled by such midline point equivalent dipoles see Dehaene, Posner, & Tucker, 1994; Dien et al., 2003b). Consistent with volume conduction, every channel reflected the two components and with the same time course. The two components were correlated at .73 and .76 in the small and large Component 1 cells respectively (when considering only subject variance), but essentially uncorrelated (less than +/-.12) between the two conditions. The scalp topographies of the two components alone are correlated at .44. Across all the observations (waveforms) the correlation between the two components is reduced to an overall mean (correlation calculated for each simulation, Fisher-Z transformed, averaged, backtransformed) .43 correlation.

To enhance comparability to real ERP datasets, background EEG from a real dataset (Dien, Frishkoff, Cerbonne, & Tucker, 2003a) were added to the dataset. The signal in these EEG was canceled out by inverting every other trial during the averaging, which has the effect of canceling out the signal while leaving the noise level intact (Schimmel, 1967). This procedure resulted in twenty noise subject averages. The data were low pass filtered at 30 Hz. The standard deviation of the noise ranged from .46 to 1.37 (median 1.04) microvolts across the epoch. Consistent with the simulation, the dataset has a 184 ms baseline and 125 Hz sampling rate. The reference for both simulated and real background EEG was the average reference (Bertrand, Perrin, & Pernier, 1985; Dien, 1998b), although the background EEG was rereferenced from an original right mastoid site. The twenty averaged background EEGs were then added to the twenty subjects in each of the simulated average datasets. The simulated data and background noise is presented in Figure 1.

Figure 1

To control for confounds with the relative sizes of the two simulated components, three additional simulations were run in a second study. For each simulation, the four variations were run using the same 100 simulated datasets and four factors were retained according to the Scree test. In the first simulation the order of the components were switched to test for possible confounding with the background EEG. Component 2 was moved earlier to coincide with Component 1's original start time while Component 1 was moved later so that its end time coincided with Component 2's original end time. In this fashion, the two components retain the same amount of overlap but the former Component 1 now overlaps with the former Component 2's trailing edge rather than its leading edge. In the second simulation, Component 1 was given the condition effect. In the third simulation, the scalp topographies of the two components were switched. Aside from these changes, the four sets of 100 simulated datasets were identical in all respects including the pattern of randomized component amplitudes. Only the restricted four-factor solution was examined in this second study due to computational limitations and since the effects of factor restriction were already evaluated in Study 1.

As noted earlier, degree of success in extracting the original waveforms was measured for three aspects: time course, scalp topography, and misallocation of condition effects.

1) Time course accuracy was operationalized as the fit between the time course and the factor with the best fit to it, measured by a correlation. Since inferential analysis is not really appropriate for this use of the correlation measure, no significance values are calculated.

Before the fit was calculated, the factor waveforms (factor pattern matrix since, unlike the factor structure matrix, it reflects only the factor and not the factors correlated with it) were first rescaled to microvolts by multiplying them by the time point standard deviations (Dien, 1998a). A similar evaluation was performed for the spatial topographies as described by the factor scores. For this measurement, the factor scores across the entire dataset (twenty subjects and two cells) were first averaged together. Modeling success is reported as the range and the median of the correlation measures for both the Component 1 and the Component 2 factors. This provides a measure of the overall performance of the simulation run for each simulated component.

Two aspects of this measurement require further explanation: scaling metric and the use of relative magnitudes rather than absolute magnitudes. Regarding scaling metrics, it is critical that any comparisons be made between numbers that are consistently scaled. For example, correlation loadings are essentially in standard deviation units whereas covariance loadings are in the original microvolt loadings. Correlation loadings cannot therefore be directly compared to either covariance loadings or the original ERP waveforms until they have been converted to microvolt scaling or vice versa (cf. Dien, 1998a; Dien & Frishkoff, in press). Consider for example, if one wished to compare car sales over the past decade in the United States to that of the European Common Market. If one scaled the U.S. data by dividing each year's price by the standard deviation of that year alone (as in a covariance loading) but scaled the European data by dividing all ten annual prices by the same number (as in a correlation loading) then it would be difficult to compare the two graphs since the shape of the U.S. graph would have been changed. When two things are compared, they need to be compared in the same metric (both in microvolts or both in standard deviation units); otherwise even identical waveforms can look quite different. Thus, although it is common to directly compare a graph of the factor loadings directly to the ERP waveforms, this can be misleading. In the current report, all factor loading information will be converted to microvolt scaling before comparison and interpretation.

The second issue that requires consideration is the use of relative magnitudes for the comparisons. The issue is that factor loadings (or more specifically the factor structure matrix) are the correlation between the factors and the variables. This correlation represents the amount of the variable variance accounted for by the factor compared to the amount not accounted for by the factor. Thus, the correlation can be reduced not just by a poorer modeling of the signal in the variable; it can also be reduced by overlapping signals or increased levels of background noise. If one compares the absolute factor loadings yielded by the PCA of two different datasets, differences in the absolute factor loadings (whatever the scaling) do not necessarily reflect differences in the quality of the PCA factor solutions. The magnitude of two identically successful factor solutions for a given ERP component might look quite different depending on what else is going on in the datasets. The same logic applies to the factor pattern matrix (which is different from the factor structure matrix only for oblique rotations).

The absolute magnitude of the factor loadings is only meaningful when taken in conjunction with the factor scores (as in multiplying them together to recreate the amount of an ERP accounted for at a particular electrode for a particular subject in a particular condition). While one could compare absolute values in this way, doing so confounds the quality of the time course reproduction with the quality of the scalp topography and condition effect reproductions. In order to keep the evaluation of the time course replication separate from the evaluation of these other aspects of the results, only the relative magnitudes of the factor waveforms will be examined. In other words, only the overall shape of the factor waveforms will be compared, not their sizes.

2) Scalp topography can be somewhat difficult to summarize. One way to do so is to compute the corresponding equivalent point dipole. Although multiple inverse solutions can produce a given scalp topography when the number and the size of the dipoles is allowed to vary, when the solution is constrained to a single point dipole the result generally appears to be a unique summary of the scalp topography. Dipole analyses were conducted using BESA5

using a four-shell elliptical head model and a single dipole. Modeling was conducted on the grand average data, following conventional practice. An iterative algorithm was utilized in which the program automatically shifted the position of the dipoles until it found a position of maximum fit. To maintain uniformity, all reported solutions are based on a central starting position. To guard against local minima issues, solutions were rechecked against front and rear starting locations; in all cases solutions were not dependent on the starting location.

In order to allow evaluation of the results in the context of ERP/fMRI co-registration, the source localizations were transformed into a Talairach coordinate system (Talairach & Tournoux, 1988) and rendered using Brain Voyager 2000 (4.4). While the intricacies of co-registration procedures is beyond the scope of this paper, we choose to use this combination of software in this paper because BESA is arguably the leading ERP source localization software and the BESA/BrainVoyager combination is the only commercially available combination for converting the BESA results into Talairach space for comparison with fMRI data. The MRI used for rendering is based on an example head included with the software.

3) In order to characterize the implications for ANOVA results, misallocation of the condition effects was examined with a two within subject-factors repeated measures ANOVA of Cell (condition1, condition 2) * Site (Cz, Pz) with twenty simulated subjects. For reasons illustrated elsewhere (McCarthy & Wood, 1985), the cell effect was mostly expected to appear in the Cell * Site interaction. Of course, in the presence of a significant interaction one does not interpret main effects so the interaction test results are the more important. SPSS 6.1 calculated the repeated measures statistics.

In order to provide a sense of the practical relevance of the effects for an actual ERP study, a representative waveform and source solution is provided for each permutation. These are intended to allow readers to directly relate the measures to the end result and thus evaluate how much of an effect (such as a .91 correlation versus a .99 correlation) is of practical import for their studies. The simulation with the median spatial correlation is utilized as a representative simulation (so that the time course presented is congruent with the source localization and may be evaluated jointly as coming from the same solution). The ranking is based on the Component 2 factor since (as will be seen) it shows the greatest sensitivity to the variations.

The PCAs were conducted on the simulated average data using the Matlab PCA Toolbox 1.091, freely available for download from: http://www.people.ku.edu/~jdien/downloads.html. Each individual PCA had 125 variables (the time points) and 2600 observations (65 channels x 2 conditions x 20 subjects). All analyses were conducted with double-precision arithmetic and identical parameters such as convergence criterion (no PCAs failed to reach convergence). Since the Kaiser normalization is applied to the Varimax step but not the Promax relaxation step, the same approach was used with the covariance loadings (weighted during Varimax but not Promax steps). For the Promax rotations, a Kappa of 3 was adopted, following the default used by SAS (see online documentation at http://support.sas.com/onlinedoc/913/docMainpage.jsp for the Power subcommand of PROC FACTOR).

Results

Study #1.

1. Covariance Matrix - As seen in Table 1, the use of a correlation matrix (Conditions 4-6, 10-12) instead of a covariance matrix (Conditions 1-3, 7-9) resulted in notably lower accuracies for the restricted solution. Although these high correlations might seem to be at ceiling, the waveforms in Figures 2 and 3 illustrate how the differences between these numbers correspond to noticeable changes in the waveforms. Examination of the unrestricted solutions indicates that in this case the two matrices result in largely identical solutions (Conditions 13-15, 19-21 versus 16-18, 22-24), suggesting that correlation matrices are capable of yielding equivalent results but are less efficient with respect to numbers of factors retained.

Figures 2 & 3

Likewise, the ANOVA results summarized in Table 2 indicate a dramatically higher rate of misallocation of condition variance to the Component 2 factor when using the correlation matrix, but only for the restricted solution (Conditions 4-6, 10-12). Equally dramatic increases in source modeling errors are seen in Table 3 for restricted solutions (Conditions 4-6, 10-12). Given these results, only the covariance matrices will be considered for the remainder of the results section.

2. Covariance Loadings – As occurs in Table 1, with covariance matrices and Varimax rotations (Conditions 1-3), the use of covariance loadings yielded lower accuracies than with both Kaiser normalization and unweighted loadings for the Component 1 factors and just a touch higher for the Component 2 factors. With covariance matrices and Promax rotations (Conditions 7-9), covariance loadings yielded lower accuracies for both factors. Turning to the ANOVA results in Table 2, focusing on the covariance matrix results, the covariance loadings performed much worse for the Varimax rotations (Conditions 1-3), with a 58% misallocation rate for the main effect (versus 14 and 15%). For the Promax rotations (Conditions 7-9), the results were less clear with more misallocations in the main effect test but fewer misallocations for the interaction test. Finally, for the source localization analyses in Table 3 the covariance loadings were roughly equivalent to the others (less by a millimeter) for the Varimax rotation (Conditions 1-3) and much worse (about 4 mm) for the Promax rotation (Conditions 7-9) for the restricted solutions. For the unrestricted solutions the covariance loadings were better by about 5 mm for the Varimax rotation (Conditions 13-15) and worse by about 2 mm for the Promax rotation (Conditions 19-21). For all the comparisons, the Kaiser normalization and the unweighted solutions were approximately equivalent.

3. Unrestricted Solutions – Looking at Table 1, the results were virtually identical to that obtained with only four factors for the covariance matrix (Conditions 1-3, 7-9 versus 13-15, 19-21) and dramatically better for the correlation matrix (Conditions 4-6, 10-12 versus 16-18, 22-24). For the covariance matrices, Component 1 was more accurate in the unrestricted solutions by about 1 percent for the Varimax rotation and about 1 percent worse for the Promax rotation. Note that the results for the Kaiser normalization and the unweighted loadings were identical for the unrestricted solutions (excepting the effect of rounding errors), since the communalities will be one for all variables when all factors are retained, resulting in no weighting changes. A similar picture is seen for the ANOVA results in Table 2. For the source localization results in Table 3 the results are somewhat worse for the Varimax rotation and better for the Promax rotation. Overall, the results are mixed.

4. Promax Rotation – As occurs in Table 1, the accuracy rates for Promax rotations (Conditions 1-3 versus 7-9) are consistently higher for the covariance matrix results in all cases except for the Component 2 factor of the covariance loading case. For the ANOVA results in Table 2, the restricted solutions yield overall better results for the Promax rotation, especially with the covariance loadings (Condition 7), except for a slightly higher misallocation rate for Component 2 when using the unweighted and Kaiser Normalized loadings (Conditions 8 & 9). Similar results are seen for the unrestricted analyses except that Promax provides improved results across the board (Conditions 13-15 versus 19-21). The source localization results in Table 3 display a strongly improved total error for the Promax rotation.

<u>Study #2.</u>

a) To determine if any of the results were due to a confound with the background EEG noise, the analysis was repeated with the temporal positions of the two components reversed but otherwise identical parameters. Only the accuracy measures are presented since the purpose is to determine if the differences in the accuracies of the two simulated components are due to their differing sizes. Only the restricted solutions are presented due to computational limits and since the Study #1 results should be sufficient for the purpose of evaluating that parameter.

As seen in Table 4, essentially the same pattern of results occurs. Overall, use of a correlation matrix was more detrimental for the smaller Component 1 for the restricted solution. Likewise, the covariance loadings were detrimental to the smaller component, especially for the Varimax rotation. Promax was beneficial to both components (except for the covariance matrix-Varimax rotation case) but most beneficial to the larger Component 2.

b) To determine if any of the results were due to a confound with the presence of cell effects, the first analysis was repeated with the cell effect in the Component 2 instead of the Component 1 but otherwise identical parameters.

Essentially the same pattern of results is seen in Table 5. Overall, use of a correlation matrix was more detrimental for the smaller Component 1 for the restricted solution. Likewise, the covariance loadings were detrimental to the smaller component, especially for the Varimax rotation. Promax was beneficial to both components (except for the covariance matrix-Varimax rotation case) but most beneficial to the larger Component 2.

c) To determine if any of the results were due to a confound with the scalp topographies, the first analysis was repeated with the scalp topographies reversed but otherwise identical parameters.

A slightly different pattern of results is seen in Table 6. Overall, use of a correlation matrix was still more detrimental for the smaller Component 1 factor. Promax was still most beneficial for the larger Component 2, but to an even greater degree. The covariance loading effect no longer clearly favors the smaller component.

Discussion

Reasonable arguments can be made regarding each of the options addressed in this report. The choices of relationship matrix, factor loading weighting, solution restriction, and factor rotation were examined using a simulation dataset. For this dataset, the results indicated that a covariance matrix was equivalent to the correlation matrix for an unrestricted solution and better for a restricted solution, supporting a prior report (Kayser & Tenke, 2003). For factor loading weights, the Kaiser Normalization was largely equivalent to the unweighted solution and both were better than the covariance loadings. We suggest Kaiser Normalization be used if for no other reason than it has become accustomed practice to use it. Regarding solution restriction, for the recommended covariance matrix the restricted solution was largely equivalent to the unrestricted solution for the time course measure. We argue that any improvements seen in the misallocation and dipole measures are more than outweighed by the multiple comparison problem, as noted in the introduction. Finally, the Promax rotation yielded strongly improved results for the time course and the spatial measures, with only a slight increase in misallocation in the case of the restricted covariance matrix solutions using unweighted or Kaiser normalized loadings. The results of Study 2 did not support the hypothesis that some of these parameters might favor larger or smaller components (defined in terms of time course for a temporal PCA).

These conclusions agree with some recommendations made by a recent paper in this journal (Kayser & Tenke, 2003) in some respects and disagree in some other respects. We completely endorse their conclusion that the covariance matrix yields better results than the correlation matrix, at least for restricted solutions. The current report also confirms their observation that correlation and covariance matrix results converge for unrestricted solutions.

Contrary to their report, we did not find improved results from the covariance loadings. They based their recommendation primarily on the basis of a visual examination of the factor waveforms (p. 2314-5) and on the basis of stability of ANOVA effects (P. 2320). Unfortunately, the use of covariances in the relationship matrix, the factor loadings, and the graphs were confounded, making it difficult to determine the independent effects of each issue. Frequently, these three separate scaling decisions were treated as being a single decision, referred to as "covariance-based" and "correlation-based" solutions. Fortunately, their analyses include a feature that resolves this ambiguity. As described in Footnote 1 of the present report, Kaiser normalization cancels out the effects of the covariance loadings. Since Kayser and Tenke (2003) used Kaiser normalization in the entire report (as noted in their appendix), the only real difference between their correlation condition and their covariance condition was the relationship matrix choice; the effects of covariance loadings were never actually tested in their report. Although this decision had the unintended effect of canceling out the covariance loading manipulation, it does increase the value of their report for evaluating the relationship matrix issue.

What, then, is to be made of the difference in the factor waveforms as seen in their Figure 3? This figure represents one place where two of the three scaling decisions are unconfounded (i.e., the relationship matrix and factor loading scaling decisions). Despite our contention that the two solutions should be mathematically identical, a difference is seen between correlation and covariance loadings (termed by Kayser and Tenke as the standardized and unstandardized loadings) with the covariance matrix. This anomaly can be explained as due to the remaining confound with the graph scaling decision. As we noted in the introduction, even identical waveforms will look different if one is graphed in standard deviation units and the other is graphed in microvolt units. The problem is that this type of scaling change alters not just the overall amplitude of the waveforms but also their shapes (since each time point has a different standard deviation). They apparently graphed the correlation loading results in standard deviation units and the covariance loading results in microvolts. This issue affects both Figures 3 and 4 of their report.

We also differ to some extent with their recommendation to avoid truncation (or restriction) of factor solutions. We do agree that factor underextraction can be problematic but do not therefore conclude that it should not be done at all. The relevant statistical papers (Fava & Velicer, 1992, 1996; Velicer & Jackson, 1990; J. M. Wood et al., 1996) also warn of the dangers of overextraction (it can cause factors to be broken down into spurious subfactors). Regarding the evidence Kayser and Tenke present against underextraction, we suggest that a more judicious use of the scree test might have yielded different results. Although a bend can be seen in their Figure 5 at Factor 4, an additional bend can be seen at Factor 7. We suspect more bends are present in eigenvalues past that shown in the figure. The logic of the scree test (Cattell, 1966; Cattell & Jaspers, 1967) requires that one take the last bend counting from the right (i.e., the first place where the eigenvalues start becoming larger than would be expected from noise alone), not the first bend counting from the left. Their results appear to be consistent with about 15 retained factors. It would be interesting to see the chart for the Scree in this vicinity. Unfortunately, their Figure 5 only shows the first ten eigenvalues. In any case, we suggest that the multiple comparison issues outlined in the introduction outweigh any improvements provided by an unrestricted solution. Ultimately, expert judgment will be required to determine if the results are affected by factor underextraction or overextraction issues. There is no replacement for expert judgment but its role does need to be restricted to the point that it can be suitably documented.

Finally, Kayser and Tenke (2003) caution against the use of oblique rotations such as Promax, although their paper is not directly concerned with this issue. They state that "the advantage of Promax and any oblique rotation method is at the same time a disadvantage, as the analyzed components are no longer independent" (Kayser & Tenke, 2003, p. 2310) and that "As the probability of Type I errors increases with the number of dependent variables (i.e., extracted factors) considered for statistical analysis, the orthogonality of the Varimax solution counteracts this undesired effect" (Kayser & Tenke, 2003, p. 2309). We are indebted to them for vocalizing these issues so that they can be discussed.

The first concern can be addressed by analogy to the related issue of balanced ANOVA designs. For between subject conditions, it is desirable to have a balanced design in which each cell has an equal number of subjects. If the ANOVA factors are correlated, this can result in unbalanced designs. For example, if the two ANOVA factors are median-split depression and anxiety groups (highly correlated scores) then most of the subjects will fall into the low-depressed/low-anxious or the high-depressed/high-anxious cells. Such unbalanced designs are problematical because a standard ANOVA assumes that each cell is an equally reliable estimate of the error variance; a cell with only two subjects is certainly not as reliable as a cell with two hundred subjects. One addresses this issue by either careful pre-screening to ensure a balanced sample or one utilizes an ANOVA algorithm that is specially adapted for unbalanced designs such as unweighted-means analysis (Keppel, 1982; Winer, 1971). Ignoring the problem by applying a standard ANOVA does not solve the problem. While the purpose of PCA is descriptive rather than inferential, there are similar issues regarding maximizing interpretability if one's ultimate goal is for each factor to reflect different ERP components. There is no way that an orthogonal solution for correlated ERP components can avoid being linear mixes of the ERP components (ignoring noise variance). Ignoring correlated components by applying a factor analysis with uncorrelated factors does not solve the problem[2].

Orthogonal solutions are only appropriate when the latent variables in the dataset are in fact orthogonal. This is often the case, which is why Varimax rotations are popular. In the case of ERP datasets, however, the effect of differing scalp topographies virtually ensures that the latent variables will be correlated to a significant degree in a temporal PCA, as described elsewhere (Dien, 1998a). Even if the components are otherwise unrelated to each other, the way spatial variance is used in temporal PCA means that part of the correlation between the two components will be determined by the similarity of the two scalp topographies; only in the rare situation of sources that are more or less (depending on the montage) at right angles to each other will scalp topography not ensure a sizeable correlation between the two components. Furthermore, since the head is a three-dimensional object, no more than three components can be at right angles to each other; any more than three components ensures that at least some of them will have sizeable correlations with each other due to spatial similarity. For this reason, we suggest that, at least in principle, oblique rotations are more appropriate for temporal PCAs; this recommendation is tempered by the continuing need to evaluate in different contexts whether available oblique rotations such as Promax are sufficiently effective in practice.

As for the second objection (that orthogonal solutions control multiple comparison problems and that oblique solutions therefore presumably do not), we cannot endorse this position at all. Keeping the variables orthogonal does nothing to control the multiple comparison problem. Multiple comparison problems (cf. Toothaker, 1991) arise because if one examines enough null effects, random noise in some of the effects will by chance reach the significance threshold and produce a spurious result. Keeping the factors orthogonal will not have any effect on the presence of random noise in the factor variables. Thus, using Varimax rotations will not protect against the ill effects of utilizing unrestricted solutions.

It would be impossible to examine all possible combinations of ERP components and to identify a procedure that will always in all cases produce the best results. The goal of this report is therefore to examine a representative situation and then to recommend a standardized protocol that we suggest will yield the best results in typical datasets. In this way, investigators may obtain protection from the concern that they are massaging the data by manipulating the many parameters of the PCA process. Since there will always be special cases where the present protocol will not be appropriate, investigators should consider the option of tailoring the protocol when appropriate. One possible procedure in cases where such a situation is suspected is to present the PCA results using both the recommended protocol and the tailored protocol and then use outside considerations to support the use of tailoring (cf. Dien et al., 2003b).

In conclusion, these results demonstrate that the choice of PCA parameters can have visible impact on the quality of the results. Keeping in mind our caveats regarding simulation studies, we recommend that PCA studies utilize a covariance matrix, Kaiser normalization, factor retention, and Promax rotation. We make this suggestion on the basis of the relative rankings of the different permutations, although whether these choices ultimately make a meaningful difference to a study depend on the goals of the analysis and the required level of accuracy. We note that the choice of the PCA parameters can make as much as a five centimeter difference in localization results, a substantive distance when co-registering with fMRI data. We also strongly recommend using microvolt-scaled factor loadings when visually comparing factor loadings to raw microvolt scaled averaged data. We would also like to take this moment to again affirm that although we have outlined a number of disagreements with Kayser and Tenke (2003), we felt this paper made important contributions in raising the issues it did and in providing graphic demonstrations of the effects of retaining too few factors.

Table 1.

#	Condition	Component 1 Median	Component 2 Median	Component Correlation
1	COVcVAR	0.89 (0.89 - 0.90)	0.98 (0.97 - 0.99)	0.0
2	COVkVAR	0.98 (0.98 - 0.98)	0.97 (0.97 - 0.98)	0.0
3	COVnVAR	0.98 (0.98 - 0.99)	0.97 (0.97 - 0.97)	0.0
4	CORcVAR	0.59 (0.53 - 0.65)	0.89 (0.87 - 0.90)	0.0
5	CORkVAR	0.56 (0.52 - 0.63)	0.90 (0.89 - 0.91)	0.0
6	CORnVAR	0.68 (0.54 - 0.75)	0.90 (0.89 - 0.91)	0.0
7	COVcPRO	0.99 (0.99 - 0.99)	0.97 (0.97 - 0.98)	.43
8	COVkPRO	1.00 (0.99 - 1.00)	0.99 (0.99 - 0.99)	.47
9	COVnPRO	1.00 (0.99 - 1.00)	0.99 (0.99 - 1.00)	.47
10	CORcPRO	0.67 (0.55 - 0.72)	0.88 (0.86 - 0.90)	.23
11	CORkPRO	0.65 (0.55 - 0.71)	0.89 (0.88 - 0.90)	.23
12	CORnPRO	0.67 (0.54 - 0.74)	0.89 (0.88 - 0.91)	.21
13	65fCOVcVAR	0.89 (0.89 - 0.90)	0.98 (0.97 - 0.99)	0.0
14	65fCOVkVAR	0.99 (0.99 - 0.99)	0.97 (0.97 - 0.97)	0.0
15	65fCOVnVAR	0.99 (0.99 - 0.99)	0.97 (0.97 - 0.97)	0.0
16	65fCORcVAR	0.89 (0.89 - 0.90)	0.98 (0.97 - 0.99)	0.0
17	65fCORkVAR	0.99 (0.99 - 0.99)	0.97 (0.97 - 0.97)	0.0
18	65fCORnVAR	0.99 (0.99 - 0.99)	0.97 (0.97 - 0.97)	0.0
19	65fCOVcPRO	0.99 (0.99 - 1.00)	0.97 (0.96 - 0.97)	.53
20	65fCOVkPRO	0.99 (0.98 - 0.99)	0.99 (0.99 - 0.99)	.48
21	65fCOVnPRO	0.99 (0.98 - 0.99)	0.99 (0.99 - 0.99)	.48
22	65fCORcPRO	0.99 (0.99 - 1.00)	0.97 (0.96 - 0.97)	.53
23	65fCORkPRO	0.99 (0.99 - 0.99)	0.99 (0.99 - 0.99)	.48
24	65fCORnPRO	0.99 (0.99 - 0.99)	0.99 (0.99 - 0.99)	.48

Correlations between the original waveforms and the factors for each of the rotations for the standard condition. Listed are the median values for Component 1 and for Component 2 (considered separately), with the low and high values listed in parentheses. The correlation column presents the correlation between the two factors (correlation calculated for each simulation, Fisher-Z transformed, averaged, backtransformed), leaving out simulations where the same factor was the best fit for both components. The original correlation was .43. COV=covariance matrix. COR=correlation matrix. c=covariance loading. k=Kaiser normalization. n=not weighted loadings. VAR=Varimax rotation. PRO=Promax rotation. 65f=unrestricted solution.

Table 2.

#	Condition	C1 F C	C1 sig C	C2 F C	C2 sig C	C1 F C*S	C1 sig C*S	C2 F C*S	C2 sig C*S	C1 Total	C2 Total
1	COVcVAR	15.5	98	6.2	58	16.4	99	0.6	0	99	58
2	COVkVAR	26.5	100	2.0	14	9.7	86	1.1	7	100	14
3	COVnVAR	25.0	100	2.1	15	9.5	83	1.2	8	100	15
4	CORcVAR	1.4	0	.6	0	.9	8	8.3	81	8	81
5	CORkVAR	.7	1	1.0	7	1.6	14	7.4	73	14	73
6	CORnVAR	.6	0	.9	5	.4	0	7.0	73	0	73
7	COVcPRO	9.7	83	2.5	17	22.6	100	1.8	11	100	17
8	COVkPRO	16.1	98	1.6	13	17.7	99	2.6	16	99	17
9	COVnPRO	15.2	98	1.7	13	17.7	99	2.6	16	99	17
10	CORcPRO	1.7	0	.9	6	.1	0	6.6	71	0	71
11	CORkPRO	.6	0	1.0	6	.2	0	6.4	68	0	68
12	CORnPRO	.8	0	1.0	6	.2	0	6.3	66	0	66
13	65fCOVcVAR	14.6	96	5.6	49	18.2	99	0.7	0	99	49
14	65fCOVkVAR	27.3	100	2.1	15	9.5	82	1.4	9	100	15
15	65fCOVnVAR	27.3	100	2.1	15	9.5	82	1.4	9	100	15
16	65fCORcVAR	14.7	96	5.6	49	18.3	99	0.7	0	99	49
17	65fCORkVAR	27.2	100	2.1	15	9.4	82	1.4	9	100	15
18	65fCORnVAR	27.2	100	2.1	15	9.4	82	1.4	9	100	15
19	65fCOVcPRO	8.2	78	2.1	15	24.1	100	1.2	7	100	15
20	65fCOVkPRO	12.4	93	1.6	12	20.1	99	1.6	8	99	12
21	65fCOVnPRO	12.4	93	1.6	12	20.1	99	1.6	8	99	12
22	65fCORcPRO	8.8	77	2.1	15	23.5	100	1.2	7	100	15
23	65fCORkPRO	13.5	95	1.6	12	20.0	99	1.7	8	99	12
24	65fCORnPRO	13.5	95	1.6	12	20.0	99	1.7	9	99	12

Misallocation of condition effects in ANOVAs. Table provides the mean F score and the number of significant tests out of the 100 simulations. Each test has 1 degree of freedom in the numerator and 19 in the denominator. Summary provided for both the main cell effect (C) as well as the interaction between site and cell (C*S). The Total columns provide the total number of simulations showing significant effects in either/both tests. C1=Component1. C2=Component 2. COV=covariance matrix. COR=correlation matrix. c=covariance loading. k=Kaiser normalization. n=not weighted loadings. VAR=Varimax rotation. PRO=Promax rotation. 65f=unrestricted solution.

Table 3.

#	Condition	Component 1 RV	Component 1 Talairach	Component 2 RV	Component 2 Talairach	Error
	Original	0.075%	2 -29 58	0.321%	0 -69 36	
1	COVcVAR	0.249%	3 -29 58	3.681%	-2 -71 49	14.30
2	COVkVAR	1.932%	3 -35 59	0.619%	-2 -74 44	15.81
3	COVnVAR	2.285%	3 -35 60	0.546%	-2 -74 44	16.05
4	CORcVAR	13.598%	0 -51 67	2.306%	0 -58 30	36.38
5	CORkVAR	1.865%	0 -60 30	1.865%	0 -60 30	52.64
6	CORnVAR	15.123%	1 -43 63	1.765%	0 -60 30	25.72
7	COVcPRO	0.712%	3 -27 55	0.561%	-1 -71 40	8.32
8	COVkPRO	0.225%	3 -28 57	0.523%	-1 -67 35	4.18
9	COVnPRO	0.211%	3 -28 57	0.539%	-1 -67 35	4.18
10	CORcPRO	15.546%	-1 -53 66	2.095%	0 -60 30	36.29
11	CORkPRO	15.736%	0 -52 67	1.928%	0 -60 30	35.60
12	CORnPRO	14.688%	0 -52 67	1.984%	0 -60 30	35.60
13	65fCOVcVAR	0.288%	3 -30 58	3.644%	-3 -71 49	14.90
14	65fCOVkVAR	2.829%	3 -39 61	0.718%	-3 -75 43	20.18
15	65fCOVnVAR	2.829%	3 -39 61	0.717%	-3 -75 43	20.18
16	65fCORcVAR	0.285%	3 -30 58	3.660%	-3 -71 49	14.90
17	65fCORkVAR	2.817%	3 -39 61	0.720%	-3 -75 43	20.18
18	65fCORnVAR	2.818%	3 -39 61	0.720%	-3 -75 43	20.18
19	65fCOVcPRO	0.781%	3 -28 56	0.715%	-2 -69 38	5.28
20	65fCOVkPRO	0.350%	2 -29 58	0.649%	-2 -67 35	3.00
21	65fCOVnPRO	0.356%	2 -29 58	0.692%	-2 -66 35	3.74
22	65fCORcPRO	0.708%	2 -28 57	0.664%	-2 -69 38	4.24
23	65fCORkPRO	0.348%	2 -29 58	0.672%	-2 -67 35	3.00
24	65fCORnPRO	0.348%	2 -29 58	0.672%	-2 -67 35	3.00

Effect of different rotations on solutions for representative simulation. Listed is the residual variance (RV) for the solutions for the two components, their Talairach coordinates (in millimeters), and the sum of the Pythagorean distance errors for the two components. For the CORcVAR and the CORkVAR simulations, the same factor was the best fit for both components. COV=covariance matrix. COR=correlation matrix. c=covariance loading. k=Kaiser normalization. n=not weighted loadings. VAR=Varimax rotation. PRO=Promax rotation. 65f=unrestricted solution.

Table 4.

#	Condition	Component 1 Median	Component 2 Median
1	COVcVAR	0.87 (0.86 - 0.88)	0.98 (0.98 - 0.99)
2	COVkVAR	0.98 (0.97 - 0.98)	0.97 (0.97 - 0.98)
3	COVnVAR	0.98 (0.98 - 0.99)	0.97 (0.96 - 0.97)
4	CORcVAR	0.56 (0.54 - 0.59)	0.88 (0.86 - 0.89)
5	CORkVAR	0.64 (0.56 - 0.69)	0.89 (0.88 - 0.91)
6	CORnVAR	0.71 (0.61 - 0.76)	0.90 (0.89 - 0.91)
7	COVcPRO	0.98 (0.97 - 0.98)	0.96 (0.95 - 0.97)
8	COVkPRO	0.99 (0.99 - 1.00)	0.99 (0.98 - 0.99)
9	COVnPRO	0.99 (0.99 - 1.00)	0.99 (0.99 - 0.99)
10	CORcPRO	0.58 (0.54 - 0.64)	0.89 (0.87 - 0.91)
11	CORkPRO	0.57 (0.53 - 0.63)	0.90 (0.89 - 0.91)
12	CORnPRO	0.60 (0.53 - 0.67)	0.91 (0.90 - 0.92)

Correlations between the original waveforms and the factors for each of the rotations for the reversed order condition. Listed are the low, median, and high correlations for Component 1 and for Component 2 (considered separately). In this study, the Component 1 has actually been moved to a longer latency while the Component 2 has been moved to be the earlier component. COV=covariance matrix. COR=correlation matrix. c=covariance loading. k=Kaiser normalization. n=not weighted loadings. VAR=Varimax rotation. PRO=Promax rotation. 65f=unrestricted solution.

Table 5.

#	Condition	Component 1 Median	Component 2 Median
1	COVcVAR	0.87 (0.86 - 0.88)	0.98 (0.98 - 0.99)
2	COVkVAR	0.98 (0.97 - 0.98)	0.97 (0.97 - 0.98)
3	COVnVAR	0.98 (0.98 - 0.99)	0.97 (0.96 - 0.97)
4	CORcVAR	0.56 (0.54 - 0.59)	0.88 (0.86 - 0.89)
5	CORkVAR	0.64 (0.56 - 0.69)	0.89 (0.88 - 0.91)
6	CORnVAR	0.71 (0.61 - 0.76)	0.90 (0.89 - 0.91)
7	COVcPRO	0.98 (0.97 - 0.98)	0.96 (0.95 - 0.97)
8	COVkPRO	0.99 (0.99 - 1.00)	0.99 (0.98 - 0.99)
9	COVnPRO	0.99 (0.99 - 1.00)	0.99 (0.99 - 0.99)
10	CORcPRO	0.58 (0.54 - 0.64)	0.89 (0.87 - 0.91)
11	CORkPRO	0.57 (0.53 - 0.63)	0.90 (0.89 - 0.91)
12	CORnPRO	0.60 (0.53 - 0.67)	0.91 (0.90 - 0.92)

Correlations between the original waveforms and the factors for each of the rotations for the reversed cell effect condition. Listed are the low, median, and high correlations for Component 1 and for Component 2 (considered separately). COV=covariance matrix. COR=correlation matrix. c=covariance loading. k=Kaiser normalization. n=not weighted loadings. VAR=Varimax rotation. PRO=Promax rotation. 65f=unrestricted solution.

Table 6.

#	Condition	Component 1 Median	Component 2 Median
1	COVcVAR	0.97 (0.97 - 0.98)	0.97 (0.97 - 0.98)
2	COVkVAR	0.95 (0.91 - 0.96)	0.99 (0.98 - 0.99)
3	COVnVAR	0.98 (0.97 - 0.98)	0.98 (0.98 - 0.98)
4	CORcVAR	0.49 (0.42 - 0.62)	0.96 (0.95 - 0.96)
5	CORkVAR	0.53 (0.48 - 0.57)	0.96 (0.96 - 0.97)
6	CORnVAR	0.50 (0.45 - 0.57)	0.96 (0.95 - 0.97)
7	COVcPRO	0.96 (0.95 - 0.97)	1.00 (1.00 - 1.00)
8	COVkPRO	0.95 (0.91 - 0.97)	1.00 (1.00 - 1.00)
9	COVnPRO	0.96 (0.95 - 0.97)	1.00 (1.00 - 1.00)
10	CORcPRO	0.48 (0.40 - 0.61)	0.96 (0.95 - 0.97)
11	CORkPRO	0.50 (0.40 - 0.57)	0.96 (0.96 - 0.97)
12	CORnPRO	0.50 (0.40 - 0.57)	0.96 (0.96 - 0.97)

Correlations between the original waveforms and the factors for each of the rotations for the reversed topography condition. Listed are the low, median, and high correlations for Component 1 and for Component 2 (considered separately). COV=covariance matrix. COR=correlation matrix. c=covariance loading. k=Kaiser normalization. n=not weighted loadings. VAR=Varimax rotation. PRO=Promax rotation. 65f=unrestricted solution.

Footnotes

1. Given a simple dataset with only two factors, the factor loadings for variable X are X_1 and X_2. The covariance loadings are SX_1 and SX_2 where S is the standard deviation of the variable. The communality C of this variable is computed as the sum of the squared loadings:

$$C = (SX_1)^2 + (SX_2)^2 = S^2(X_1 + X_2)^2$$

When the covariance loadings are divided by the square root of the communality they end up being:

$X_1/(X_1 + X_2)$ and $X_2/(X_1 + X_2)$

A caveat for this conclusion is that if the communalities were based on the correlation loadings rather than on the covariance loadings, then the normalization would not cancel out the covariance loading procedure. We are not aware of any statistical packages using such a procedure but it is possible.

2. The argument that an orthogonal solution is preferable no doubt arises from the intuition that if the variable (factor) that has no condition effect is allowed to be correlated with the variable (factor) that does have a condition effect, then the former variable will end up with a condition effect too. This concern can be addressed by clarifying that there are multiple sources of variance in these variables (condition, subject, channels). The overall correlation between the two variables (factors) can be conceptualized as the sum of the different sources of partial correlation (Cohen & Cohen, 1983). Two variables can be correlated overall due to two sources of partial correlation (subject and channels) without the other source of variance (condition) being correlated. If the two variables (factors) are forced to be uncorrelated, this is likely to be accomplished by introducing a correlation in the condition component to cancel out

the existing subject and channel partial correlations. The result would be variables that are overall uncorrelated but that now include misallocated condition effects.

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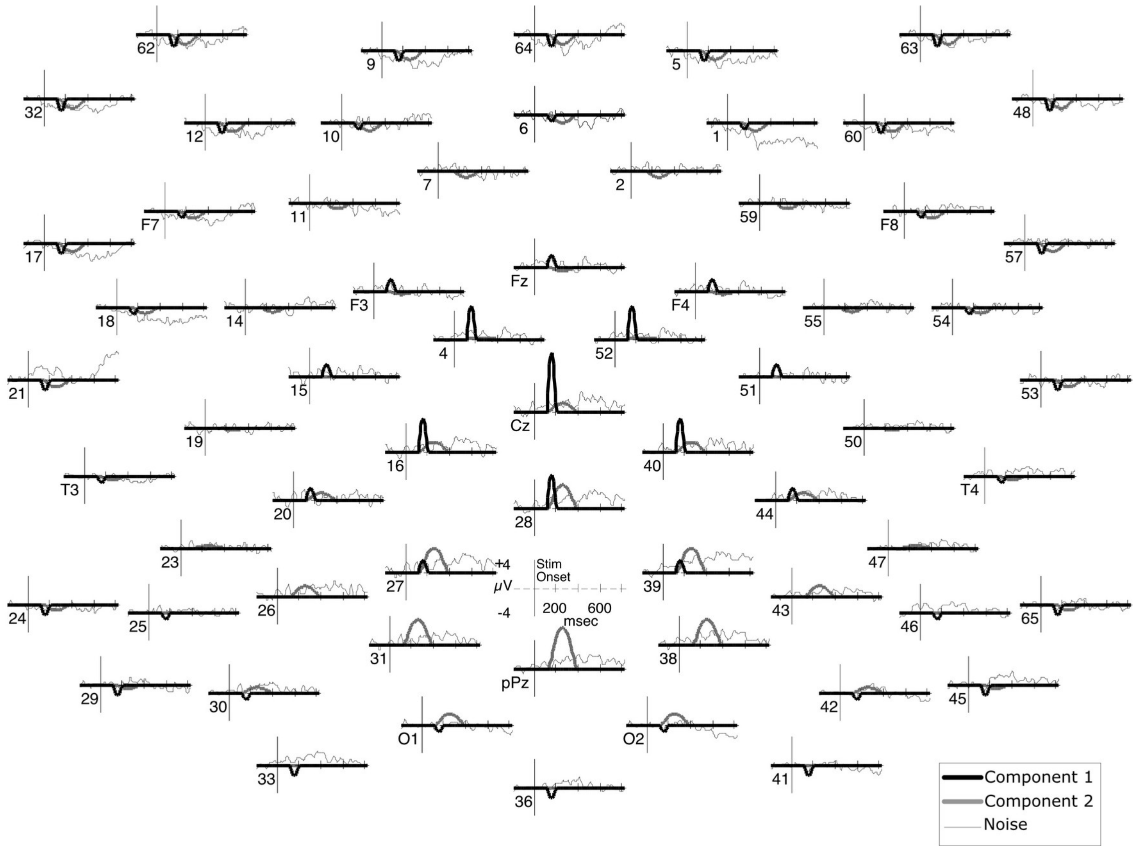
Figure Captions

Figure 1. Scalp Topography of Simulated Components and Background Noise. Waveforms represent grand average of background noise summed across both conditions. Simulated components are presented with an amplitude at the middle of the random range (3 microvolts). The channels are laid out topographically with the top being the front of the head.

Figure 2. Effect of PCA Variations on Four Factor Waveforms. The bottom graph presents the original waveforms. The other graphs present the factor loadings (factor patterns scaled to microvolts) for the representative simulation (median reconstruction of Component 2). For comparison's sake, each waveform is scaled so that the maximum amplitude is set to the top of the graph. For the CORkVAR simulation the same factor was the best fit for both components. COV=covariance matrix. COR=Correlation matrix. c=covariance loading. k=Kaiser normalization. n=not weighted loadings. VAR=Varimax rotation. PRO=Promax rotation.

Figure 3. Effect of PCA Variations on Sixty-Five Factor Waveforms. The bottom graph presents the original waveforms. The other graphs present the factor loadings (factor patterns scaled to microvolts) for the representative simulation (median reconstruction of Component 2). For comparison's sake, each waveform is scaled so that the maximum amplitude is set to the top of the graph. COV=covariance matrix. COR=Correlation matrix. c=covariance loading. k=Kaiser normalization. n=not weighted loadings. VAR=Varimax rotation. PRO=Promax rotation.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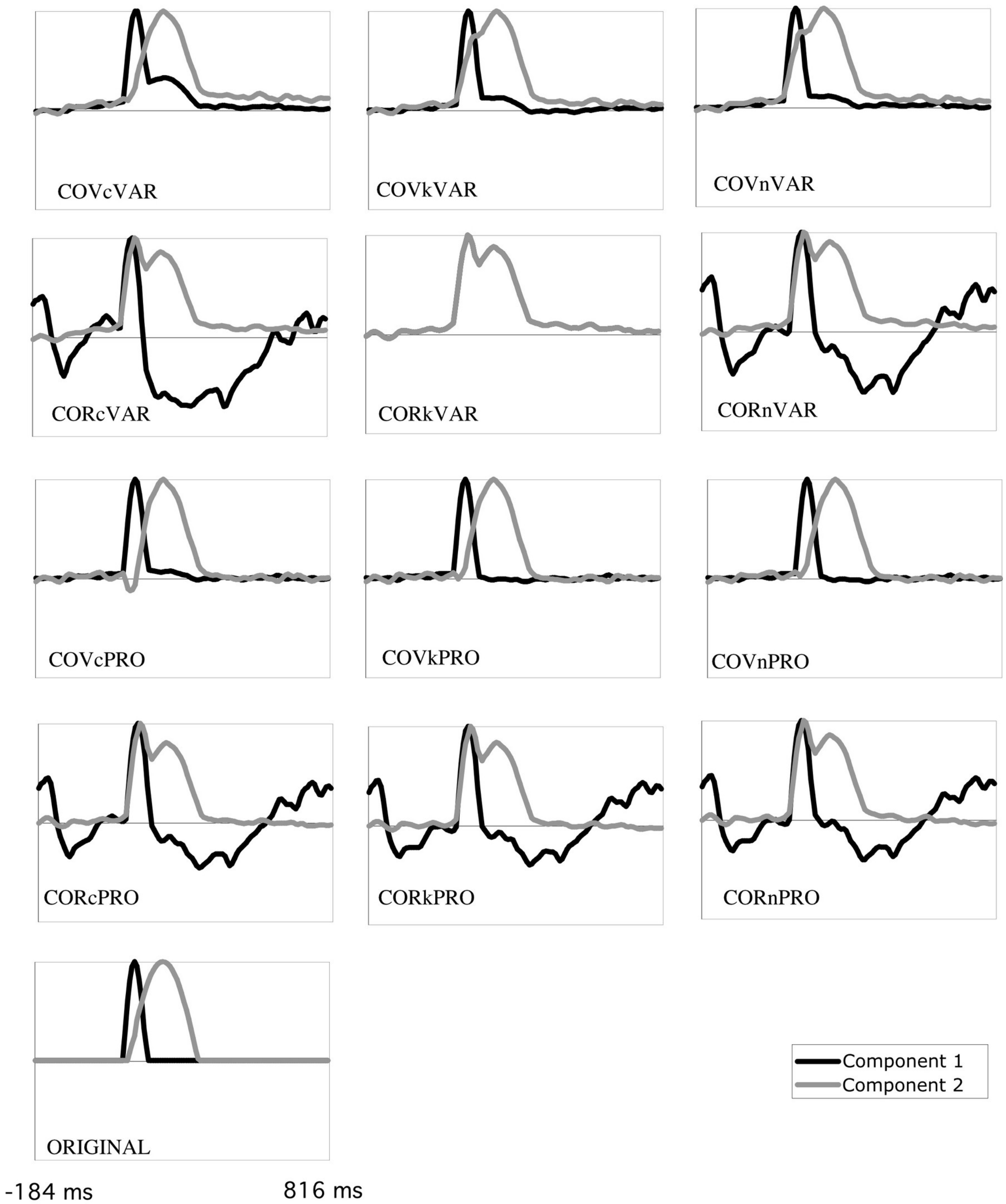
Component 1
Component 2
Noise

4 factors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CORnPRO
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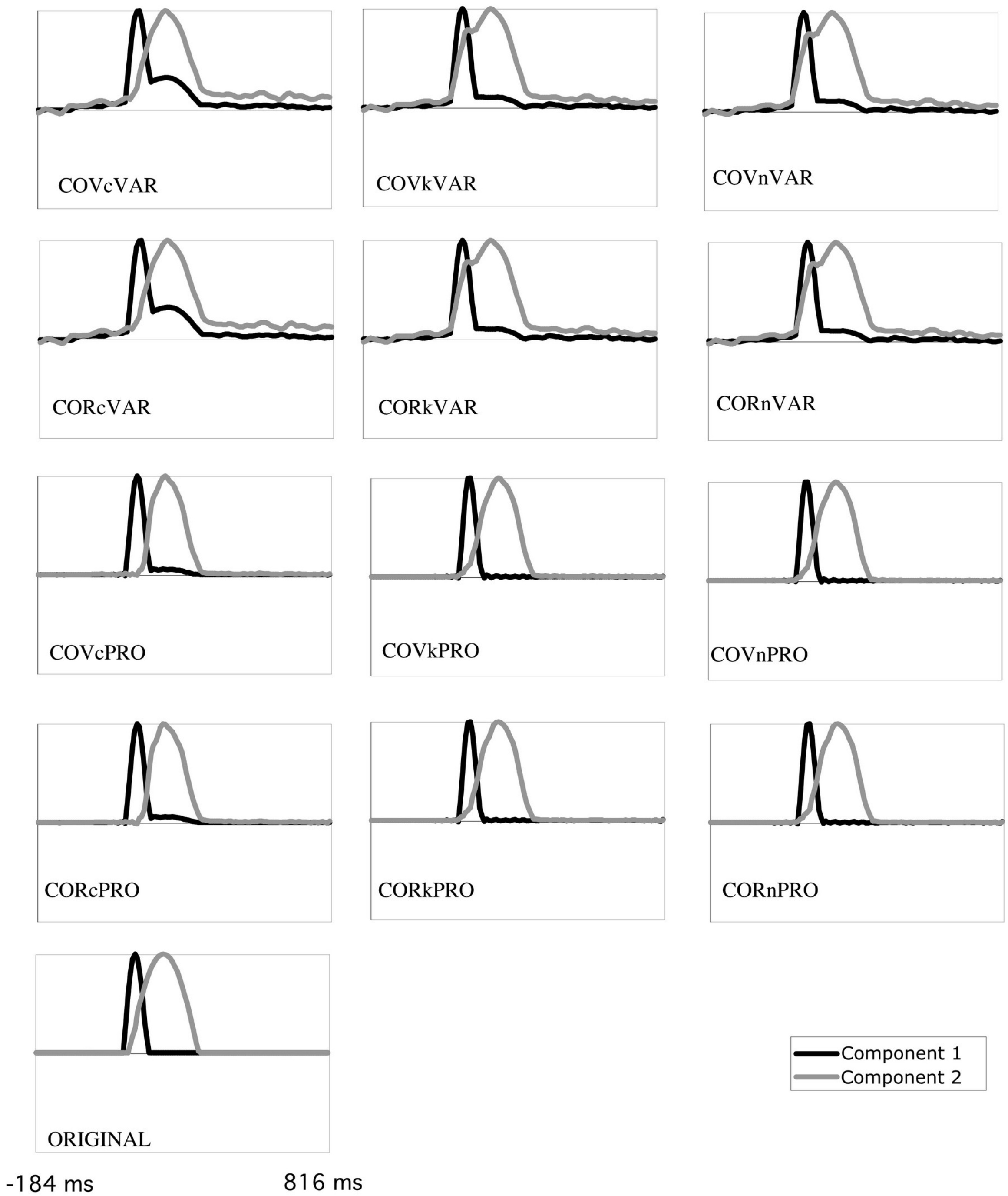
Component 1
Component 2
-184 ms
816 ms

65 factors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ORIGINAL
Component 1
Component 2
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816 ms