Tellus (1988), *40B*, 50–58

A cautionary note concerning a commonly applied eigenanalysis procedure

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(Manuscript received 31 March; in final form 8 July, 1987)

ABSTRACT

Owing to the complex nature of eigenanalysis programming algorithms, most atmospheric science research utilizing empirical orthogonal functions (EOFs), principal component analysis (PCA), or common-factor analysis (CFA) use the "canned" computer programs on statistical packages such as EISPACK, IMSL, SAS, BMDP, etc. These programs usually encourage truncation of the eigenvector series according to some criterion to exclude noise and facilitate data reduction; the EOFs/PCs/CFs retained are then often physically interpreted (with or without further linear transformations) according to which variables have salient magnitudes. Results presented here illustrate that following this type of analysis procedure can lead to the interpretation of coefficients as being physically significant, when they are purely noise. Several checks to avoid such a pitfall are suggested.

1. Introduction

Eigentechniques are frequently employed in meteorological exploratory analyses for data reduction purposes (e.g., Weickmann, 1983), to group synoptic and chemical variables (e.g., Christensen and Bryson, 1966; Gatz, 1984), to assist in forecasting atmospheric parameters (e.g., Brier and Meltesen, 1976), to aid in determining the variability of atmospheric fields (e.g., Horel, 1981) and to identify coherent modes of atmospheric parameters (e.g., Craddock and Flood, 1969; Richman and Lamb, 1985; Barnston and Livezey, 1987). The widespread acceptance of these techniques for the aforementioned purposes is evidenced by the frequent publication of the results of diverse applications. However, there are several aspects of the eigenmodels, and their application and interpretation, that warrant concern. Specifically:

(a) The heavy use of computer packages such as EISPACK (1976), IMSL (1980), SAS (1985), BMDP (1981) and SPSS (1979), which stems from the needed programs being very complex. For example, Press et al. (1986, p. 340) state "You have probably gathered by now that the solution of eigensystems is a fairly complicated business. It is. It is one of the few subjects covered in this book for which we do *not* recommend that you avoid canned routines." However, the existence of such canned programs and the nature of their documentation tend to foster an unquestioning reliance on the output.

(b) The need for critical decisions to be made concerning the optimal similarity coefficient, number of eigenvectors to retain, eigenmodel to apply, and application of a linear transformation, further complicate the analysis. Since the models involve these intricate steps, yielding coefficients with units different from the raw data, the analyst may be tempted to accept and interpret the results without testing their reliability and validity.

(c) Several of the high-level packages (e.g., BMDP, SAS, SPSS) offer "default" options (e.g., truncation point at some predetermined eigenvalue) to help simplify matters while yielding a reasonably accurate solution. However, the accompanying documentation typically does not warn of the possible pitfalls of using such default criteria. An example of this is the BMDP package which, as a default, will automatically truncate an eigenvalue series at 1.0 and, if rotation is desired, will use a preassigned Varimax rotation in agreement with Kaiser's (1960, 1961) *original* recommendation known as the Kaiser-Guttman "K-G" test (without rotation) or "Little Jiffy" (with Varimax rotation). However, although this recommendation has since been modified, the package has not yet followed suit (Kaiser, 1970; Kaiser and Rice, 1974). The latest version of SAS, with its simple command PROC FACTOR (DATA = XXX), will automatically select the principal component model based on correlations of XXX and apply the K-G test. Numerous published atmospheric science studies have also followed this same procedure (Christensen and Bryson, 1966; Dyer, 1975; Hastenrath and Wendland, 1979; Ladd and Driscoll, 1980; LeDrew, 1980; Salinger, 1980; Gray, 1981; Horel, 1981; Hopke, 1982; Cohen, 1983; Horel, 1984; Kalkstein and Corrigan, 1986).

(d) The degree of automation is further compounded by the manner in which most eigenanalyses are interpreted. Typically, the variables with salient loadings or coefficients (i.e., Harris, 1967, recommended interpreting PC loadings greater than $|0.30|$) on each eigenvector are inspected to determine which ones are grouped together. At that point, a name is assigned to the eigenvector in a *causal* or *summary* sense, *a posteriori* (hence generating new theory) according to the patterns of interrelationships isolated. An example of the procedure is contained in Gatz's (1984, p. 1898) work on precipitation chemistry and reproduced in Table 1. In this case the loading cutoff for physical interpretation was selected at $|0.50|$ and the first component (termed *factor*) had salient loadings on Ca, Mg, K, and total insoluble residue, and hence was named a *crustal dust factor*. The second component (Table 1) grouped together NH_4, NO_3 and SO_4, and therefore was called a *gaseous precursor factor*; while the third component clustered Na and Cl, thereby gaining the name *sea salt or road salt factor*. The fourth component grouped SO_4 with H and was not formally given a name (the reader was referred to Baker et al., 1981, who found a similar factor and termed it an *acid factor*). Similarly, Thurston

Table 1. *Loading table from factor analysis on event precipitation samples, using correlation about the mean, from Gatz (1984, p. 1898)*

	Correlation of concentrations			
	Factor			
	1	2	3	4
Ca	0.87			
Mg	0.85			
K	0.78			
Total insol	0.73			
NH_4		0.84		
NO_3		0.80		
SO_4		0.71		0.50
Na			0.90	
Cl			0.83	
H				0.95
Variance explained (%)	29	25	19	13
Cumulative variance (%)	29	54	73	86

and Spengler (1985, p. 1250) provide a larger atmospheric chemistry component analysis (their Table 3) in which PC1 is named *soil aerosol PC* (grouping the crustal elements Si, Ca, Mn, Fe), PC2 is a *motor vehicles aerosol PC* (clustering leaded auto exhaust elements Br, Pb), PC3 is a *coal-related aerosol PC* (S, Se), PC4 is termed *residual oil combustion aerosol PC* (V, Ni), and PC5 called *salt aerosol PC* (Cl).

This paper will illustrate that the types of results contained in the above examples are obtainable from a PCA of any data set, even ones representing purely noise, by following the default criteria on statistical packages and then interpreting the resulting loadings for groups of clustered variables. Several tests and procedures will then be suggested to help avoid interpreting spurious PC loadings.

2. Pseudo-random analysis

Two pseudo-random number generators were employed in this study; one used a feedback shift register algorithm (Lewis and Payne, 1973) and the other a congruential generation algorithm passing the Coveyou-Macpherson test (Knuth, 1981). Fifteen separate matrices were created with the number of variables ranging from 5 to 50 and the number of observations ranging from 100 to 10,000 which is in line with most analyses found in the atmospheric science literature. The elements of the matrices were normally distributed random variates drawn from a population of zero mean and unit variance. The probability density function, where x denotes a random variable, is given by:

$$\langle(\sigma\sqrt{2\pi})^{-1}\,e^{-\frac{1}{2}[(x-\pi)\sigma^{-1}]^2}\rangle$$

$$-\infty < x < \infty$$

$$-\infty < \mu < \infty$$

$$0 < \sigma < \infty$$

These pseudo-random matrices were subject to eigenanalysis schemes that included application of the standard eigenvalue $\geqslant 1$ default criterion that is on the statistical packages. The results of the 15 analyses were consistent in producing sets of salient loadings for both generators; representative examples will be shown for 10 variables and 100 observations versus 10 variables and 5000 observations. Mock chemical names were randomly assigned to each variable such that variables 1–10 were represented by [Si, Ca, Cl, Mn, Br, Pb, Zn, S, Fe, and Se], which is a similar group to those included in Thurston and Spengler (1985).

For the pseudo-random variables based on the normal distribution [$N(0,1)$] with a sample size of 100 (Table 2), the correlation matrix contained 20 off-diagonal entries greater than $|0.10|$ with the largest being $|0.175|$ (panel (a)), which implies little grouping of variables. Since four of the eigenvalues of this matrix were greater than or equal to 1.0, four PCs were retained by the K-G test (panel (b)) for which the PC loadings (panel (c)) are shown. The interpretation uses an arbitrary $|0.50|$ cutoff similar to Gatz (1984) to isolate salient coefficients. The chemical elements were then inspected to determine which ones were grouped by each PC. PC1 (panel (c)) clusters Si, Ca, and Fe, and might be called a soil element PC, PC2 groups Br, Pb, and Zn (motor vehicles); PC3 relates S and Se (coal), PC4 Cl (and negative Se) (maybe salt). If a chemist applied the elemental tags as used here, physically plausible results would arise from data containing no signal. This analysis represents an extreme case of the potential for placing a physical interpretation on random data. Other variations exist, such as different plausible combinations of elements, or with data, interpreting mixtures of signal and noise (see Richman (1985)).

All of the remaining analyses outlined above produced groupings of variables with maximal coefficients on each PC of approximately $|0.70|$, regardless of the number of variables or sample size. Table 3 summarizes the analysis based on 10 variables and 5000 independent cases, where the largest off-diagonal correlation was only $|0.036|$. Application of the K-G test suggested retention of five PCs. Although Table 3a is almost an identity matrix and suggests no signal, the PC loadings are nevertheless as high as $|0.743|$, with three PCs grouping 2 or more variables at the

Table 2. *Analysis information for pseudo-random variables drawn from a normal distribution with a sample size of 100. (a) Correlation matrix, (b) Eigenvalue sequence, (c) Unrotated PC loadings*
(a) Correlation matrix

	Variable									
Variable	1	2	3	4	5	6	7	8	9	10
1	1.000									
2	0.132	1.000								
3	0.150	−0.095	1.000							
4	−0.143	−0.133	0.020	1.000						
5	−0.060	0.058	−0.031	−0.101	1.000					
6	−0.090	−0.133	−0.113	0.058	0.136	1.000				
7	0.087	0.037	−0.072	−0.152	0.154	0.055	1.000			
8	−0.095	−0.112	0.058	0.109	0.052	0.130	0.053	1.000		
9	0.145	0.138	0.139	0.012	0.035	−0.068	0.135	0.050	1.000	
10	0.039	−0.005	0.024	0.052	−0.054	−0.112	0.175	0.083	0.134	1.000

Table 2 *continued*

(b)

Root number	Eigenvalue
1	1.562
2	1.352
3	1.318
4	1.065
5	0.962
6	0.877
7	0.815
8	0.733
9	0.680
10	0.636

(c) Unrotated PC loadings

	PC			
Variable	1	2	3	4
Si	0.597	−0.149	−0.006	0.318
Ca	0.503	0.052	−0.357	−0.195
Cl	0.212	−0.347	0.427	0.619
Mn	−0.421	−0.242	0.443	−0.196
Br	0.032	0.641	−0.117	0.301
Pb	−0.431	0.502	0.016	0.267
Zn	0.373	0.620	0.154	−0.162
S	−0.233	0.295	0.572	0.109
Fe	0.515	0.088	0.408	0.088
Se	0.294	0.076	0.529	−0.544

Table 3. *Analysis information for pseudo-random variables drawn from a normal distribution with a sample size of 5000*
(a) Correlation matrix

	Variable									
Variable	1	2	3	4	5	6	7	8	9	10
1	1.000									
2	0.021	1.000								
3	0.009	0.008	1.000							
4	−0.026	0.003	0.008	1.000						
5	−0.013	−0.024	0.031	0.009	1.000					
6	0.026	0.012	0.007	−0.022	0.000	1.000				
7	0.004	0.001	−0.005	−0.029	−0.005	0.009	1.000			
8	0.002	−0.009	0.010	0.002	0.012	0.020	0.008	1.000		
9	−0.020	0.005	0.019	0.000	0.009	−0.036	0.007	0.002	1.000	
10	0.017	−0.006	0.021	−0.014	−0.018	−0.000	−0.033	−0.002	0.008	1.000

(b) Eigenvalue sequence

Root number	Eigenvalue
1	1.081
2	1.047
3	1.044
4	1.024
5	1.012
6	0.991
7	0.966
8	0.960
9	0.942
10	0.934

(c) Unrotated PC loadings

	PC				
Variable	1	2	3	4	5
1	−0.521	0.276	−0.004	−0.069	0.067
2	−0.242	0.103	0.235	−0.231	0.743
3	0.116	0.552	−0.369	−0.198	0.252
4	0.432	0.040	0.096	0.415	0.466
5	0.309	0.097	−0.576	0.107	0.001
6	−0.512	0.073	−0.331	0.260	0.102
7	−0.205	−0.466	−0.299	−0.484	0.011
8	−0.048	0.068	−0.503	0.091	−0.020
9	0.379	0.132	−0.008	−0.654	0.018
10	−0.075	0.633	0.242	−0.063	−0.405

|0.50| level. Consequently, the generation of tables or figures of PC loadings for interpretation can create meaningful-looking coefficients from any data, even random, thereby opening the door for interpretation of spurious results. Typically, these types of tables or figures of PC loadings are all that are presented to readers in journal articles.

3. Conclusions and implications

This study examined how an eigenmodel responded to data which were purely white noise (created on pseudo-random number generators), to discern if the loadings generated appeared to differ from data believed to be comprised of signal. The resulting PC loadings typically exhibited large magnitudes of grouped variables when a standard default algorithm recommended by various statistical packages was applied, despite the lack of inter-variable correlations to support them. This can be troublesome as (a) the eigentechniques are frequently used as exploratory tools to "let the data determine the patterns" where little prior knowledge exists concerning which variables should group together and (b) the manner by which physical significance is placed on the PCs is an *a posteriori* inspection of tables or figures of eigenvector loadings to identify variables clustering together with salient magnitudes. Consequently, these techniques are open to potential misuse as they can yield reasonable looking (but spurious) PC loadings, based on random noise, where none should exist.

The result in Tables 2 and 3 point to a weakness in applying the eigenvalue 1.0 rule to an eigenvector analysis and then applying the usual interpretational strategy of inspecting columns of the loading matrix for grouped variables to name them as causal factors. All inter-variable correlation coefficients for Table 2 (Table 3) were found to be less than |0.20| (|0.04|), which is indicative of little (or no) physically meaningful inter-relationships although the loadings would appear to indicate meaningful groupings. It is therefore suggested that the researcher use caution when naming components. There are several methods available to safeguard against physically interpreting meaningless loadings:

(a) Apply Bartlett's (1950) test of sphericity. This would accept or reject the null hypothesis that the correlation matrix is indistinguishable from a multivariate normal matrix of uncorrelated variables, indicating the matrix is not worthy of further investigation. The test is computed as: $X^2 = -[N - 1 - \frac{1}{6}(2P + 5)] \ln |R|$, where N equals the number of cases, P equals the number of variables and $|R|$ equals the determinant of the correlation matrix. For a large N, the statistic is approximately distributed as chi square with $\frac{1}{2}P(P-1)$ degrees of freedom. This will screen situations where the data are purely white noise; it will not reject matrices comprised of a mixture of signal and noise which was found to be equally troublesome in a recent study (Richman, 1985, pp. 266–267).

(b) Rigorously test the eigenvalue series. There exist more sophisticated tests for an eigenvalue series than the Kaiser-Guttman 1.0 rule. The scree test (Cattell, 1966) plots up the eigenvalues in decreasing order (abscissa) against root number (ordinate) considering the last pronounced discontinuity in the eigenvector series prior to its leveling off as the division between unrotated PCs that possess non-random signals (those with larger eigenvalues) and the ones that do not. Several packages offer the scree test, however, they do not warn of potential problems in its application—lack of accuracy with certain types of data conditions (Hakstian et al., 1982), yielding multiple break points (Zwick and Velicer, 1982), no break point (Linn, 1968) and its implicit subjectivity (Crawford and Koopman, 1979). Application of the scree test to the eigenvalue series shown in Table 2 reveals one of the abovementioned weaknesses as the last break in the eigenvalue series occurs between roots three and four (this can be inferred from Fig. 1b—see below).

More accurate tests to separate signal from noise exist in the literature (e.g., Preisendorfer et al., 1981; Overland and Preisendorfer, 1982; North et al., 1982) which will usually safeguard against accepting eigenvalues representing white noise; however, the statistical packages do not offer these. Rule U (Preisendorfer et al., 1981) is constructed by drawing a number of matrices (e.g. 100) of random normal deviates the same size as the data matrix, obtaining eigenvalues of these matrices and plotting the Monte Carlo curves for eigenvalues in decreasing order with

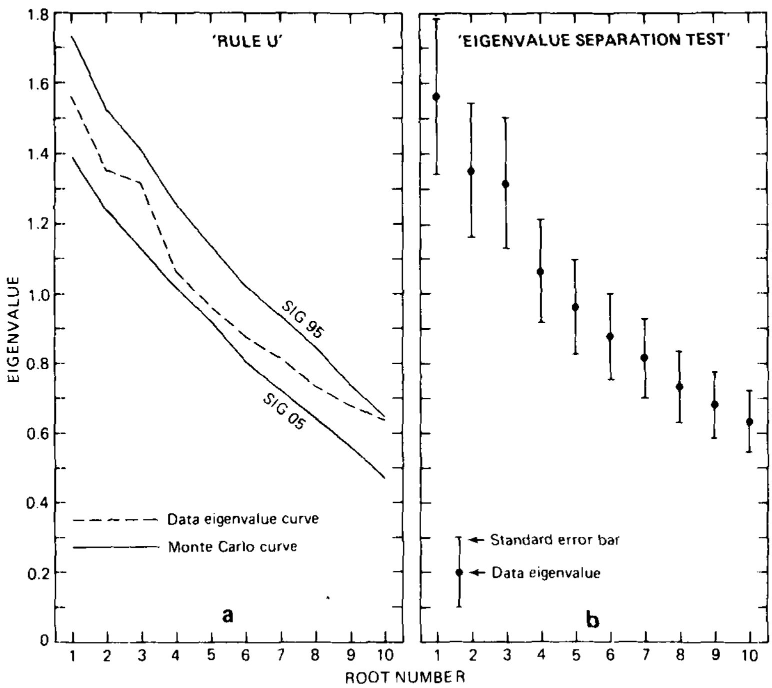

Fig. 1. Example of Preisendorfer et al. (1981) 'Rule U' (panel (a)) versus Kendall (1980)/North et al. (1982) 'eigenvalue separation test' (panel (b)) applied to the eigenvalues listed in Table 2. Note the data eigenvalue curve in panel a never crosses the Monte Carlo confidence bands and all adjacent error bars for the 10 eigenvalues in panel (b) overlap, thereby illustrating the "data" are no different from white noise. This is in sharp contrast to the K-G test indicating 4 roots for retention or the scree test indicating 3 roots.

the lower 5% and upper 5% points on a cumulative distribution of eigenvalues drawn (see application below). Data eigenvalues exceeding the upper 5% significance band are retained. Preisendorfer et al. (1981) also develop a normalized version of Rule U, known as Rule N. Storch and Hannoschöck (1985) offer a few caveats when RuleU/Rule N type tests are applied to small samples. The eigenvalue separation test (Kendall, 1980; North et al., 1982) plots up standard error bars on each individual eigenvalue in decreasing order as $\lambda(2/N)^{1/2}$ where λ is the eigenvalue and N is the sample size. The last root having a spacing exceeding the error bars can be chosen as the truncation point. Lawley and Maxwell (1971, p. 23) note that this type of test is only strictly applicable to eigenvalues belonging to a variance-covariance matrix; however, they do go on to state that the results obtained might serve as a "rough approximation" for correlation-based eigenvalues.

Fig. 1 illustrates the application of Rule U (Fig. 1a) and the eigenvalue separation criterion (Fig. 1b) to the "data" eigenvalue series from Table 2. Note that the data eigenvalue line connecting all roots never crosses outside the Monte Carlo confidence bandwidth between the upper and lower 5% of the randomly generated eigenvalues in Rule U (Fig. 1a), indicating the data lie in the white noise spectrum. Additionally, the error bars of the separation test (Fig. 1b) all overlap, indicating no two roots are sufficiently separated for truncation and the total 10-space is an effectively degenerate multiplet. North et al. (1982) illustrate the subsequent instability of individual eigenvectors when this type of overlap occurs.

More emphasis should be placed on applying the most appropriate selection rules. Testing the

Table 4. *Common factor (CF) loadings based on a principal axis decomposition with squared multiple correlations used as communalities*

(a) Unrotated CF loadings (100 observations)

	CF			
Variable	1	2	3	4
Si	0.385	0.093	−0.006	0.122
Ca	0.323	−0.018	−0.205	−0.075
Cl	0.134	0.199	0.237	0.222
Mn	−0.268	0.128	0.248	−0.076
Br	0.025	−0.348	−0.067	0.109
Pb	−0.272	−0.291	0.009	0.108
Zn	0.253	−0.364	0.081	−0.056
S	−0.139	−0.167	0.302	0.039
Fe	0.336	−0.045	0.223	0.031
Se	0.190	−0.047	0.285	−0.197

(b) Unrotated CF loadings (5000 observations)

	CF				
Variable	1	2	3	4	5
1	−0.145	0.060	0.001	−0.001	0.008
2	−0.066	0.022	−0.048	−0.035	0.086
3	0.032	0.119	0.080	−0.031	0.029
4	0.120	0.009	−0.020	0.067	0.053
5	0.085	0.020	0.122	0.017	−0.001
6	−0.143	0.015	0.070	0.042	0.011
7	−0.057	−0.102	0.062	−0.077	0.002
8	−0.013	0.013	0.104	0.014	−0.003
9	0.105	0.029	0.002	−0.104	0.003
10	−0.021	0.139	−0.050	−0.011	−0.046

Analysis procedure was otherwise identical to PC algorithm with (a) corresponding to the analysis of the correlations in Table 2 and (b) corresponding to the correlations in Table 3.

efficacy of all eigenvalue truncation rules used by analysts would be useful and, to this end, there have been a few small-scale comparative studies (Hakstian et al., 1982; Zwick and Velicer, 1982). Further research in this area on a comprehensive basis is warranted.

(c) Application of the common factor model in tandem with PC or EOF. This may be useful as CF will exclude most white noise (see Richman and Lamb, 1985; 1987). The spurious PC loadings shown in Tables 2 and 3 were subject to a common factor analysis with squared multiple correlations used to separate common variance (treated as signal under the model) from unique variance (variance not shared by two or more variables treated as noise) with positive results (Table 4). The CF loadings in Table 4a, corresponding to the PC loadings in Table 2, illustrate the considerable reduction in loading magnitude CFA offers for data containing a high degree of white noise. The 10 PC loadings in excess of $|0.50|$ have all been reduced below this threshold under the CF model, although several exceed the $|0.30|$ level suggested by Harris (1967). Similarly, Table 4b demonstrates this property of CF loadings as the PC loadings of Table 3 have all been strongly attenuated to magnitudes below $|0.15|$ with the larger sample size (5000). Consequently, the CF model may be considered both more conservative and accurate in representing the inter-variable relationships when the signal to noise ratio is low. It is, however, a more complex model with its own unique set of potential pitfalls, which Rummel (1970), Mulaik (1972) and Harman (1976) examine comprehensively.

(d) Test the reliability of the groupings generated. The standard errors of the loadings can be calculated with various resampling techniques such as jackknifing (Pennel, 1972; Clarkson, 1979). [For a recent review and discussion of resampling, see Wu (1986).] Another method to assess stability is through split samples or subgroup analysis (Richman, 1986, Richman and Lamb, 1987).

(e) Compare the loadings to the underlying correlations to test the validity of the analysis (see Richman and Lamb, 1985, 1987; Richman, 1986 for examples).

4. Acknowledgements

This study was partly supported by NSF Grant ATM 85-20877. The author would like to express thanks to Peter J. Lamb, Robert E. Livezey and two anonymous reviewers for the comments concerning the manuscript, Donald F. Gatz for graciously allowing the further use of his analysis, Rebecca Runge for typing the text and John Brother for drafting the figure.

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