EVALUATING TWO-STEP PCA OF ERP DATA WITH GEOMIN, INFOMAX, OBLIMIN, PROMAX, AND VARIMAX ROTATIONS

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ABSTRACT

Principal components analysis (PCA) can facilitate analysis of event-related potential (ERP) components. Geomin, Oblimin, Varimax, Promax, and Infomax (independent components analysis) were compared using a simulated dataset. Kappa settings for Oblimin and Promax were also systematically compared. Finally, the rotations were also analyzed in a two-step PCA procedure, including a contrast between spatio-temporal and temporo-spatial procedures.

Promax was found to give the best overall results for temporal PCA and Infomax was found to give the best overall results for spatial PCA. The current practice of kappa values of 3 or 4 for Promax and 0 for Oblimin was supported. Source analysis was meaningfully improved by temporal Promax PCA over the conventional windowed difference wave approach (from a median 32.9 mm error to 6.7 mm). It was also found that temporo-spatial PCA produced modestly improved results over spatio-temporal PCA.

Principal components analysis or PCA (for reviews, see Gorsuch, 1983; Harman, 1976) has long been applied to ERP (event-related potential) datasets (Chapman & McCrary, 1995; Dien & Frishkoff, 2005; Donchin & Heffley, 1979; Glaser & Ruchkin, 1976; Möcks & Verleger, 1991; van Boxtel, 1998) in order to obtain dependent measures and to determine the dimensionality of effects of interest. Although an early critique (Wood & McCarthy, 1984) led for a time to concerns about the technique, the "misallocation of variance" problem they reported was just a way of saying that PCA solutions are not always perfect. Furthermore, those authors noted that even the conventional windowed measure shares the same issue of misallocation of variance and therefore did not mean to discourage use of PCA. In any case, with the increasing use of high-density ERP recording montages, there has been a resurgence of interest in this data reduction technique. Furthermore, a series of studies (Carretie et al., 2004; Debener, Makeig, Delorme, & Engel, 2005; Dien, Tucker, Potts, & Hartry, 1997; Dien, Frishkoff, Cerbone, & Tucker, 2003a; Dien, Spencer, & Donchin, 2003c; Dien & O'Hare, 2008; O'Hare & Dien, 2008; O'Hare, Dien, Waterson, & Savage, 2008; Pourtois, Delplanque, Michel, & Vuilleumier, 2008; Richards, 2004; Tapia, Carretie, Sierra, & Mercado, 2008) have demonstrated that it can enhance source analysis efforts, a topic of current interest.

An important step in PCA is rotation, which is necessary because the factors[1] generated by the initial unrotated solution tend to be arbitrary uninterpretable linear combinations of the true latent variables. This happens because the initial "unrotated" solution follows the criterion that each factor (computed in succession) accounts for the maximum possible variance that has not been accounted for by prior factors, a criterion that is generally best met by combinations of the latent variables (e.g., ERP components) rather than a single latent variable, which is normally the goal of the researcher. Rotation is a method of translating these sets of factors to mathematically equivalent sets of linear combinations that are simpler and more interpretable (ideally just one latent variable per factor). The extent to which this process can succeed depends on the extent to which the rotation criteria match the characteristics of the true latent variables (e.g., the ERP components). For example, most rotations attempt to achieve some version of simple structure, defined as minimization of the number of variables loading on each factor (Thurstone, 1935; Yates, 1987), a criterion that seems especially appropriate for ERP waveforms, which will typically have loadings of zero for most of the time points (for an example of "unrotated" versus rotated ERP solutions, see Dien & Frishkoff, 2005).

Despite steady progress by statisticians in refining factor analytic techniques, much of the ERP literature still uses the basic Varimax rotation first developed in the 1950's (Kaiser, 1958). This rotation maximizes the variance of the factor loadings. One of the chief limitations of this rotation procedure is that it maintains the orthogonality of the initial unrotated solution (i.e., the resulting factors are uncorrelated with each other). If the latent variables (e.g., the ERP components) are not orthogonal, the resulting mismatch between the statistical model and the true data results in distorted factor solutions, as demonstrated in simulation studies where the true solution is known (Dien, 1998a; Dien, Beal, & Berg, 2005). This issue of orthogonality is especially an issue for ERP datasets because, at least for temporal PCA where the time points are the variables and the channels are the observations, the spatial overlap of ERP components virtually guarantees that the ERP factors should be substantially correlated (see Figure 1).

There are a number of oblique rotations available that allow factors to be correlated. One of the most widely used is the Promax rotation (Hendrickson & White, 1964), which takes the Varimax solution as a starting point and then relaxes the orthogonality restriction by performing a further rotation in which orthogonality is no longer enforced. This further rotation takes the form of rotating towards a target computed as the current factor loadings taken to a higher power. This higher power is specified by a parameter, kappa, which is typically in the range of 2 to 4 (SAS uses 3 as the default and SPSS uses 4 as the default). Higher kappas result in more correlated solutions, with the appropriate kappa depending on the dataset (Hakstian & Abell, 1974; Hakstian, 1971). This approach will succeed to the extent that the Varimax rotation has approximated the appropriate solution. When applied to ERP data, Promax has been shown to yield improved results over Varimax with both real (Dien et al., 2003c) and simulated (Dien, 1998a; Dien et al., 2005) data.

An alternative oblique rotation from a quite different background is Infomax (Bell & Sejnowski, 1995), which, as implemented by the EEGlab software (Delorme & Makeig, 2004), uses an independent components analysis (ICA) approach (Hyvärinen, Karhunen, & Oja, 2001). Infomax differs in a number of respects from the conventional PCA rotations (Dien, Khoe, & Mangun, 2007; Jennrich & Trendafilov, 2005). When used as a rotation following an initial PCA extraction, it can be treated as just another oblique rotation, albeit one with special properties since it does not seek to maximize simple structure, unlike the other rotations discussed thus far. This rotation maximizes statistical independence (minimizing the extent to which a factor raised to a set of higher powers, operationalized as a logarithmic function equivalent to a Taylor series, is correlated with other factors) between the factor scores instead of seeking simple structure in the factor loadings. Full independence would mean that the rotation would be orthogonal but in practice the second order correlations are removed prior to the rotation and then reintroduced afterwards, resulting in an oblique rotation. The practice of removing the second order correlations prior to the rotation (by a process termed sphering) also means that the often-repeated assertion that Infomax operates on more information than conventional PCA rotations is, in practice, false and so the typical Infomax analysis is in effect operating on different information, not more information. Infomax also seeks to maximize the non-normality of the factor scores, based on the principle that mixtures are more likely to be normally distributed due to the central limit theorem (Hyvärinen et al., 2001, p. 9). Both criteria influence the rotation process in combination. A more detailed discussion of the differences between Promax and Infomax is made elsewhere (Dien et al., 2007).

These differences in rotation criteria are especially pertinent to the distinction between spatial and temporal PCAs. The former involves using channels as the variables and the latter using time points as the variables (Dien, 1998a). Both approaches provide both spatial and temporal information, differing only in which is represented in the factor loadings and which is represented in the factor scores. Counter-intuitively, spatial PCA is best at characterizing the time course and temporal PCA is best at characterising the spatial topography (Dien, 1998a; Dien, Spencer, & Donchin, 2004). This distinction is especially important to the present comparisons because traditionally the Varimax rotation (the most common procedure) has been applied as a temporal PCA whereas the Infomax rotation (ICA) is normally applied as a spatial PCA (Debener et al., 2005; Johnson et al., 2001; Klein & Feige, 2005; Ku et al., 2007; Lin et al., 2007; Makeig, Jung, Bell, Ghahremani, & Sejnowski, 1997; Makeig et al., 1999a; Makeig et al., 1997b; Makeig et al., 1999b; Mehta, Jerger, Jerger, & Martin, 2009; Marco-Pallares, Grau, & Ruffini, 2005; Olbrich et al., 2002; Olbrich, Maes, Valerius, Langosch, & Feige, 2005; Pritchard, Houlihan, & Robinson, 1999; Wibral, Turi, Linden, Kaiser, & Bledowski, 2008).

For a number of reasons, the two types of analyses are not equivalent. For example, two ERP components with similar time courses but different scalp topographies cannot be separated by temporal PCA since the factors are defined in terms of a specific time course (as encoded in the factor loadings) and if they have the same time course then they must be represented by the same factor (thus relying on a temporal PCA alone to determine the dimensionality of an effect is likely insufficient, cf. Lefebvre, Marchand, Smith, & Connolly, 2007); however, these two ERP components could be separated by spatial PCA due to their different topographies (the presence of condition and individual difference variance in the observations allows the two ERP components to be separated in the latter case). For this reason, a two-step PCA procedure involving first one and then the other type of analysis is recommended over either spatial or temporal PCA alone (Dien & Frishkoff, 2005; Spencer, Dien, & Donchin, 1999; Spencer, Dien, & Donchin, 2001). Whether the spatial step should be used first (Dien et al., 2003c; Dien et al., 2004; Fishman, Goldman, & Donchin, 2008; Friederici, Mecklinger, Spencer, Steinhauer, & Donchin, 2001; Goldstein, Spencer, & Donchin, 2002; Krigolson & Holroyd, 2006; Krigolson & Holroyd, 2007; Lin et al., 2007; Lui & Rosenfeld, 2008; Rigoulot et al., 2008; Spencer et al., 1999; Spencer et al., 2001) or the temporal step should be used first (Curran & Dien, 2003; Curran & Friedman, 2004; Foti, Hajcak, & Dien, in press; O'Hare et al., 2008; O'Hare & Dien, 2008; Tapia et al., 2008) has not yet been determined, although this author has been informally recommending a temporo-spatial sequence on the basis of the observation that the temporal step provides better separation (Dien et al., 2007) and therefore seems likely to provide some additional benefit to the following spatial step. The relative merits of spatio-temporal and temporo-spatial two-step PCA will therefore be examined as well.

Whereas rotating to simple structure is appropriate for a temporal PCA since a given time point should only be affected by a subset of the ERP components, it is not appropriate for a spatial PCA where volume conduction ensures that nearly all channels are affected by a given ERP component. Indeed, a comparison (Dien et al., 2007) of Promax and Infomax on simulation datasets revealed that whereas Promax yielded more accurate results for temporal PCA, Infomax yielded more accurate results for spatial PCA. This conclusion built on prior studies (Makeig, Jung, Ghahremani, & Sejnowski, 2000; Richards, 2004) that reported only advantages for Infomax. The former study (Makeig et al., 2000) examined only spatial PCA (conditions now known to favor Infomax). The second study (Richards, 2004) did not rotate the PCA solutions, a practice that results in factors that are complex uninterpretable combinations of the latent variables and that are uncorrelated rather than oblique, both problematic. Another study (Bugli & Lambert, 2007) that compared conventional PCA with ICA (albeit a different variant than Infomax) also concluded in favor of ICA but it seemed to be using only spatial PCA and it is unclear what rotation it used for the PCA, if any.

While Promax is the most commonly used oblique PCA rotation, it is far from the only one. It is unclear whether its prevalence is due to merit or just inertia. Indeed, published papers suggest there are better alternatives. The one study (Gorsuch, 1970) that recommended the use of Promax over the alternatives did so on the basis of it being faster to compute, a consideration that modern computers have rendered moot; however, the conclusions of these papers may not generalize to the unique characteristics of ERP datasets. This manuscript is therefore dedicated to evaluating two other oblique rotations that have been claimed to provide better rotations than Promax and which have not been compared to Infomax.

The first alternative rotation is the Oblimin rotation (the only oblique rotation offered by SPSS other than Promax). The original rotation (Carroll, 1957) was later refined (Jennrich & Sampson, 1966) in a form termed Direct Quartimin (which corresponds to Direct Oblimin with a kappa of zero). In this latter form, the rotation criterion is balanced between an overly oblique criterion in which the sum of the squared cross-products of the factor loadings is minimized and an overly orthogonal rotation criterion in which sum of the covariances of the squared cross-products is minimized. The degree of balance between the two criteria is controlled by a parameter termed kappa. Kappa is usually varied between -4 (essentially orthogonal) and .8 (very correlated), based on the view that values over .8 can be problematical (Harman, 1976) but see (Jennrich, 1979). A comparison (Hakstian & Abell, 1974) of Promax and Direct Oblimin (and some other rotations) concluded that Oblimin generally yielded better solutions than Promax, although no one level of kappa seemed to be best for all datasets. It has been suggested (Gorsuch, 1983) that one might optimize the Oblimin rotation by running it multiple times with the entire range of kappa values and then choosing the one that maximized a measure of simple structure. In the present report, this approach will be termed a Variable Oblimin (in that the kappa parameter is variable).

A second alternative is Geomin (Yates, 1987), which operates by seeking to minimize the product of a variable's loading (or more specifically, its reference vector coefficient) across all the factors in an effort to meet Thurstone's original definition of simple structure. Against a number of rotations, Geomin seemed to perform best in one test (Browne, 2001). Likewise, in a direct comparison with Direct Oblimin it yielded superior results (Yates, 1987); however, effectiveness of a rotation is dependent on the characteristics of the data and they have not yet been evaluated with respect to ERP data.

A simulation ERP dataset was therefore constructed to evaluate the Geomin and Oblimin rotations. The background noise was made to be realistic by using real background noise. The simulated components were also made to be realistic by using real data to form them. They were also given realistic individual difference variance both spatially and temporally by using subject averages rather than grand averages to form them. The decision was made to include only two simulated components in each simulation so that the cause of PCA failures could be understood and generalizations drawn on the boundary conditions of these procedures. Using only pairs of components has the drawback of being less realistic, however. It has already been shown elsewhere (Dien et al., 2007) that including more than two simulated components does not change the conclusions.

Regarding the analysis approach, a number of decisions had to be made about how to evaluate a simulated dataset. First of all, since the true answer is known, it was possible to precisely measure the degree of accuracy of the reconstructions. Of course, it will not be readily evident to a reader how much of a difference in accuracy (e.g., .97 vs. .96) is "meaningful." Meaningfulness will be provided by presenting the effects on the bottom line measures of ANOVA effects and source analysis. It is up to the reader to decide whether the differences obtained are "meaningful." Accuracy of ERP component reconstruction is provided to facilitate the long-term goal of incrementally improving the quality of the factor analysis procedures. Statistical tests were applied to the results since they provide a convenient criterion for identifying noteworthy differences; however, since the data are simulated, it is not clear what these statistical tests signify. The observations are not random samples from a larger population of interest and thus significant results do not signify generalizability. These comparisons were made against the rotations currently recommended: Promax for temporal PCA and Infomax for spatial PCA (Dien et al., 2007).

Finally, the accuracy and the source analysis results will be presented on a casewise basis, averaging together the scores of each pair, rather than on the basis of individual components. This approach will be taken partly in order to reduce the information load being induced by the tables. This approach will also be taken because interpretation of the effects will focus on the pairwise relationships (e.g., a particular rotation has difficulties with differentiating ERP components with similar scalp topographies). Although it might be tempting to wish to know which rotation is especially good for a particular component, this simulation study was not designed to characterize real ERP components and so the labels should not be taken literally. For example, the "N400" is not a negativity as it is comprised of all the ERP activity present in the N400 window collapsed into a single dimension (although it was extracted from an N400 dataset). These simulated components were constructed solely to provide a diverse range of characteristics.

In the present report, Geomin and Oblimin are compared to Varimax, Promax, and EEGlab's Infomax implementation in order to ascertain whether either of them provide an improvement for ERP data with respect to accurately extracting individual ERP components, enhancing statistical power of ANOVAs, and optimizing source localizations. Furthermore, the effects of different kappa levels for Promax and Oblimin are examined, as well as a Variable Oblimin algorithm. This simulation study also extends prior such efforts (Dien, 1998a; Dien et al., 2005; Dien et al., 2007) by measuring not just accuracy of the factor reconstructions but also the bottom line effects on ANOVAs and source analyses. These comparisons will be made against the existing recommendation (Dien et al., 2007), based on empirical results, that Infomax is best for spatial PCA and Promax is best for temporal PCA. Finally, these analyses will be extended to the two-step PCA procedure to verify whether these observations generalize to it and also to determine whether the spatial or the temporal step should be applied first.

METHODS

Simulation Construction

A simulation dataset was derived from a prior study (Simulation #4, Dien et al., 2007) to compare the rotation methods. This simulation set consists of 100 simulated sets of data, each with 16 participants, 2 conditions, 65 channels, and 125 time points (125 Hz digitization rate). Background electroencephalographic (EEG) activity was added from 16 real participants (55 trials per average) from a previously published study (Dien et al., 2003a). event-related potentials (ERPs) were eliminated by using a +/- reference (Schimmel, 1967), which flips every other trial prior to averaging. The noise average was filtered with a 30 Hz low pass filter and average referenced (Bertrand, Perrin, & Pernier, 1985; Dien, 1998b). The standard deviation of the noise ranged from 0.44 to 1.38 (median 1.05) microvolts across the epoch.

Pairs of real components were added to each dataset (Figure 2). A total of five ERPs were obtained from prior experiments (a visual P1, an auditory N1, an auditory P300, an auditory P2, and a visual N400). In order to ensure that these ERPs have a known unitary dimensionality, they were constructed from the cross-product of the time course at the peak electrode of the grand average and the scalp topography at the peak time point of the grand average (i.e., they had an identical time course at all electrodes and an identical scalp topography at all time points). Realistic subject variability in time course and scalp topography was included by using the subject averages rather than the grand average to construct these ERP components. Ten different pairs of these components were generated, resulting in ten replicates for each type of pair (total of one hundred simulations). Each simulation had random shared amplitude variability of the two ERP components (individual difference variance) as well as separate random variability for each individual ERP component. In order to be able to examine misallocation of condition effects, a modest condition effect was introduced into one of the two ERP components (amplitude was multiplied by .7 in one condition and by 1.3 in the other condition). The size of the condition effect was intended to be realistic to avoid exaggerating the size of any misallocation effects (Beauducel & Debener, 2003) and to evaluate the impact of the principal components analysis (PCA) techniques under challenging circumstances.

To be more specific about the amplitude parameters, for each pair, the first component's amplitude was multiplied by a random parameter (0.5 to 1.5) and the second component's parameter was an average of the first amplitude parameter and a separate random number (0.5 to 1.5). The means of the first parameter was 0.996 and 0.992 respectively for the two conditions (standard deviation of .28). For the second parameter, the means of the first parameter was 0.700 and 1.294 respectively for the two conditions (standard deviations of 0.14 and 0.26).

Principal Components Analysis Procedures

The ERP PCA (EP) Toolbox versions 1.2 and 1.31 (https://sourceforge.net/projects/erppcatoolkit/) were used to analyze the simulated datasets. The implementations used in the EP Toolkit are the EEGlab implementation of Infomax (Delorme & Makeig, 2004), the gradient projection implementations of Geomin and Oblimin (Bernaards & Jennrich, 2005), and the published algorithms for Varimax (Kaiser, 1959) and Promax (Hendrickson & White, 1964). The variable Oblimin algorithm follows a suggestion (Gorsuch, 1983) to apply a range of kappa values to each analysis (in this case: -4 -3 -2 -1 0 .2 .4 .6 .8) and then use a measure of factor simplicity (in this case Hofmann, 1977) to select the optimal solution.

The PCAs were conducted using covariance matrices and Kaiser normalization of the loadings for Varimax and Promax (Dien et al., 2005). Based on Scree plots (Cattell, 1966; Cattell & Jaspers, 1967), six factors were retained for spatial PCAs and seven for temporal PCAs. The factor loadings were converted into microvolts by multiplying the factor pattern matrix with the standard deviations of the variables (Dien et al., 1997; Dien, 2006).

Evaluation of Principal Components Analysis Results

The accuracy of the resulting waveforms and scalp topographies was measured using a simple correlation between the known values and the factor that had the closest match. If the same factor matched both ERP components then it was matched with the closest component and the second closest match was found for the other component. Matches were made on the basis of the factor pattern matrix loadings (even for Infomax) scaled to microvolts (Dien, 2006) and the grand average data (matching by loadings generally yielded better results than by factor scores for both spatial and temporal PCAs).

For tests of misallocation of variance in the analysis of variance (ANOVA) results, the peak time point (for spatial PCA) and peak channel (for temporal PCA) of the matched ERP component was used for an ANOVA of the factor score. A repeated measures one-way ANOVA was conducted for each of the factors corresponding to an ERP component. Type I errors were defined as significant p-values for the ERP component with no condition effect and Type II errors were defined as non-significant p-values for the ERP component with the condition effect. For comparison's sake, a conventional windowed analysis was also conducted on the simulated datasets with a 50 ms window centered on the peak time point at the peak channel.

For tests of localization accuracy, the scalp distribution as encoded in the factor pattern matrix loadings rescaled to microvolts (for spatial PCA) and the factor scores (for temporal PCA) was utilized. Robert Oostenveld's Dipfit 2.2 of the FieldTrip software (http://www2.ru.nl/fcdonders/fieldtrip) was used to perform the source localization analyses. A three-shell boundary element model was used to provide a realistic head shape. Symmetric paired dipoles were used and an automatic grid scan was conducted first to identify the starting location most likely to be close to the global minimum, prior to an iterative gradient descent search for the optimal source solution. The results were compared to that obtained by a source analysis of the original synthetic ERP component (prior to the addition of the background EEG noise and without any other overlapping ERP components). Error was defined as the Pythagorean distance from this "correct" solution. For comparison's sake, source analysis was also conducted on the difference wave of the experimental ERP component using a 50 ms window centered on the peak time point. When evaluating the results, it should be kept in mind that the simulation ERP components were created by collapsing together all the activity within the window of interest in order to produce an artificial component of known dimensionality; for this reason, it is not expected that a source solution would correspond to any real anatomical source site as it should reflect the central tendency of all the ERP components that were collapsed together.

Robust Statistics for Inference Testing

For the inferential tests of the simulation results, SAS/IML code (Keselman, Wilcox, & Lix, 2003) for conducting robust statistical tests (made available athttp://www.umanitoba.ca/faculties/arts/psychology/) was ported to Matlab (available for download at http://homepage.mac.com/jdien07/). A 5% symmetric trim rule was used (1 observation dropped at either extreme within each cell). The seed for the number generation was set at 1000. The number of simulations used for the bootstrapping routine was set at 50,000 to ensure stable *p*-values. The robust statistic (T_{WJt}/c) is meant to improve on (more closely comply with the nominal alpha rate than) the conventional ANOVA by: 1) using boostrapping to estimate the population distribution rather than assuming a normal distribution, 2) using trimmed means to be more resistant to outliers, and 3) using a Welch-James statistic to not assume a homogenous variance-covariance structure. Further description of the inferential issues, as they apply to ERP data, is available elsewhere (Dien, Franklin, & May, 2006). P-values are rounded to the second significant digit. The ANOVAs of the experimental effects themselves were conducted using conventional ANOVAs since it is expected that they are what most readers use themselves.

RESULTS

One-Step PCA

Starting with the temporal PCA waveform results (Table 1), the current standard, Promax, yielded the best accuracy, along with Oblimin. Promax was significantly better than Varimax (T_{WJt}/c [1,89]=20.53, $p<.00001$) and Geomin (T_{WJt}/c [1,89]=6.20, $p=.017$) only. Turning to the temporal PCA scalp topography results (Table 2), the Promax rotation produced the best result, which was significantly better than Geomin (T_{WJt}/c [1,89]=6.71, $p=.025$) and Infomax (T_{WJt}/c [1,89]=5.44, $p=.025$).

The waveform results for spatial PCA (Table 3) indicate a substantial advantage for the current standard, the Infomax rotation, versus the other rotations (Varimax: T_{WJt}/c [1,89]=66.23, $p<.00001$; Promax: T_{WJt}/c [1,89]=51.08, $p<.00001$; Geomin: T_{WJt}/c [1,89]=48.26, $p<.00001$; Oblimin: T_{WJt}/c [1,89]=23.03, $p=.00005$). Likewise, Infomax yielded the best performance for scalp topography (Table 4), which was significantly better than the alternatives (Varimax: T_{WJt}/c [1,89]=28.21, $p<.00001$; Promax: T_{WJt}/c [1,89]=61.42, $p<.00001$; Geomin: T_{WJt}/c [1,89]=118.91, $p<.00001$; Oblimin: T_{WJt}/c [1,89]=167.27, $p<.00001$).

The comparison of kappa values for Oblimin and Promax (Table 5) suggest that the default values used (zero for Oblimin and 3 for Promax) were appropriate. For Promax, the kappa made little difference across the values tested for temporal PCA and even the best kappa (4) did not approach Infomax for spatial PCA. For Oblimin, the kappa of zero was nearly the best, although a kappa of .2 did produce a slight increase (0.96 versus 0.95) for waveforms using temporal PCA. For the remaining analyses the Oblimin kappa will be kept at zero since the difference from a kappa of .2 seems insufficient to justify moving away from the commonly accepted value of zero. The Variable Oblimin algorithm underperformed Oblimin with a kappa of zero.

Turning to the bottom line measures in Table 6, there were no significant differences between the rotations with respect to the Type I and Type II error rates for both spatial and temporal rotations. The p-values appeared to be a more sensitive measure of rotation effects. For spatial PCA, Infomax correctly yielded significantly higher p-values for the ERP component with no experimental effect (Varimax: T_{WJt}/c [1,89]=9.20, p=.0033; Promax: T_{WJt}/c [1,89]=65.32, p<.00001; Geomin: T_{WJt}/c [1,89]=12.1, p=.00082; Oblimin: T_{WJt}/c [1,89]=36.05, p<.00001) and lower p-values for the correct ERP component than Promax (T_{WJt}/c [1,89]=65.32, p<.00001). Infomax also outperformed the windowed measure for both the Type I (T_{WJt}/c [1,89]=699.48, p<.00001) and Type II errors (T_{WJt}/c [1,89]=20.15, p=.00072). For temporal PCA, Promax produced significantly higher p-values for the ERP component with no experimental effect than Varimax (T_{WJt}/c [1,89]=8.21, p=.0057), Geomin (T_{WJt}/c [1,89]=7.75, p=.0066), and Oblimin (T_{WJt}/c [1,89]=6.36, p=.015). For the ERP component with the experimental effect, Promax was significantly different from the other rotations but only notably so from Infomax, where it was correctly lower (T_{WJt}/c [1,89]=6.21, p=.023).

Turning to source localization analyses, Table 6 indicates a substantial improvement by all methods over a conventional windowed difference wave approach. For spatial PCA, Infomax was significantly more accurate than the alternative rotations (Varimax: T_{WJt}/c [1,89]=44.35, p<.00001; Promax: T_{WJt}/c [1,89]=46.39, p<.00001; Geomin: T_{WJt}/c [1,89]=18.01, p=.00004; Oblimin: T_{WJt}/c [1,89]=37.43, p<.00001). For temporal PCA, Promax was more accurate than Geomin (T_{WJt}/c [1,89]=9.50, p=.0051) and Infomax (T_{WJt}/c [1,89]=11.67, p=.0017). Both spatial Infomax (T_{WJt}/c [1,89]=20954, p<.00001) and temporal Promax (T_{WJt}/c [1,89]=21.37, p=.00002) were more accurate than the windowed difference wave approach. Table 7 provides a comparison between temporal Promax and conventional windowing for each case.

<u>Two-Step PCA</u>

Starting with the waveform results (Table 8), the current informal recommendation, Temporal Promax/Spatial Infomax yielded the best accuracy (.97), with temporospatial rotations that started with Geomin or Oblimin being significantly less accurate but essentially equivalent: for example, Temporal Geomin/Spatial Infomax (.965: $T_{WJt}/c[1.0,89.0]=12.45$, $p=0.0023$) and Temporal Oblimin/Spatial Infomax (.965: $T_{WJt}/c[1.0,89.0]=14.34$, $p=0.00052$). Although Spatial Infomax/Temporal Promax was better (.92) than all other spatio-temporal PCA results (except for Spatial Oblimin/Temporal Promax at .93), it was notably lower than the temporo-spatial equivalent (.97): $T_{WJt}/c(1.0,89.0)=42.07$, $p<0.00000001$.

The results for Temporal Promax/Spatial Infomax were also strong, but less clear-cut, for scalp topography results (Table 9). Although the spatio-temporal results were stronger when the spatial rotation was Infomax (.90 vs. .86), they were not significantly so. Examination of the individual results indicated that there were a substantial number of poor results with the Infomax rotation that were not reflected in the median summary statistic of the table but that affected the inferential statistics (even with the use of trimmed means). It could be said that the spatial Infomax rotations (for spatio-temporal procedures) often worked better when it worked but was not as consistent as the Temporal Promax/Spatial Infomax procedure. Some sense of this can be had from the casewise breakdown of the localization results in Table 7. Thus, this procedure was significantly better, or at least equal to, all of the spatio-temporal procedures. There were some better temporo-spatial procedures including Temporal Varimax/Spatial Infomax ($T_{WJt}/c[1.0,89.0]=68.16$, $p<0.00000001$), Temporal Geomin/Spatial Infomax ($T_{WJt}/c\ [1.0,89.0]=31.55$, $p<0.00000001$), and Temporal Oblimin/Spatial Infomax ($T_{WJt}/c[1.0,89.0]=12.97$, $p=0.00058$).

Moving on to bottom line measures of localization errors (Table 10), Temporal Promax/Spatial Infomax yielded results that were stronger or statistically equivalent to all the spatio-temporal procedures. Results were also better than, or equivalent to, all the temporal-spatial alternatives except for Temporal Geomin/Spatial Infomax: $T_{WJt}/c(1.0,89.0)=5.88$, $p=0.021$.

For performance with ANOVAs (Table 11), Temporal Promax/Spatial Infomax yielded results that were either better or statistically comparable to all the other rotations for Type I and Type II error rates: for example, Spatial Infomax/Temporal Promax Type II errors ($T_{WJt}/c\ [1.0,89.0]=2.02$, $p=0.037$). For raw p-values, Spatial Promax/Temporal Geomin ($T_{WJt}/c\ (1.0,89.0)=6.07$, $p=0.016$), Spatial Oblimin/Temporal Oblimin ($T_{WJt}/c\ (1.0,89.0)=4.46$, $p=0.039$), Temporal Varimax/Spatial Varimax ($T_{WJt}/c\ (1.0,89.0)=12.53$, $p=0.0038$), Temporal Varimax/Spatial Promax ($T_{WJt}/c\ (1.0,89.0)=10.19$, $p=0.0058$), Temporal Varimax/Spatial Geomin ($T_{WJt}/c\ (1.0,89.0)=5.59$, $p=0.023$), Temporal Geomin/Spatial Infomax ($T_{WJt}/c\ (1.0,89.0)=23.64$, $p=0.00026$), Temporal

Oblimin/Spatial Varimax (T_{WJt}/c (1.0,89.0)=9.31, p=0.0043), Temporal Oblimin/Spatial Promax (T_{WJt}/c (1.0,89.0)=8.60, p=0.0038), and Temporal Oblimin/Spatial Infomax (T_{WJt}/c (1.0,89.0)=20.65, p=0.00056) yielded significantly lower p-values for the simulated ERP component with the true experimental effect. For the incorrect ERP component, only Spatial Oblimin/Temporal Promax generated a higher (good) p-value: T_{WJt}/c (1.0,89.0)=3.98, p=0.050.

DISCUSSION

The comparison of Geomin and Oblimin against Infomax (as implemented in EEGlab) for spatial PCA and Promax for temporal PCA yielded a variety of results. The present analyses strengthened an earlier recommendation (Dien et al., 2007) to use Infomax for spatial PCA and Promax for temporal PCA by showing that the improvements are reflected in bottom line of ANOVA and source analysis results. In general, temporal PCA proved to be a more effective approach for optimizing source analysis than spatial PCA. Varimax was once again generally shown not to be the optimal approach for either type of PCA. It was also found that kappa values of 3 or 4 for Promax and 0 for Oblimin were generally supported. The Variable Oblimin algorithm was inferior to the normal Oblimin rotation. Finally, the two-step PCA results generally support the use of a temporo-spatial sequence rather than a spatio-temporal sequence.

Regarding the rotation comparisons, the results provide grounds for making empirically informed choices for ERP datasets. The Geomin and Oblimin rotations did not outperform the competing oblique rotations despite promising initial reports (Browne, 2001; Hakstian & Abell, 1974; Yates, 1987). One possible reason is that ERP datasets have characteristics that do not favor these particular rotation criteria. Another possible reason is that the gradient projection implementation of these rotation criteria (Bernaards & Jennrich, 2005) was not as efficacious as those used in these reports.

For temporal PCAs, the overall best choice was Promax, although Oblimin was not significantly different (Tables 1 and 2). Figure 3 displays an example of the reconstructed waveforms to help provide a sense for the meaningfulness of the accuracy numbers. Examination of the cases suggests that although Promax is overall better for temporal PCA, Infomax does have an advantage for cases where the two components have very similar time courses, as in Cases 3 and 5 ("case" meaning particular pairings of simulated components, as the degree of similarity between components is more relevant to success in separating them than is the characteristics of any individual component).

The Infomax rotation as implemented in EEGlab was much more effective for spatial PCA than the other rotations evaluated herein (Tables 3 and 4), as found in a prior comparison with Promax (Dien et al., 2007) and thus it continues to be the recommended approach for spatial PCAs. The casewise numbers of Table 3 suggest that this advantage is especially pronounced for ERP components that have a similar scalp topography, as in Cases 4 and 5. There did not appear to be any cases that were notably more difficult for Infomax.

As seen in Table 5, these conclusions were not modified by changes in the kappa values of the two rotations as this analysis suggested that the original kappa choices (zero for Oblimin and three for Promax) were appropriate, although a kappa of .2 did yield an incremental improvement for Oblimin. Such a minor change is unlikely to be robust across different datasets and so it is recommended to continue using the commonly accepted kappa value of zero for Oblimin. Likewise, it appears that, for ERP data, the commonly used kappa values of 3 and 4 are both appropriate, in contrast with a study (Cureton, 1976) of non-ERP data which concluded that 4 was optimal.

Although the accuracy measures provide some sense of rotation performance, the ultimate question is whether the different accuracies recorded herein makes a meaningful difference for analyses. With respect to ANOVAs of experimental effects, as seen in Table 6, nearly all rotations seemed to improve statistical specificity over the conventional windowed measure (reducing Type I errors in the non-experimental component from 0.10 to between 0.00 and 0.10), although they were not statistically different. The p-values were, however, significantly improved by spatial Infomax and temporal PCA. Both also yielded significant differences in p-values for the Type II rate of the experimental component but in practice the p-values were not meaningfully different. The Type I and Type II effects could be mediated by either reductions in the error variance or by misallocation of the condition effect to the wrong factor. Since the effects were mostly seen in the Type I effects, it seems likely that they were mediated mostly by reduction in the noise variance. When one considers the Type I and Type II effects in aggregate, it is apparent that the recommendation to use Infomax for spatial PCA and Promax for temporal PCA was further supported.

The most dramatic results of this report involve source analysis. There were considerable improvements in source solutions, with a 32.9 mm error with difference wave data being reduced to 17.5 mm with spatial PCA using

Infomax and just 6.7 mm error with temporal PCA using Promax. Given that functional cortical areas (such as Brodmann areas) are often on the order of 10 mm across, these improvements in accuracy are of notable practical significance. It is therefore concluded that PCA can be quite helpful for optimizing the success of source analysis. The advantage of PCA over the difference wave approach is that it can make use of the entire amplitude of an ERP component rather than just the portion that differs between conditions, resulting in a higher signal-to-noise ratio. Contrary to what intuition might suggest, temporal PCA appears to be preferable to spatial PCA for source analysis, regardless of which rotation is used. Of the rotations tested, Promax performed best for such temporal PCAs. Figure 4 provides some sense of how these results translate into functional neuroanatomy.

When evaluating a method, it is important to examine its failures as well as its successes in order to arrive at a full understanding of its capabilities. In Table 7 the efficacy of spatial Infomax is compared to temporal Promax, as well as Varimax, is compared to the conventional windowing procedure for each of the ten cases. In all but Case #5 the Promax solution provided a clearly improved solution over the conventional approach. Examination of Table #1 indicates that Case #5 was especially problematic for all but the Infomax rotation. For this case only did spatial Infomax clearly outperform temporal Promax.

For Case #5 the difficulty was that temporal PCA essentially attempts to divide the epoch into non-overlapping windows and the simulated P1 entirely overlaps with the simulated N1. Further refinements of the PCA procedure will be needed to address such situations. It is notable that although Infomax overall did not function as well as Promax, it did perform better in this case. It may therefore be prudent to verify results with an Infomax analysis when such cases of total overlap are thought to be present.

For three further cases (#1, #6 and #8) temporal Promax yielded improved source analysis results over conventional windowing but the error was still unacceptably large (over 20 mm). The commonality between these three cases is that the experimental ERP component (the "P1" and the "P300") had a small amplitude compared to the other ERP components (see Figure 2). Thus, this is just an unsurprising observation that PCA may not be sufficient to overcome the low signal-to-noise ratio of small ERP components. For the larger components, however, the error was quite small (less than 6 mm).

Finally, the rotations were evaluated in the context of the two-step PCA procedure (Spencer et al., 1999; Spencer et al., 2001). The two questions of primary concern were how it compares with the regular one-step PCA (which continues to be the most common approach) and whether the spatial or the temporal step should be conducted first. The results generally favored the use of a Temporal Promax/Spatial Infomax procedure over the alternative two-step procedures. The closest contender was the Temporal Geomin/Spatial Infomax procedure, which did well in the localization analysis but not as well in the ANOVA analysis. The spatio-temporal procedures were consistently worse, or at best equivalent, than the Temporal Promax/Spatial Infomax procedure.

The two-step procedure was generally did not produce results as strong as that of the one-step PCA procedures for both the ANOVA and the localization analyses. It is suggested that the reason is that the simulated dataset represents a situation favoring the conventional one-step PCA. For example, in the dataset originally used to present the two-step PCA procedure (Spencer et al., 1999; Spencer et al., 2001), there were multiple ERP components with nearly identical time courses, peaking at about 300 ms. A temporal PCA cannot separate ERP components with nearly identical time courses (Dien, 1998a) as the factors are defined in terms of the time course (all activity peaking at 300 ms must necessarily be allocated to the same factor). The same is true for spatial PCA and scalp topographies. In the present simulated dataset, most of the simulated components have different time courses and scalp topographies. Thus, the present report indicates that when the ERP components are sufficiently distinct, the one-step PCA can and does have an advantage over the two-step PCA. A examination of the case where the ERP components were not readily separated in either domain (Case #3 with the "P300" and the "N400"), the two-step PCA did indeed provide stronger results, with a localization error of 25.2 compared to 67.8 for temporal Promax and 70.1 for spatial Infomax (Table 7). With respect to the localization results (Table 7), the two-step procedure produced much better results in one case, slightly better in one case (within 10 mm), intermediate results in two cases, slightly worse in five cases (within 10 mm), and much worse in one case (where "case" is a particular pairing of simulated ERP components). Closer inspection of the worst case did not clarify why it was problematic for the two-step procedure.

It should also be noted that one-step analyses are also preferred for certain analytical goals. For example, spatial PCA allows the time course to differ between conditions and is therefore better for examining latency shifts (Dien, 1998a; Dien et al., 2004). Conversely, temporal PCA allows the scalp topography to shift and therefore may be better for examining laterality effects (Dien, 1998a) and fine-grained parametric analyses (Dien et al., 2003a). On the other hand, both the spatial and the temporal PCA will be vulnerable to confounding ERP components that are similar in the spatial and the temporal domains respectively so there is always a trade-off. Thus, the choice of whether to use a spatial PCA, a temporal PCA, or a two-step PCA depends on the analytical goals and the characteristics of the dataset.

It is therefore recommended that a two-step PCA be used for general analysis situations, especially when the componentry of the ERP is not fully known. If there is a mix of ERP components with some best separable temporally and others best separated spatially (as seems likely for most ERP datasets) then the two-step PCA procedure provides a generally applicable procedure. On the other hand, if the componentry is well-known and the ERP components of interest can be clearly distinguished in either the spatial or the temporal domain alone, then the corresponding one-step PCA should be used to take advantage of its stronger statistical power. Thus, the two-step PCA is the more general approach but its generality results in some loss of power compared to more specifically tailored approaches.

Finally, the results generally favored the use of a temporo-spatial sequence to a spatio-temporal sequence for two-step PCA. This may be understood in the following manner. Because the temporal Promax step generally produced cleaner separations than the spatial Infomax step, it is beneficial to apply it first. If one applies the less effective step first then the resulting factors will be more likely to be mixtures of the underlying ERP components. One might, for example, end up with two spatial factors, each a mix of the P2 and the P3. A subsequent temporal PCA step would result in four factors, two each for the P2 and the P3. Furthermore, when the second temporal step was applied, the mixing of the two ERP components increases the likelihood that the second step would be unsuccessful in correctly separating the ERP components in each of the two initial spatial factors. If the more effective temporal PCA step had been applied first then the initial two factors would have been a more-or-less pure P2 and P3 factor and the spatial step would not even be needed.

These conclusions must be tempered by some caveats. The efficacy of the conventional difference wave approach will vary as a function of the size of the condition effect; a larger condition effect will increase the size of the signal compared to the background noise. In the present case, the signal was moderate (100% modulation). It is also not claimed that this analysis constitutes a test of localization accuracy per se. The comparison in the present case is between the "correct" result obtained under ideal conditions (no background noise or other ERP components) and the result under non-ideal conditions as addressed by PCA and conventional difference waves. Thus, these results address only the errors introduced by background noise, overlapping ERP components, and inaccuracies in the PCA solutions, and not other influences (such as the quality of the head model). Thus, while the simulation results provide empirical guidance on which rotations provide more optimal solutions, they should not necessarily be taken as indicating that the accuracy of such a procedure would be 6 mm or so for real data. The present results also do not pertain to analyses where temporal PCA is not an option (as in frequency-domain data), where spatial PCA, and hence the Infomax rotation, are clearly preferable.

It is also important to note that the source solutions should not be taken literally as being likely generators for the simulated ERP components. The process for constructing the simulated components almost certainly fused together multiple ERP components. No effort was made during the process to obtain a pure ERP component and the procedure used to generate unidimensional simulated components would make it impossible to separate the constituent ERP components. The challenge of isolating pure ERP components will be left to future studies explicitly designed to do so and the current results may help to do so more effectively.

In conclusion, these results reinforce prior reports of the utility of PCA for ERP analysis. Furthermore, they reinforce the existing conclusion that Promax is preferable for temporal PCA and Infomax for spatial PCA. Geomin and Oblimin did not prove to be better alternatives to Promax, contrary to published reports, at least for ERP data. The present results also strengthen the argument that PCA can provide a promising approach for optimizing source analyses. Finally, the ultimate recommendation is not so much to favor Promax over Infomax as to suggest that they each be used in a two-step PCA approach (Spencer et al., 1999), using an initial temporal Promax followed by a spatial Infomax (see Franklin, Dien, Neely, Waterson, & Huber, 2007) when a broadly general approach is needed, while one-step temporal Promax and spatial Infomax can provide more powerful tools if chosen to fit the characteristics of the dataset.

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AUTHOR NOTES

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FOOTNOTES

1) Although it is customary to term the statistical variables produced by both PCA and ICA "components", since features of the ERP are also termed "components", in this treatment they will be termed "factors" instead to avoid confusion.

	C1	C2	Vmax	Pmax	Imax	Gmin	Omin
1	N400	P1	0.97	0.98	0.96	0.98	0.96
2	N400	N1	0.97	0.99	0.95	0.99	0.97
3	N400	P300	0.67	0.67	0.90	0.71	0.71
4	N400	P2	0.96	0.98	0.91	0.97	0.98
5	P1	N1	0.65	0.72	0.96	0.62	0.59
6	P1	P300	0.92	0.94	0.80	0.86	0.87
7	P1	P2	0.96	0.96	0.92	0.96	0.97
8	N1	P300	0.87	0.84	0.83	0.89	0.89
9	N1	P2	0.97	0.98	0.93	0.98	0.99
10	P300	P2	0.93	0.93	0.74	0.92	0.94
Totals	Median		0.94*	0.95#	0.92	0.94*	0.95
Totals	SD		0.12	0.11	0.07	0.12	0.12

Table 1. Waveform Results for Temporal PCA. C1 and C2 are the two simulated components in the dataset. Imax = Infomax ICA rotation. Omin = Oblimin rotation. Gmin = Geomin rotation. Pmax = Promax rotation. Vmax = Varimax rotation. The values are the accuracy of the reconstructions of the time courses, expressed as the correlation between the scaled factor results and the matching original component. The values are the median value of the ten replications. For each analysis, the accuracy was calculated for both simulated components and the mean accuracy of the two factors was recorded. The bottom rows are the median score across the entire 100 simulations and the standard deviation of the scores. # = Comparison score. * = Significantly different from the comparison score.

	C1	C2	Vmax	Pmax	Imax	Gmin	Omin
1	N400	P1	0.98	0.97	0.98	0.97	0.97
2	N400	N1	0.94	0.98	0.97	0.98	0.98
3	N400	P300	0.68	0.59	0.78	0.80	0.82
4	N400	P2	0.98	0.98	0.98	0.98	0.98
5	P1	N1	0.95	0.96	0.91	0.90	0.85
6	P1	P300	0.94	0.87	0.84	0.90	0.90
7	P1	P2	0.99	0.99	0.98	0.99	0.99
8	N1	P300	0.86	0.78	0.74	0.89	0.90
9	N1	P2	0.98	1.00	0.96	0.99	1.00
10	P300	P2	0.91	0.90	0.62	0.89	0.87
Totals	Median		0.95	0.97#	0.92*	0.94*	0.94
Totals	SD		0.10	0.12	0.12	0.06	0.08

Table 2. Scalp Topography Results for Temporal PCA. C1 and C2 are the two simulated components in the dataset. Imax = Infomax ICA rotation. Omin = Oblimin rotation. Gmin = Geomin rotation. Pmax = Promax rotation. Vmax = Varimax rotation. The values are the accuracy of the reconstructions of the scalp topographies, expressed as the correlation between the scaled factor results and the matching original component. The values are the median value of the ten replications. For each analysis, the accuracy was calculated for both simulated components and the mean accuracy of the two factors was recorded. The bottom rows are the median score across the entire 100 simulations and the standard deviation of the scores. # = Comparison score. * = Significantly different from the comparison score.

	C1	C2	Vmax	Pmax	Imax	Gmin	Omin
1	N400	P1	0.83	0.80	0.94	0.82	0.90
2	N400	N1	0.89	0.88	0.92	0.88	0.87
3	N400	P300	0.81	0.88	0.83	0.86	0.86
4	N400	P2	0.56	0.56	0.92	0.59	0.75
5	P1	N1	0.58	0.88	0.91	0.89	0.97
6	P1	P300	0.63	0.62	0.58	0.62	0.64
7	P1	P2	0.76	0.75	0.94	0.75	0.93
8	N1	P300	0.74	0.73	0.79	0.77	0.70
9	N1	P2	0.92	0.91	0.92	0.91	0.88
10	P300	P2	0.61	0.53	0.66	0.52	0.51
Totals	Median		0.74*	0.75*	0.90#	0.77*	0.85*
Totals	SD		0.13	0.13	0.12	0.13	0.14

Table 3. Waveform Results for Spatial PCA. C1 and C2 are the two simulated components in the dataset. Imax = Infomax ICA rotation. Omin = Oblimin rotation. Gmin = Geomin rotation. Pmax = Promax rotation. Vmax = Varimax rotation. The values are the accuracy of the reconstructions of the time courses, expressed as the correlation between the scaled factor results and the matching original component. The values are the median value of the ten replications. For each analysis, the accuracy was calculated for both simulated components and the mean accuracy of the two factors was recorded. The bottom rows are the median score across the entire 100 simulations and the standard deviation of the scores. # = Comparison score. * = Significantly different from the comparison score.

	C1	C2	Vmax	Pmax	Imax	Gmin	Omin
1	N400	P1	0.81	0.77	0.90	0.76	0.78
2	N400	N1	0.90	0.84	0.89	0.81	0.81
3	N400	P300	0.66	0.68	0.84	0.69	0.63
4	N400	P2	0.83	0.76	0.89	0.76	0.74
5	P1	N1	0.63	0.60	0.88	0.66	0.78
6	P1	P300	0.88	0.85	0.74	0.82	0.78
7	P1	P2	0.85	0.84	0.96	0.84	0.83
8	N1	P300	0.88	0.87	0.90	0.86	0.76
9	N1	P2	0.93	0.90	0.91	0.81	0.82
10	P300	P2	0.49	0.76	0.83	0.68	0.82
Totals	Median		0.84*	0.81*	0.88#	0.80*	0.78*
Totals	SD		0.14	0.11	0.06	0.09	0.06

Table 4. Scalp Topography Results for Spatial PCA. C1 and C2 are the two simulated components in the dataset. Imax = Infomax ICA rotation. Omin = Oblimin rotation. Gmin = Geomin rotation. Pmax = Promax rotation. Vmax = Varimax rotation. The values are the accuracy of the reconstructions of the scalp topographies, expressed as the correlation between the scaled factor results and the matching original component. The values are the median value of the ten replications. For each analysis, the accuracy was calculated for both simulated components and the mean accuracy of the two factors was recorded. The bottom rows are the median score across the entire 100 simulations and the standard deviation of the scores. # = Comparison score. * = Significantly different from the comparison score.

Rotation	Temp Waves	Temp Topo	Spat Waves	Spat Topo
Promax 2	0.95(0.12)	0.97(0.14)	0.75(0.13)	0.82(0.13)
Promax 3	0.95(0.11)	0.97(0.12)	0.75(0.13)	0.81(0.11)
Promax 4	0.95(0.11)	0.97(0.12)	0.76(0.13)	0.80(0.10)
Oblimin -4	0.91(0.12)	0.94(0.11)	0.89(0.14)	0.76(0.05)
Oblimin -3	0.91(0.12)	0.94(0.11)	0.87(0.14)	0.76(0.05)
Oblimin -2	0.92(0.11)	0.94(0.12)	0.87(0.14)	0.76(0.05)
Oblimin -1	0.93(0.10)	0.94(0.11)	0.86(0.14)	0.77(0.06)
Oblimin 0	0.95(0.13)	0.94(0.08)	0.85(0.14)	0.78(0.06)
Oblimin .2	0.96(0.13)	0.94(0.08)	0.85(0.14)	0.79(0.06)
Oblimin .4	0.95(0.11)	0.83(0.13)	0.84(0.14)	0.78(0.09)
Oblimin .6	0.88(0.10)	0.71(0.20)	0.83(0.12)	0.76(0.09)
Oblimin .8	NaN	NaN	NaN	NaN
Variable Oblimin	0.94(0.13)	0.94(0.10)	0.83(0.13)	0.76(0.09)

Table 5. Factor Results for Different Rotation Parameters for Promax and Oblimin Rotations. The Oblimin and Promax parameters are for kappa. Temp = temporal PCA. Spat = spatial PCA. Waves = timecourse. Topo = scalp topography. The values are the accuracy of the reconstructions of the time course and scalp topography, expressed as the correlation between the scaled factor results and the matching original component. The values are the median value across all 100 simulations with the standard deviation in parentheses. For each analysis, the accuracy was calculated for both simulated components and the mean accuracy of the two factors was recorded. NaN means that the rotation failed, resulting in "not a number."

PCA Type	Rotation	Type I Errors	Type II Errors	Type I p-values	Type II p-values	Localization Error
Spatial	Varimax	0.00	0.34	0.544*	0.003	37.0 (24.9)*
	Promax	0.09	0.32	0.391*	0.007*	38.7 (21.2)*
	Infomax	0.00#	0.34#	0.648#	0.004#	17.5 (30.2)#
	Geomin	0.04	0.34	0.538*	0.008	38.9 (15.4)*
	Oblimin	0.10	0.40	0.417*	0.007	46.1 (23.4)*
Temporal	Varimax	0.08	0.31	0.390*	0.005*	11.8 (24.3)
	Promax	0.02#	0.31#	0.545#	0.006#	6.7 (22.5)#
	Infomax	0.08	0.36	0.420	0.021*	18.0 (24.2)*
	Geomin	0.02	0.29	0.383*	0.004*	21.0 (29.4)*
	Oblimin	0.04	0.32	0.394*	0.006*	8.4 (27.6)
Conventional		0.10	0.34	0.305*	0.006*	32.9 (21.1)*

Table 6. Effects of Rotation on ANOVA and Source Localization errors. The Type I Errors were the proportion of false positives for the ERP factor with no condition effect. The Type II Errors were the proportion of false negatives for the ERP factor with a condition effect. The Type I and Type II p-values are the median of the actual p-values, so higher is better for the inactive component and lower is better for the active component. The localization error is the median distance in mm from the correct source solution for the experimental ERP component with the standard deviation in parentheses. The conventional row reports the results using a conventional windowed measure (50 ms window) for the ANOVAs and source localization error based on the difference wave for the experimental ERP component. # = Comparison score. * = Significantly different from the comparison score.

	C1	C2	Spatial Infomax	Temporal Promax	Spatial Varimax	Temporal Varimax	T-Pmax/S-Infomax	Windowed
1	N400	P1	45.5	32.1	60.1	31.8	33.1	33.4
2	N400	N1	19.2	5.8	26.3	8.1	29.0	12.6
3	N400	P300	70.1	67.8	85.6	86.1	25.2	81.1
4	N400	P2	4.5	4.2	39.5	7.0	9.9	11.4
5	P1	N1	17.4	52.9	37.4	53.2	18.8	13.7
6	P1	P300	70.3	23.8	71.3	17.2	21.3	93.2
7	P1	P2	2.3	3.4	24.7	2.9	8.5	10.8
8	N1	P300	72.8	26.3	57.7	37.2	79.9	93.8
9	N1	P2	2.4	3.8	19.3	9.1	10.6	11.7
10	P300	P2	2.3	3.7	25.7	4.1	11.1	12.6

Table 7. Localization Error For Each Case. C1 and C2 are the two simulated components in the dataset. Figures are the distance in mm, average of the two components, median such score across the ten replicates. The conventional row reports the results using a conventional windowed measure (50 ms window) based on the difference wave for the experimental ERP component.

	Spatial Varimax	Spatial Promax	Spatial Infomax	Spatial Geomin	Spatial Oblimin
			Spatial First		
Temporal Varimax	0.87*	0.89*	0.91*	0.88*	0.92*
Temporal Promax	0.87*	0.88*	0.92*	0.88*	0.93*
Temporal Infomax	0.77*	0.76*	0.84*	0.77*	0.81*
Temporal Geomin	0.87*	0.87*	0.93*	0.88*	0.91*
Temporal Oblimin	0.87*	0.87*	0.92*	0.87*	0.92*
			Temporal First		
Temporal Varimax	0.96*	0.96*	0.96*	0.96*	0.96*
Temporal Promax	0.97	0.97	0.97#	0.97	0.97
Temporal Infomax	0.92*	0.92*	0.92*	0.92*	0.92*
Temporal Geomin	0.97*	0.97*	0.97*	0.97*	0.97*
Temporal Oblimin	0.97*	0.97*	0.97*	0.97*	0.97*

Table 8. Waveform Results for Two-Step PCA. The values are the accuracy of the reconstructions of the time courses, expressed as the correlation between the scaled factor results and the matching original component. The numbers are the median values. For each analysis, the accuracy was calculated for both simulated components and the mean accuracy of the two factors was recorded. # = Comparison score. * = Significantly different from the comparison score.

	Spatial Varimax	Spatial Promax	Spatial Infomax	Spatial Geomin	Spatial Oblimin
			Spatial First		
Temporal Varimax	0.86	0.84*	0.90	0.83*	0.79*
Temporal Promax	0.86	0.84*	0.90	0.83*	0.79*
Temporal Infomax	0.86	0.84*	0.90	0.83*	0.79*
Temporal Geomin	0.86	0.84*	0.90	0.83*	0.79*
Temporal Oblimin	0.86	0.84*	0.90	0.83*	0.79*
			Temporal First		
Temporal Varimax	0.89	0.82*	0.91*	0.84*	0.80*
Temporal Promax	0.88	0.84*	0.86#	0.81*	0.79*
Temporal Infomax	0.89	0.83*	0.89	0.85*	0.80*
Temporal Geomin	0.89	0.84*	0.87*	0.83*	0.79*
Temporal Oblimin	0.88	0.83*	0.88*	0.83*	0.79*

Table 9. Scalp Topography Results for Two-Step PCA. The values are the accuracy of the reconstructions of the scalp topographies, expressed as the correlation between the scaled factor results and the matching original component. The numbers are the median values. For each analysis, the accuracy was calculated for both simulated components and the mean accuracy of the two factors was recorded. # = Comparison score. * = Significantly different from the comparison score.

	Spatial Varimax	Spatial Promax	Spatial Infomax	Spatial Geomin	Spatial Oblimin
			Spatial First		
Temporal Varimax	37.5*	38.7*	20.2	32.9*	47.6*
Temporal Promax	37.5*	38.7*	17.8	31.3*	47.6*
Temporal Infomax	37.1*	38.7*	26.0	32.8*	47.6*
Temporal Geomin	36.3*	38.7	16.1	34.0*	47.5*
Temporal Oblimin	37.5*	38.7*	21.7	31.9*	47.6*
			Temporal First		
Temporal Varimax	26.3*	31.6*	17.0	32.5*	54.5*
Temporal Promax	24.5*	29.1*	18.8#	31.0*	38.8*
Temporal Infomax	31.5*	32.0*	23.9	27.0*	52.1*
Temporal Geomin	28.6*	33.0*	18.1*	32.9*	48.4*
Temporal Oblimin	31.6*	32.6*	19.0	30.5*	43.1*

Table 10. Localization Error Results for Two-Step PCA. The localization error is the median distance in mm from the correct source solution for the experimental ERP component. # = Comparison score. * = Significantly different from the comparison score.

	Spatial Varimax	Spatial Promax	Spatial Infomax	Spatial Geomin	Spatial Oblimin
			Spatial First		
Temporal Varimax	0.01/0.34	0.02/0.33*	0.05/0.32	0.02/0.32	0.12/0.36*
Temporal Promax	0.05/0.37	0.05/0.33*	0.08/0.33*	0.03/0.35	0.10/0.35
Temporal Infomax	0.07/0.40*	0.11/0.38*	0.04/0.33*	0.13/0.43*	0.15/0.37
Temporal Geomin	0.06/0.39*	0.07/0.36*	0.07/0.34	0.06/0.36*	0.10/0.36*
Temporal Oblimin	0.10/0.37	0.10/0.33*	0.10/0.33*	0.11/0.33	0.10/0.35
			Temporal First		
Temporal Varimax	0.05/0.32	0.10/0.30	0.02/0.30	0.06/0.31	0.11*/0.35*
Temporal Promax	0.02/0.31	0.08/0.30	0.04#/0.31#	0.03/0.32	0.09/0.35
Temporal Infomax	0.03/0.43	0.11/0.36	0.14*/0.41*	0.12/0.39*	0.10/0.51*
Temporal Geomin	0.05/0.33	0.09/0.32	0.10/0.33*	0.03/0.33*	0.08/0.35
Temporal Oblimin	0.04/0.34	0.09/0.32	0.08/0.32	0.03/0.34	0.09/0.36*

Table 11. ANOVA Error Results for Two-Step PCA. The first number is the Type I error rate and the second number is the Type II error rate. The Type I Errors were the proportion of false positives for the ERP factor with no condition effect. The Type II Errors were the proportion of false negatives for the ERP factor with a condition effect. # = Comparison score. * = Significantly different from the comparison score.

	Spatial Varimax	Spatial Promax	Spatial Infomax	Spatial Geomin	Spatial Oblimin
			Spatial First		
Temporal Varimax	0.476/0.005	0.520/0.004	0.542/0.005	0.546/0.007	0.427*/0.009*
Temporal Promax	0.575/0.010*	0.627/0.007*	0.540/0.007	0.603/0.010	0.504*/0.010
Temporal Infomax	0.393*/0.028	0.429*/ 0.018*	0.565/0.009	0.417*/ 0.030*	0.524/0.014
Temporal Geomin	0.517/0.016*	0.635/0.006*	0.599/0.005	0.616/0.008	0.467*/0.007
Temporal Oblimin	0.502/0.011	0.562/0.009	0.552/0.006	0.531/0.013*	0.388*/0.008*
			Temporal First		
Temporal Varimax	0.394*/ 0.007*	0.426*/ 0.004*	0.475/0.009	0.513/0.007*	0.441*/0.013
Temporal Promax	0.511/0.006	0.569/0.006	0.485#/ 0.009#	0.592/0.005	0.573/0.013*
Temporal Infomax	0.478/0.034	0.445/0.021*	0.462/ *0.025*	0.450/0.028	0.378*/0.051
Temporal Geomin	0.538/0.005	0.532/0.005	0.496/0.007*	0.597/0.006	0.571/0.018
Temporal Oblimin	0.549/0.005*	0.577/0.005*	0.496/0.008*	0.621/0.005	0.571/0.011*

Table 12. ANOVA p-Value Results for Two-Step PCA. The first number is the p-value for the simulated component with no condition effect (larger is better) and the second number is the p-value for the simulated component with a condition effect (smaller is better). # = Comparison score. * = Significantly different from the comparison score.

FIGURE LEGENDS

Phi	Correlation
0	1.00
10	0.97
20	0.88
30	0.76
40	0.60
50	0.42
60	0.24
70	0.10
80	-0.01
90	-0.11

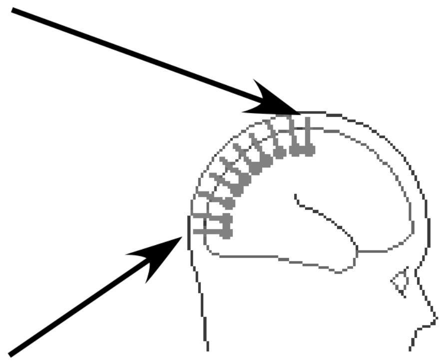


Figure 1. Effects of scalp topography on component correlations in temporal PCA. The figure indicates the component correlations due to similarity of scalp topography for a series of dipole locations with a second dipole located at Cz. Dipole Simulator was used to generate the expected scalp topography from each of these dipole locations for the 64-channel montage of the present study. Results may differ depending on the montage used. Phi indicates the Phi coordinate of the dipole in spherical coordinates.

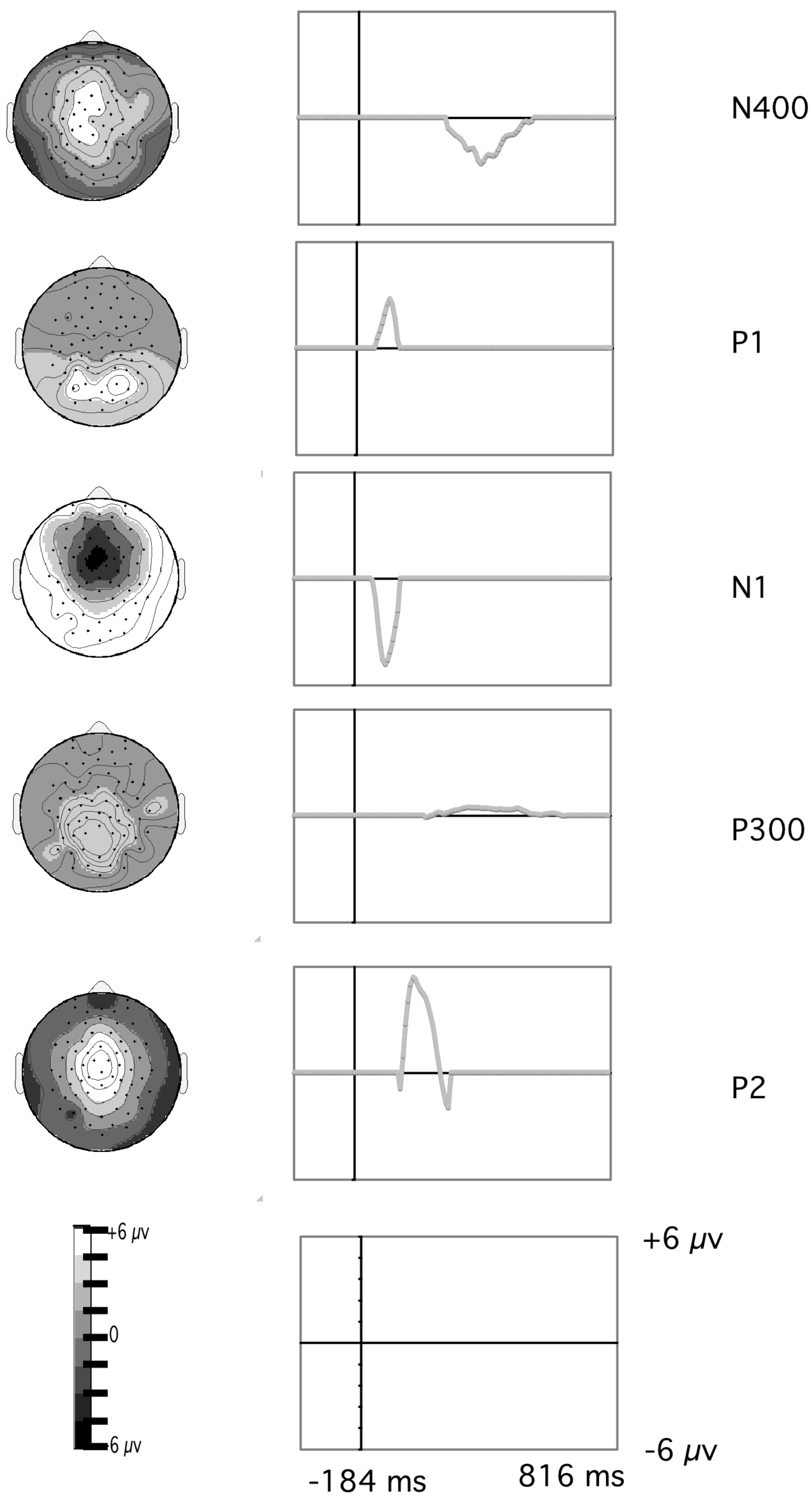
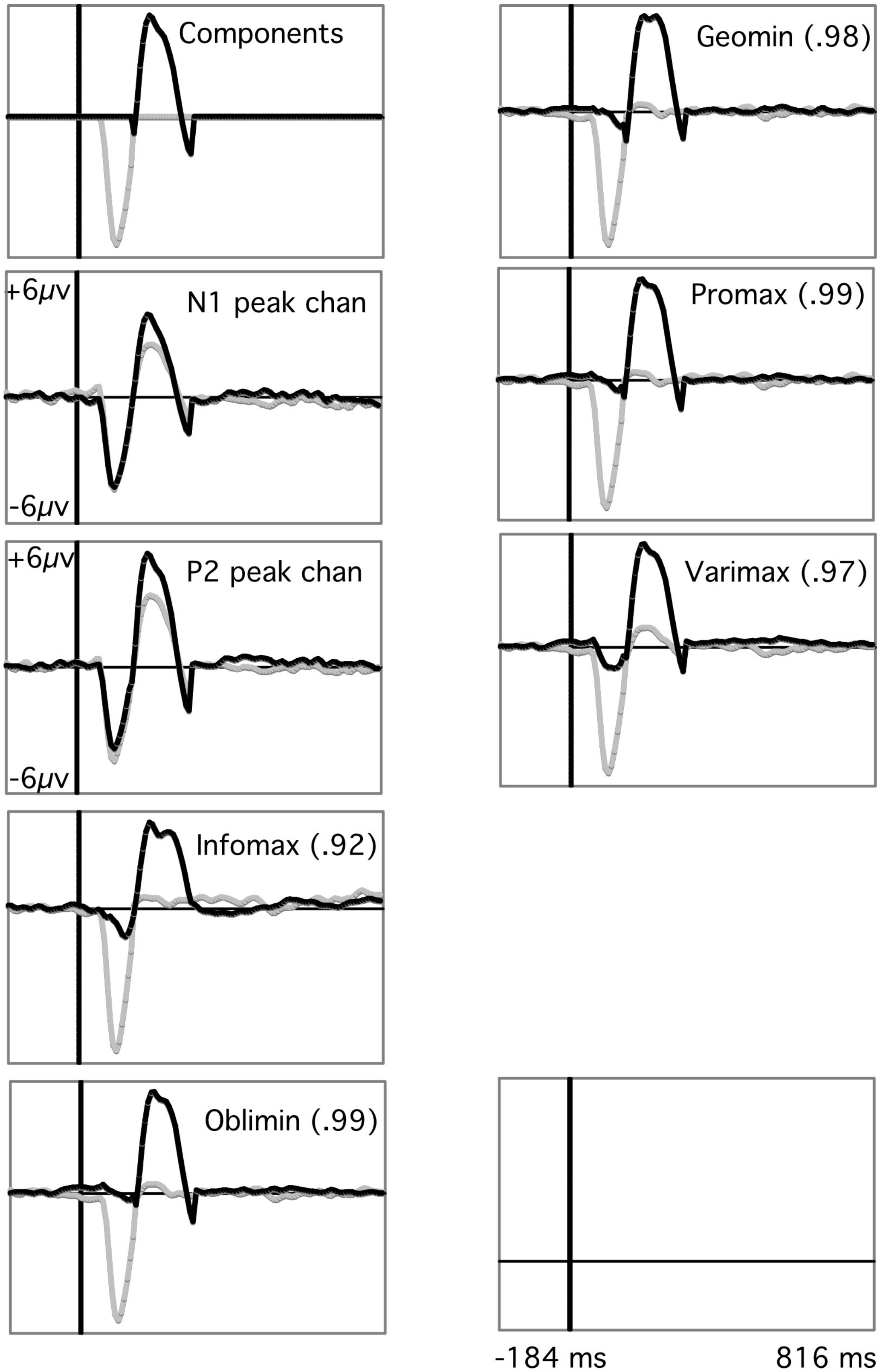

N400
P1
N1
P300
P2
+6 μv
0
6 μv
+6 μv
-6 μv
-184 ms
816 ms

Figure 2. Simulated ERP Components. The scalp topographies represent the voltage map at the peak time point. The time courses represent the voltages at the peak channel. The "N400" component is fused with other ERP components that make it overall a positivity at the vertex. The time course is negative since the peak channel is at a lateral electrode site that is negative at the peak time.



Components
Geomin (.98)
+6μv
N1 peak chan
-6μv
Promax (.99)
+6μv
P2 peak chan
-6μv
Varimax (.97)
Infomax (.92)
Oblimin (.99)
-184 ms
816 ms

Figure 3. Example Effects of Rotations on Waveforms. The waveforms are for the temporal PCA of the first replicate of Case #9, which consists of the N1 and the P2 components. The "Components" box shows the two artificial components (N1 gray and P2 black). The dips at the edges of the P2 peak are an artifact of the method of its construction. The next two (N1 and P2 Peak Channel) show the grand average of the simulated data at the peak channels for the P2 and the P3 components. The condition effect can be seen in the P2 component (the gray and black lines are the two conditions). The remaining waveforms show the factor reconstructions of the two ERP components, scaled to microvolts. Since factor loadings apply to all channels, no matter how small or large the ERP component at that channel, they necessarily have no inherent absolute scaling and are displayed scaled to maximum values. Misallocation of variance can be seen when one factor has non-zero loadings during the time points corresponding to the other component. The numbers are the accuracy scores as computed for Table 1.

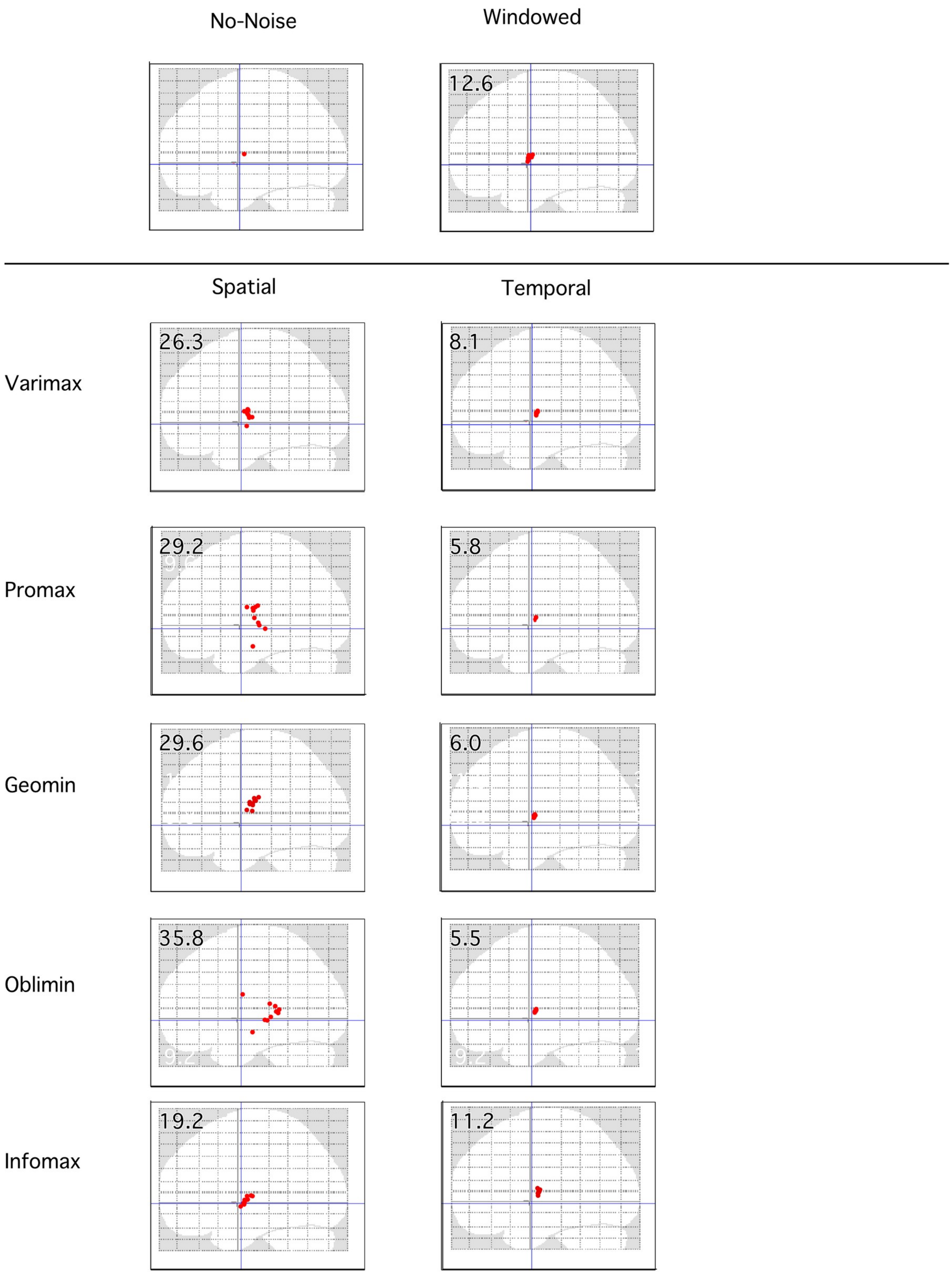


Figure 4. Example Effects of Rotations on Source Analysis. The source analyses are for the temporal PCA of Case #2, which consists of the N1 and the N400 components. The solutions are for the N1, the

component with the experimental effect. The locations are projected onto the x-y plane. Keep in mind that the simulation components are constructed from all ERP activity in the window and so the source analysis should not be considered a true solution for any of the real N1 components, of which there are many (see Näätänen & Picton, 1987). The No-Noise result is the solution under ideal conditions with no background noise and no other components and hence represents the "correct" solution insofar as successfully excluding the effects of these other aspects of the data on the source solution. For the remaining solutions, each red dot represents one of the ten replicates. The Windowed result is the solution using a conventional difference wave. The remaining solutions are the effects of using the various oblique rotations under both spatial and temporal approaches. The median error in mm for each solution is provided in the upper left hand corner. The median error is based on all three dimensions whereas the figures only show two dimensions so they may not correspond exactly. The blue cross-hairs denote the origin.