Sensitivity Test of POP System Matrices—An Application of Spectral Portrait of a Nonsymmetric Matrix

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ABSTRACT

By using the POP (principal oscillation pattern) system matrices as examples, this study introduces to the meteorological community the concept and application of spectral portrait (or pseudospectra) of a nonsymmetric matrix. An analytical formula is provided to estimate the system error of a POP matrix due to the inversion of a covariance matrix. By comparing the spectral portrait and the system error, this study demonstrates a possible tool to test the sensitivity of a POP analysis.

1. Introduction

The purpose of this study is to demonstrate a new approach to examine the sensitivity of a nonsymmetric linear system.

North et al. (1982) discussed the perturbation of a covariance matrix ($\hat{\mathbf{C}}_0$) due to sampling errors. They pointed out that, in practice, when we estimate a covariance matrix from samples, what we really obtain is the unknown covariance $\mathbf{C}_0$ plus a perturbation $\delta(\mathbf{C}_0)$ [i.e., $\hat{\mathbf{C}}_0 = \mathbf{C}_0 + \delta(\mathbf{C}_0)$]. This perturbation can be due to many different factors, and in their cases, they discussed the sampling errors. To obtain a robust eigensolution, the perturbation has to be small relative to $\mathbf{C}_0$ (i.e., $\|\delta(\mathbf{C}_0)\| \leq \varepsilon\|\mathbf{C}_0\|$, where $\varepsilon \ll 1$ and $\|\cdot\|$ refers to a matrix norm, which is chosen to be the largest singular value of the corresponding matrix). For a symmetric matrix, the eigenspace consists of a complete set of orthogonal vectors, and an analytic formula to estimate the size of the sampling error for each eigenvector can be obtained (North et al. 1982). For a given sample, the spacing between the adjacent eigenvalues determines the stability of the eigenanalysis. When two eigenvalues are too close, their error bars due to sampling errors will overlap and the corresponding eigenvectors are not distinguishable. This means that the linear system is ''effectively'' degenerate and eigensolutions can be different from one sample to the other.

The problem of the perturbation of a linear system matrix discussed by North et al. (1982) is a general problem of any matrix analysis technique, including not only symmetric, but also nonsymmetric matrices like the system operator of POP (principal oscillation pattern) analysis.

POP analysis is a well-established method for finding propagating modes in geophysical fields (Hasselmann 1988; von Storch et al. 1995). Let $x(t)$ represent an n-dimensional stochastic process [for practical purposes, the original process is usually reduced into the subspace of leading empirical orthogonal functions or EOFs, hence, $x(t)$ is the first n leading Principal Components, or PCs]. The evolution of the vector x can be represented as a first-order multivariate Markov process: $x(t + 1) = Ax(t) + r(t + 1)$, where $r(t)$ is the ratio of noise/forcing which is generally nonwhite, non-Gaussian, and with zero mean. It can be shown that in order to minimize $\langle r^2\rangle$ ($\langle\cdot\rangle$ refers to a time average), $\mathbf{A}$ has to be chosen as $\mathbf{A} = \mathbf{C}_1 \cdot \mathbf{C}_0^{-1}$, where $\mathbf{C}_1$ denotes the lag-1 coveriance matrix of $x(t)$ and $\mathbf{C}_0$ the lag-0 covariance matrix. To perform a POP analysis is to solve the eigenproblem for A and to find the temporal variation of each eigenvector or POP.

The usefulness of POP analysis has been clearly demonstrated in the forecasting of ENSO (El Niño–Southern Oscillation) (Xu and von Storch 1990). It seems to yield satisfactory results when the signals under investigation have a periodic behavior, such as the equatorial quasi-biennial oscillation (QBO) and ENSO (Xu and von Storch 1990; Xu 1992). However, when trying to apply the POP analysis to find the lagged connection between the tropical sea surface temperature (SST) and extratropical atmospheric circulation, we found it to be quite sensitive to the number of EOF modes kept for calculation. Even the leading modes can appear different when different numbers of EOF modes are retained for the POP analysis.

Like in EOF analysis, any estimated POP system matrix $\hat{A}$ is the sum of an unbiased system matrix A and

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its perturbation δA. Here the perturbation is not only due to sampling errors, but also due to EOF truncation errors and errors related to inverting a covariance matrix. Because eigenvalues and eigenvectors for a nonsymmetric matrix can be either real or complex, and the eigenvectors are not necessarily orthornormal, the rule of thumb derived in North et al. (1982) is not suitable here. Hence, a closer investigation of the sensitivity of this analytical tool will provide us with a better understanding of this statistical method. The paper is organized as follows. In section 2, we will introduce the definition of spectral portrait of a matrix. In section 3, an analytical formula is obtained to estimate the POP system error related to the inversion of a covariance matrix. Some examples are shown in section 4 and summary and discussion in section 5.

2. Spectral portrait of a linear system y = Ax

The spectral portrait of a matrix A for a given ε, Λ_ε, consists of neighborhoods around each eigenvalue of A in the complex plane and is defined as follows: $\lambda \in \Lambda_\varepsilon$ if there exists a matrix perturbation $\delta A(\|\delta A\| \le \varepsilon\|A\|)$, which satisfies

$$det[\lambda \mathbf{E} - (\mathbf{A} + \delta\mathbf{A})] = 0 \tag{1}$$

or equivalently (as proved by Godunov et al. 1990), if

$$\frac{\sigma_{\min}(\mathbf{A} - \lambda_i\mathbf{E})}{\sigma_{\max}(\mathbf{A})} \le \varepsilon, \tag{2}$$

where $\sigma_{\min}$ and $\sigma_{\max}$ represent the smallest and largest singular values of the respective matrices. Here, $\mathbf{E}$ is the identity matrix. Hence, to find the spectral portrait of a matrix, one will give different perturbation amplitudes (ε), and for each eigenvalue and each ε, find all the λ that satisfy Eq. (2).

Examining the spectral portrait of a nonsymmetric system matrix will allow us to see how much perturbation the system matrix can tolerate before all or some of the eigenvalues are mixed and the system matrix becomes degenerate. For each eigenvalue, the maximum perturbation it can tolerate before its spectral portrait overlaps with those of others is called ''tolerance'' of this eigenvalue. Different eigenvalues may have different tolerances. By comparing the spectral portraits of two different matrices, or just comparing their tolerance values, we can compare their sensitivities. Furthermore, if we can estimate the system error, then compare it with the tolerances of the system matrix, we can determine whether or not the system matrix is effectively stable or effectively degenerate. In the next section, we will derive an analytical formula to estimate the system error for a POP system matrix.

3. System error of the POP system matrix due to the inversion of the covariance matrix

As discussed earlier, the POP system matrix is given by

$$\mathbf{A} = \mathbf{C}_1 \cdot \mathbf{C}_0^{-1}, \tag{3}$$

where

$$\mathbf{C}_{1ij} = \langle x_i(t + 1)x_j(t)\rangle \tag{4}$$

and

$$\mathbf{C}_{0ij} = \langle x_i(t)x_j(t)\rangle. \tag{5}$$

The error in $\mathbf{A}$ due to errors in estimation of $\mathbf{C}_0^{-1}$ and $\mathbf{C}_1$ is given by

$$\delta A \cong \mathbf{C}_1 \cdot \delta(\mathbf{C}_0^{-1}) + \delta(\mathbf{C}_1) \cdot \mathbf{C}_0^{-1}. \tag{6}$$

Here, we consider only the perturbation due to the first term on the right-hand side of (6), since we are particularly interested in examining how much error the inversion of the covariance matrix $\mathbf{C}_0$ contributes to δA.

Therefore,

$$\|\delta A\| \le \|\mathbf{C}_1\| \cdot \|\delta(\mathbf{C}_0^{-1})\|, \tag{7}$$

where $\mathbf{C}_0$ is a diagonal matrix since it is constructed by the first n leading PCs in EOF subspace, and $\mathbf{C}_{0ii} = \lambda_i$. Here, λ_i represents the ith diagonal element or ith eigenvalue of $\mathbf{C}_0$. It follows that $\mathbf{C}_0^{-1}$ is also a diagonal matrix with the diagonal elements $\mathbf{C}_{0ii}^{-1} = 1/\lambda_i$. We assume that the perturbation of $\mathbf{C}_0^{-1}$ is mainly contributed by the perturbations in its diagonal elements and the perturbations in the off-diagonal elements are small enough to be neglected [i.e., $\delta(\mathbf{C}_{0ii}^{-1}) = \delta(1/\lambda_i)$ and $\delta(\mathbf{C}_{0ij}^{-1}) = 0$, when $i \ne j$] so that $\delta(\mathbf{C}_0^{-1})$ is also a diagonal matrix. For simplicity in notation, we use the absolute value of the diagonal elements of $\delta(\mathbf{C}_0^{-1})$ to examine the perturbation, since $\|\delta(C_0^{-1})\|$ is the largest diagonal element by definition. Therefore,

$$\left|\delta(\mathbf{C}_{0ii}^{-1})\right| = \left|\delta\left(\frac{1}{\lambda_i}\right)\right| = \left|\frac{\delta\lambda_i}{\lambda_i^2}\right| \le \left|\frac{1}{\lambda_i}\right| \cdot \left|\frac{\delta\lambda_i}{\lambda_i}\right|,$$

where

$$\left|\frac{1}{\lambda_i}\right| \le \frac{1}{\lambda_{\min}}.$$

Here, $\lambda_{\min} = \lambda_{\min}(\mathbf{C}_0)$, the smallest eigenvalue or the smallest diagonal element of $\mathbf{C}_0$. By applying the approach of North et al. (1982), we have $\delta\lambda_i/\lambda_i \approx (2/N)^{1/2}$, where N is the number of temporal degrees of freedom in the sample. Here, $\delta\lambda_i/\lambda_i \approx (2/N)^{1/2}$ represents the part of error due to the sampling error. We then obtain

$$\|\delta(\mathbf{C}_0^{-1})\| \approx \left(\frac{2}{N}\right)^{1/2} \cdot \frac{1}{\lambda_{\min}}. \tag{8}$$

Furthermore, Eq. (3) is equivalent to $C_1 = \mathbf{A} \cdot \mathbf{C}_0$, therefore, $\|\mathbf{C}_1\| \le \|\mathbf{A}\| \cdot \|\mathbf{C}_0\|$, or

$$\|\mathbf{A}\| \ge \frac{\|\mathbf{C}_1\|}{\|\mathbf{C}_0\|}. \tag{9}$$

By combining (7), (8), and (9), we can obtain the relative error due to the perturbation of inversion of the covariance matrix:

$$\frac{\|\delta A\|}{\|\mathbf{A}\|} \le \frac{\left(\frac{2}{N}\right)^{1/2} \cdot \frac{1}{\lambda_{\min}} \cdot \|\mathbf{C}_1\|}{\|\mathbf{A}\|} \le \frac{\left(\frac{2}{N}\right)^{1/2} \cdot \frac{1}{\lambda_{\min}} \cdot \|\mathbf{C}_1\| \cdot \|\mathbf{C}_0\|}{\|\mathbf{C}_1\|}$$

$$= \left(\frac{2}{N}\right)^{1/2} \cdot \frac{\lambda_{\max}}{\lambda_{\min}} \sim \varepsilon.$$

Hence, we obtain the rule of thumb for the perturbation amplitude of POP analysis due to the first term on the right-hand side of (6):

$$\varepsilon \cong \left(\frac{2}{N}\right)^{1/2} \cdot \mathrm{cond}(\mathbf{C}_0)$$

where $\mathrm{cond}(\mathbf{C}_0) = \dfrac{\lambda_{\max}}{\lambda_{\min}}$ is the condition number of $\mathbf{C}_0$. (10)

Hereafter, we will refer to ε obtained from (10) simply as the POP system error. The system error estimated by this formula is consistent with Eq. (7) in that it is the product of two factors: one is the sampling error, which is represented as $(2/N)^{1/2}$; the other is the error related to the inversion of the covariance matrix $\mathbf{C}_0$, which is representd as the condition number of $\mathbf{C}_0$. In the next section, we will show some examples where the EOF truncation error can lead to a large $\mathrm{cond}(\mathbf{C}_0)$ and hence to a large system error.

4. Examples

a. Example 1: A perfect propagating signal and Monte Carlo experiment

As we mentioned earlier, POP analysis is generally successful in capturing periodic signals. As a first example, we therefore generate a 24×24 dimensional covariance matrix from a process that contains one perfectly propagating signal. This process is represented by the equation

$$y(t) = \cos\left[\left(\omega_1 t - \frac{\pi}{6}x\right)\right]. \quad (11)$$

Here, t represents time, x represents space. Applying an EOF analysis to the covariance matrix, PCs for the first two leading EOFs are retained to form a 2×2 POP system matrix. The POP analysis captures the propagating mode well in terms of the amplitude and frequency of the signal (not shown). The two complex eigenvalues are presented as two dots in Fig. 1a. All the contours surrounding the two eigenvalues in Fig. 1a together constitute the spectral portrait of the system matrix. The area enclosed by each contour in the figure represents all the possible values that one or both eigenvalues can assume under a specified amount of perturbation (here, 20%, 50%, 75%, and 120%, respectively). The tolerance for both eigenvalues is between 75% and 80%. At a perturbation of 75% the contours of eigenvalues are still well separated. When the perturbation increases to 80% (not shown), the corresponding contours start to merge, representing the mixing of the eigenvalues and eigenvectors. Hence the system matrix is degenerate at a perturbation level somewhere between 75% and 80%.

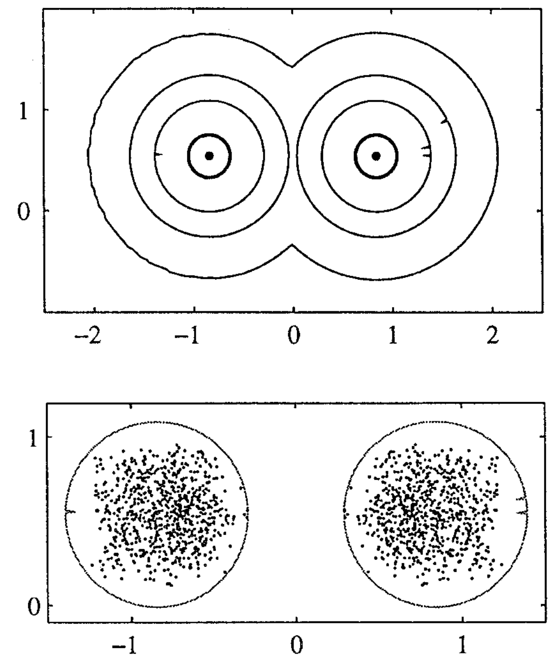

FIG. 1. (a) Spectral portraits of POP system matrix when being applied to a perfect propagating signal. The abscissa represents the real part and the ordinate the imaginary part. The perturbations applied to the system are 20%, 50%, 75%, and 120%. The 20% contour is thickened. (b) Eigenvalues of the system matrix under random perturbation with its norm less than 50% of that of the original matrix.

To test our results, we performed a Monte Carlo experiment. We randomly added perturbation matrices to the system matrix under the condition that the norm of the perturbation does not exceed 50% of the norm of the matrix. All the eigenvalues for the disturbed system matrix are plotted in Fig. 1b. As we can see, all the eigenvalues for the perturbation matrices fall within the expected neighborhoods.

b. Example 2: A perfect propagating signal and a standing wave

Similar to example 1, we generated a 24×24 dimensional covariance matrix from a process that contains one propagating mode and one standing mode. This process is represented by the equation

$$y(t) = \cos\left[\left(\omega_1 t - \frac{\pi}{6}x\right)\right] + \sin\left(\frac{\pi}{6}x\right)\cos(\omega_2 t). \quad (12)$$

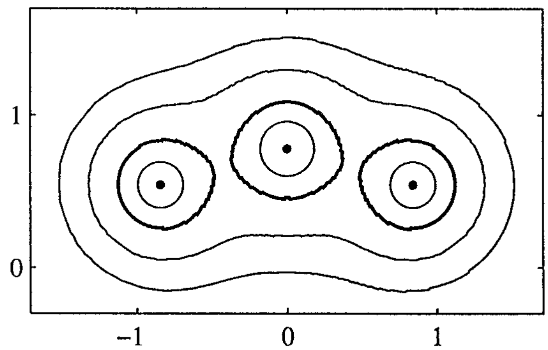

FIG. 2. As in Fig. 1a but for a system with a perfect propagating mode and a standing mode. The perturbations applied to the system are 10%, 20%, 30%, and 50%. The 20% contour is thickened.

Also applying an EOF analysis to the 24 × 24 covariance matrix, we keep the first three PCs to form a 3 × 3 POP system matrix. The three eigenvalues are presented as three dots in Fig. 2. As in example 1, the POP analysis captures the propagating mode well in terms of its amplitude and frequency. However, the standing mode is captured only to about 70% in terms of the amplitude of the signal. In this case (Fig. 2), the tolerance for all three eigenvalues is between 20% and 30%, compared to 75%–80% in the previous example. The reason that the system tends to be less stable might be because a nonpropagating signal is mixed in with the data.

c. *Example 3: Quasi-biennial oscillation (QBO)*

As presented in Xu and von Storch (1990), POP analysis can successfully capture the QBO signal. Here, we will investigate the sensitivity of the corresponding POP system matrix.

The dataset we used here consists of 38 yr (1956–93) of monthly zonal wind at Singapore measured at the levels of 70, 60, 50, 40, 30, 20, 15, and 10 mb. We apply an EOF analysis to this dataset. The two leading modes explain 99.6% of the total variance. The third mode explains only 0.2% of the total variance, and so it is considered to be noise. We performed a POP analysis by first retaining PCs for the first two leading EOF modes, then for the first three, to see how the sensitivity of the POP system matrix changes. Figure 3a shows the spectral portrait of the two-PC POP system matrix under the perturbations of 5%, 15%, and 20%. It shows that the tolerance of the perturbation for the system matrix is between 15% and 20% (the 15% curve is thickened). The system error is about 11%, which is smaller than the tolerance of the perturbations, hence the POP system matrix is stable.

We then form the POP system matrix by retaining PCs of the first three EOF modes, which is equivalent to adding some noise to the system. The spectral portraits of the system matrix under the perturbations of

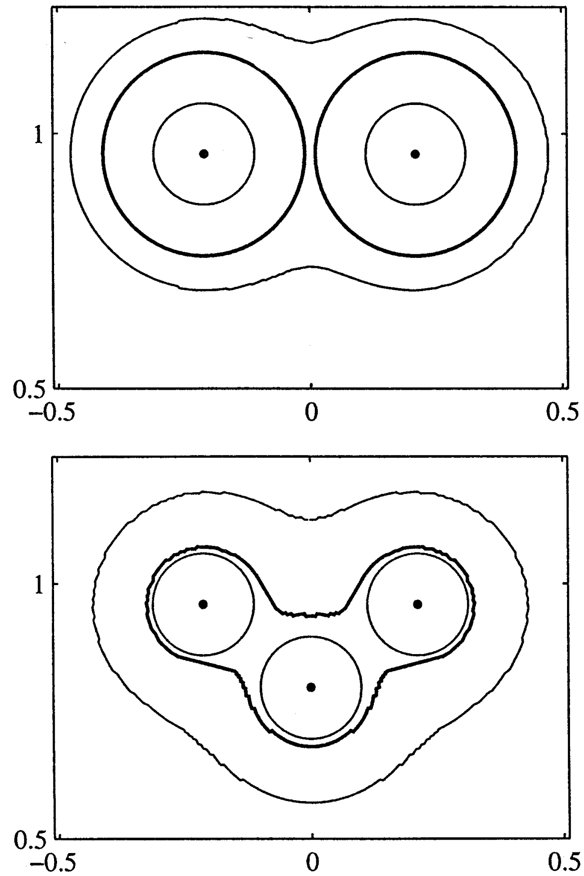

FIG. 3. (a) Same as Fig. 1a but using real QBO data with 2 EOF modes. The perturbations are 5%, 15%, and 25%. The contour for 15% perturbation is thickened. (b) As (a) but with 3 EOF modes. The perturbations are 5%, 10%, and 20%. The 10% contour is thickened.

5%, 10%, and 20% (10% contour is thickened) are shown in Fig. 3b. Apparently, even though the leading modes change very little, the tolerance of the perturbation drops to some value between 10% and 5%. This decrease in the stability of the system matrix is due to the EOF truncation error. Furthermore, the system error increases significantly from 11% to 125% due to the error in the inversion of the covariance matrix, which is related to truncation problems (the condition number increases from 1.6 to 18.7) when the third mode is retained. Therefore, the system error exceeds the tolerance of the perturbation, and the system is unstable.

d. *Example 4: Capturing the ENSO signal from tropical SST and Southern Hemispheric SLP*

Xu and von Storch (1992) showed that the POP analysis can capture the ENSO process when the process is presented by Southern Hemisphere SLP anomalies. Here, we will also analyze ENSO, but first by using an SST anomaly field over the tropical Pacific. We retained three and five EOF modes (total variances explained are 58% and 71%), respectively, to form two different POP

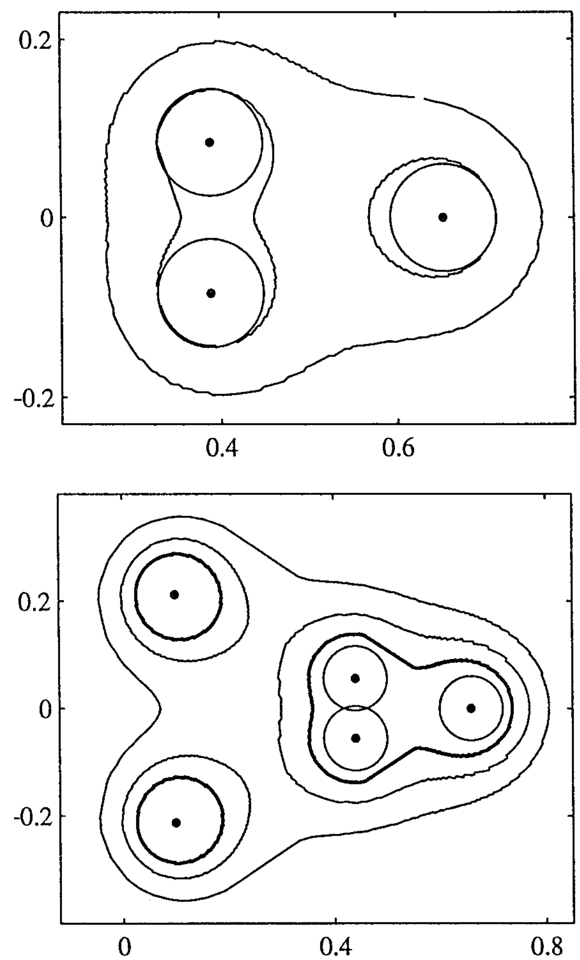

FIG. 4. Spectral portraits of POP system matrix based on PCs of tropical SST anomalies. (a) Retaining three modes, for perturbations of 3%, 5%, and 10%; (b) retaining five modes, for perturbations of 2%, 5%, 7%, and 10%. The 5% contour is thickened

system matrices in order to further examine the effect of EOF truncation. Figure 4a shows the spectral portrait of the system matrix when three EOF modes are retained. The tolerance of the perturbations for this system matrix lies between 3% and 5%, which is considerably lower than for QBO indicating that this system matrix is much more sensitive than that of QBO. The system error estimated by using Eq. (10) is 115%, which is significantly larger than the tolerance. Hence, the system is unstable. It is worth noting that the first mode of the system is a standing mode, and the second and third modes shown as a pair of propagating modes do not have the same frequency as ENSO modes would have. Hence, we did not capture any propagating ENSO mode by applying POP to monthly SST data. This strong sensitivity can be further demonstrated by Fig. 4b, spectral portraits of the POP system matrix for five EOF modes under perturbations of 2%, 5%, 7%, and 10%. The tolerance is about 2%, but the system error is much larger (180%). The lack of robustness of this POP system matrix hints to the possibility that when POP analysis is applied to a physical process that is not clearly periodic, this method might tend to be more sensitive or less effective (see, e.g., Bürger 1993).

For the same analysis, we also calculated the spectral portraits of POP matrices formed from monthly SLP anomalies (not shown). When only two EOF modes, which explains 35% of the total variance, were kept, we obtained a stable system. However, the corresponding period and damping time indicate that this pair of modes does not represent ENSO. Spectral portraits of the POP matrix with nine EOFs done in the way similar in Xu and von Storch (1992) were also examined. By examining the temporal variation (including both the frequency and the *e*-folding time) of the time coefficient and the spatial patterns, we know that modes 5 and 6 in this case are Southern Oscillation patterns. However, one has to be aware that this system is an unstable one, indicating that the same mode might not be captured in another sample.

5. Summary and conclusions

The examples shown above introduce the concept of spectral portrait of a nonsymmetric matrix, and illustrate the use of spectral portrait in examining the sensitivity of a matrix. Example 3 stresses an important issue about POP analysis: its sensitivity to the EOF truncation error and to the inversion of the covariance matrix. Adding minor EOF modes can change the POP system from a stable linear system to an unstable one. Example 4 demonstrates that, when a system does not contain a clearly periodic mode, the POP system matrix can be more sensitive. The tolerance value for the perturbations of the POP system matrix due to the inversion of the covariance matrix provides an indicator for the robustness of a POP system matrix. As we see, in practice, POP analysis system matrices can be ill-conditioned not only because of the inversion of a system matrix, but also because of the sampling error associated with limited data records.

Examining spectral portraits of a matrix is a simple and practical way of assessing the robustness of a linear system and can be generally applied to any type of matrix analysis technology. The sensitivity test of POP system matrices discussed here is just one example. It is important to examine the sensitivity of a linear system matrix before drawing conclusions from its results.

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