EIGENVALUES AND EIGENVECTORS OF SPECTRAL DENSITY MATRICES

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EIGENVALUES AND EIGENVECTORS OF SPECTRAL DENSITY MATRICES

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ABSTRACT

This report describes some interpretations and uses of eigenvalues and eigenvectors of spectral and sample spectral density matrices of multiple stationary time series.

The spectral density matrix of a zero-mean multiple stationary time series is defined. Eigenvalues and eigenvectors of the spectral density matrix are discussed and principal component theory is presented. Statistical distribution theory and related results are used to investigate the eigenvalues of a sample spectral density matrix. This investigation gives methods for obtaining simultaneous confidence bounds on the elements of the true spectral density matrix and its inverse, and also methods for obtaining confidence bounds on the eigenvalues of the true spectral density matrix.

CONTENTS

EIGENVALUES AND EIGENVECTORS OF SPECTRAL DENSITY MATRICES

The present report describes some interpretations and uses of eigenvalues and eigenvectors of spectral and sample spectral density matrices of multiple stationary time series.

1. SPECTRAL REPRESENTATION OF A ZERO-MEAN MULTIPLE STATIONARY TIME SERIES

A zero-mean multiple stationary time series $\overline{X}(t)$ has the spectral representation

$$X(t) = \begin{bmatrix} X_1(t) \\ X_2(t) \\ \cdot \\ \cdot \\ \cdot \\ X_p(t) \end{bmatrix} = \int_{-\infty}^{\infty} e^{i\omega t} \begin{bmatrix} dZ_1(\omega) \\ dZ_2(\omega) \\ \cdot \\ \cdot \\ \cdot \\ dZ_p(\omega) \end{bmatrix} \qquad (1)$$

One has

$$E \begin{bmatrix} dZ_1(\omega) \\ \cdot \\ \cdot \\ \cdot \\ dZ_p(\omega) \end{bmatrix} \left[\overline{dZ_1}(\omega), \ldots, \overline{dZ_p}(\omega)\right] = \Sigma(\omega)\, d\omega \qquad (2)$$

where the p x p Hermitian nonnegative definite matrix $\Sigma(\omega)$ is the spectral density matrix at frequency ω of $\overline{X}(t)$.

2. EIGENVALUES AND EIGENVECTORS OF A SPECTRAL DENSITY MATRIX

There exists a p x p unitary matrix $\beta(\omega)$, i. e.

$$\overline{\beta}'(\omega)\,\beta(\omega) = I = \beta(\omega)\,\overline{\beta}'(\omega) \tag{3}$$

such that

$$\overline{\beta}'(\omega)\,\Sigma(\omega)\,\beta(\omega) = \begin{bmatrix} \lambda_1(\omega) & & & & \\ & \lambda_2(\omega) & & 0 & \\ & & \cdot & & \\ & & & \cdot & \\ & 0 & & \cdot & \\ & & & & \lambda_p(\omega) \end{bmatrix} \equiv \Lambda(\omega) \tag{4}$$

where the $\lambda_j(\omega)$, $(j = 1, \ldots, p)$, are the eigenvalues (real and nonnegative) of $\Sigma(\omega)$ and

$$\lambda_1(\omega) \geq \lambda_2(\omega) \geq \cdots \geq \lambda_p(\omega) \geq 0 \tag{5}$$

Consider

$$\begin{bmatrix} dW_1(\omega) \\ \cdot \\ \cdot \\ \cdot \\ dW_p(\omega) \end{bmatrix} \equiv \bar{\beta}'(\omega) \begin{bmatrix} dZ_1(\omega) \\ \cdot \\ \cdot \\ \cdot \\ dZ_p(\omega) \end{bmatrix} \tag{6}$$

one has

$$E \begin{bmatrix} dW_1(\omega) \\ \cdot \\ \cdot \\ \cdot \\ dW_p(\omega) \end{bmatrix} \left[\overline{dW_1}(\omega), \ \ldots, \ \overline{dW_p}(\omega) \right] = E\, \bar{\beta}'(\omega) \begin{bmatrix} dZ_1(\omega) \\ \cdot \\ \cdot \\ \cdot \\ dZ_p(\omega) \end{bmatrix} \left[\overline{dZ_1}(\omega), \ \ldots, \ \overline{dZ_p}(\omega) \right] \beta(\omega) \tag{7}$$

$$= \bar{\beta}'(\omega)\, \Sigma(\omega)\, \beta(\omega)\, d\omega = \begin{bmatrix} \lambda_1(\omega) & & & \\ & \cdot & & 0 \\ & & \cdot & \\ 0 & & \cdot & \\ & & & \lambda_p(\omega) \end{bmatrix} d\omega = \Lambda(\omega)\, d\omega$$

From (7) one observes that the complex random variables $dW_1(\omega), \ldots, dW_p(\omega)$ are uncorrelated, and that

$$\mathrm{Var}\,(dW_j(\omega)) \equiv E\left|dW_j(\omega)\right|^2 = \lambda_j(\omega)\, d\omega, \quad (j = 1, \ldots, p) \tag{8}$$

Let $\beta_j(\omega)$, $(j = 1, \ldots, p)$, denote the jth column vector of the unitary matrix $\beta(\omega)$. Since $\beta(\omega)$ is unitary

$$\bar{\beta}_j'(\omega)\, \beta_{j'}(\omega) = \begin{cases} 0 \text{ if } j \neq j' \\ 1 \text{ if } j = j' \quad , \quad (j = 1, \ldots, p) \end{cases} \tag{9}$$

Equation (9) expresses that the column vectors $\beta_j(\omega)$ of $\beta(\omega)$ are orthonormal, i.e., they are orthogonal and of unit norm. From (4) one has

$$\Sigma(\omega)\, \beta(\omega) = \beta(\omega)\, \Lambda(\omega) \tag{10}$$

i.e.

$$\Sigma(\omega)\, \beta_j(\omega) = \lambda_j(\omega)\, \beta_j(\omega) \quad , \quad (j = 1, \ldots, p) \tag{11}$$

so that the column vectors $\beta_j(\omega)$ of $\beta(\omega)$ are the (normalized) eigenvectors of the spectral density matrix $\Sigma(\omega)$.

From (6),

$$dW_j(\omega) = \bar{\beta}_j'(\omega) \begin{bmatrix} dZ_1(\omega) \\ \cdot \\ \cdot \\ \cdot \\ dZ_p(\omega) \end{bmatrix} , \quad (j = 1, \ldots, p) \tag{12}$$

so that $dW_j(\omega)$ is a linear combination of $dZ_1(\omega), \ldots, dZ_p(\omega)$ with coefficients equal to the complex conjugate of the components of the column vector $\beta_j(\omega)$, $(j = 1, \ldots, p)$.

3. PRINCIPAL COMPONENTS

The $dW_1(\omega), \ldots, dW_p(\omega)$ are called principal components. With the eigenvalues $\lambda_1(\omega), \ldots, \lambda_p(\omega)$ in the order indicated by (5), $dW_1(\omega)$ is called the first principal component, $dW_2(\omega)$ the second principal component, etc.

Consider the problem of determining $c_{11}(\omega), c_{21}(\omega), \ldots, c_{p1}(\omega)$ satisfying

$$\sum_{j=1}^{p} \left| c_{j1}(\omega) \right|^2 = 1 \tag{13}$$

such that the linear combination $\sum_{j=1}^{p} \bar{c}_{j1}(\omega)\, dZ_j(\omega) = d\widetilde{W}_1(\omega)$ has maximum variance, i.e., such that

$$\operatorname{Var}(d\widetilde{W}_1(\omega)) \equiv \operatorname{Var}\left(\sum_{j=1}^{p} \bar{c}_{j1}(\omega)\, dZ_j(\omega)\right) \equiv E\left|\sum_{j=1}^{p} \bar{c}_{j1}(\omega)\, dZ_j(\omega)\right|^2 = \text{maximum} \tag{14}$$

The general solution to that problem is

$$\left[c_{11}(\omega),\ c_{21}(\omega),\ \ldots,\ c_{p1}(\omega)\right] = u_1(\omega)\, \beta_1'(\omega) \tag{15}$$

where $u_1(\omega)$ denotes an arbitrary complex number of unit modulus and $\beta_1(\omega)$ is the eigenvector of $\Sigma(\omega)$ corresponding to the eigenvalue $\lambda_1(\omega)$ described previously. Thus, the variance of $dW_1(\omega)$ is a maximum if and only if

$$d\widetilde{W}_1(\omega) = u_1(\omega)\, dW_1(\omega) \tag{16}$$

Furthermore, that maximum variance is

$$E\left|d\widetilde{W}_1(\omega)\right|^2 = E\left|dW_1(\omega)\right|^2 = E\, \bar{\beta}_1'(\omega) \begin{bmatrix} dZ_1(\omega) \\ \cdot \\ \cdot \\ \cdot \\ dZ_p(\omega) \end{bmatrix} \left[\overline{dZ_1}(\omega),\ \ldots,\ \overline{dZ_p}(\omega)\right] \beta_1(\omega) \tag{17}$$

$$= \bar{\beta}_1'(\omega)\, \Sigma(\omega)\, \beta_1(\omega)\, d\omega = \bar{\beta}_1'(\omega)\, \lambda_1(\omega)\, \beta_1(\omega)\, d\omega = \lambda_1(\omega)\, d\omega$$

Next, consider the problem of determining $c_{12}(\omega)$, $c_{22}(\omega)$, ..., $c_{p2}(\omega)$ satisfying

$$\sum_{j=1}^{p} \left| c_{j2}(\omega) \right|^2 = 1 \tag{18}$$

such that the linear combination $\sum_{j=1}^{p} \bar{c}_{j2}(\omega)\, dZ_j(\omega) = d\widetilde{W}_2(\omega)$ is uncorrelated with $dW_1(\omega)$ and has maximum variance, i.e., such that

$$E\, d\widetilde{W}_2(\omega)\, \overline{dW_1}(\omega) = 0 \tag{19}$$

and

$$\mathrm{Var}\,(d\widetilde{W}_2(\omega)) \equiv E\left| d\widetilde{W}_2(\omega) \right|^2 = \text{maximum} \tag{20}$$

The general solution to the problem is

$$\left[c_{21}(\omega),\ c_{22}(\omega),\ \ldots,\ c_{p2}(\omega) \right] = u_2(\omega)\, \beta_2'(\omega) \tag{21}$$

where $u_2(\omega)$ denotes an arbitrary complex number of unit modulus and $\beta_2(\omega)$ is the eigenvector of $\Sigma(\omega)$ corresponding to the eigenvector $\lambda_2(\omega)$ described previously. Thus, the variance of $dW_2(\omega)$ is a maximum if and only if

$$d\widetilde{W}_2(\omega) = u_2(\omega)\ dW_2(\omega) \tag{22}$$

That maximum variance is

$$E\left|d\widetilde{W}_2(\omega)\right|^2 = E\left|dW_2(\omega)\right|^2 = \lambda_2(\omega)\ d\omega \tag{23}$$

Similarly, the $c_{13}(\omega)$, $c_{23}(\omega)$, ..., $c_{p3}(\omega)$ satisfying

$$\sum_{j=1}^{p}\left|c_{j3}(\omega)\right|^2 = 1 \tag{24}$$

such that $d\widetilde{W}_3(\omega) \equiv \sum_{j=1}^{p} \bar{c}_{j3}(\omega)\ dZ_j(\omega)$ is uncorrelated with $dW_1(\omega)$ and $dW_2(\omega)$ and has maximum variance is

$$\left[c_{13}(\omega),\ c_{23}(\omega),\ \ldots,\ c_{p3}(\omega)\right] = u_3(\omega)\ \beta_3'(\omega) \tag{25}$$

the $d\widetilde{W}_3(\omega)$ possessing maximum variance is

$$d\widetilde{W}_3(\omega) = u_3(\omega)\ dW_3(\omega) \tag{26}$$

and that maximum variance is

$$E\left|dW_3(\omega)\right|^2 = \lambda_3(\omega)\ d\omega \tag{27}$$

Proceeding inductively in the manner illustrated above it is seen that

$$d\widetilde{W}_{r+1}(\omega) = u_{r+1}(\omega)\ dW_{r+1}(\omega) \tag{28}$$

is the solution to the following problem:

Find the $d\widetilde{W}_{r+1}(\omega) \equiv \sum_{j=1}^{p} \bar{c}_{j,\,r+1}(\omega)\ dZ_j(\omega)$ possessing maximum variance subject to the constraint that $\sum_{j=1}^{p} \left|c_{j,\,r+1}(\omega)\right|^2 = 1$ and $d\widetilde{W}_{r+1}(\omega)$ is uncorrelated with $dW_1(\omega)$, $dW_2(\omega)$, ..., $dW_r(\omega)$. Furthermore, that maximum variance is

$$E\left|d\widetilde{W}_{r+1}(\omega)\right|^2 = E\left|dW_{r+1}(\omega)\right|^2 = \lambda_{r+1}(\omega)\ dW \tag{29}$$

From the foregoing discussion it is seen that the transformation (6) of the $\left[dZ_1(\omega), \ldots, dZ_p(\omega)\right]$ to the $\left[dW_1(\omega), \ldots, dW_p(\omega)\right]$, i.e., the transformation to principal components, is a transformation to uncorrelated random variables possessing the special variance properties described above. In some studies the principal components with large variance may be of special interest. When the principal components with large variance "account for most of the variability," i. e., when the total variance of the other principal components is comparatively small, restricting attention (in exploratory investigations) to the principal components with large variance may constitute an effective way of reducing the "dimensionality" of a problem.

4. STATISTICAL ESTIMATION OF EIGENVALUES AND EIGENVECTORS OF A SPECTRAL DENSITY MATRIX

Let $\hat{\Sigma}(\omega)$ denote a sample Hermitian nonnegative definite spectral density matrix constituting an estimator of the true spectral density matrix $\Sigma(\omega)$. The eigenvalues $\hat{\lambda}_j(\omega)$, $(j = 1, \ldots, p)$, of $\hat{\Sigma}(\omega)$ in descending order are, respectively, estimators for the eigenvalues $\lambda_j(\omega)$, $(j = 1, \ldots, p)$, of $\Sigma(\omega)$. Similarly, the corresponding (normalized) eigenvectors $\hat{\beta}_j(\omega)$, $(j = 1, \ldots, p)$, of $\hat{\Sigma}(\omega)$ are, respectively, estimators for the normalized eigenvectors $\beta_j(\omega)$, $(j = 1, \ldots, p)$, of $\Sigma(\omega)$. Under suitable hypotheses (i. e., hypotheses that make $\hat{\Sigma}(\omega)$ a maximum likelihood estimator for $\Sigma(\omega)$), the $\hat{\lambda}_j(\omega)$, $\hat{\beta}_j(\omega)$, $(j = 1, \ldots, p)$, are, respectively, maximum likelihood estimators for $\lambda_j(\omega)$, $\beta_j(\omega)$, $(j = 1, \ldots, p)$.

5. STATISTICAL DISTRIBUTION THEORY AND RELATED RESULTS PERTAINING TO THE RANDOM EIGENVALUES OF A SAMPLE SPECTRAL DENSITY MATRIX

To simplify notation the dependence on the frequency ω will not be indicated here. For example, $\hat{\Sigma}(\omega)$ will simply be denoted by $\hat{\Sigma}$, the frequency dependence being understood. That is, it is understood that $\hat{\Sigma}$ is a spectral density estimator pertaining to a small frequency band centered at frequency ω.

The distributional theory and related results described here are predicated on

$$\hat{\Sigma} = \frac{1}{n} A \tag{30}$$

where A is complex Wishart distributed with n degrees of freedom. The complex Wishart distribution with parameters n, p, Σ will be denoted by $W_c(\Sigma; n, p)$.

Thm. 1. If A has the distribution $W_c(I; n, p)$ with $n \geq p$, then the random eigenvalues $\hat{K}_1 \geq \hat{K}_2 \geq \ldots \geq \hat{K}_p \geq 0$ of A have the joint probability density function

$$p(\hat{K}_1, \hat{K}_2, \ldots, \hat{K}_p) = C(p, n) \left(\prod_{j=1}^{p} \hat{K}_j^{n-p} \right) e^{-\sum_{j=1}^{p} \hat{K}_j} \prod_{\substack{j<k \\ j,k=1}}^{p} \left(\hat{K}_j - \hat{K}_k \right)^2 \tag{31}$$

where the "constant" $C(p, n)$ is given by

$$C(p, n) = \left[\prod_{j=1}^{p} \Gamma(n - p + j)\, \Gamma(j) \right]^{-1} \tag{32}$$

The probability density function (31) is defined over the domain $\hat{K}_1 \geq \hat{K}_2 \geq \cdots \geq \hat{K}_p \geq 0$.

Since the eigenvalues $\hat{\lambda}_j$ of $\hat{\Sigma}$ are related to the eigenvalues $\hat{K}_j$ of A by $\hat{\lambda}_j = \frac{1}{n}\hat{K}_j$, $(j = 1, \ldots, p)$, one may regard (31) as giving the probability density function of the $\hat{\lambda}_j$, $(j = 1, \ldots, p)$.

Thm. 2. If $\hat{K}_1, \hat{K}_2, \ldots, \hat{K}_p$ are random variables distributed with the probability density function (31), then for any constants a, b such that $0 \leq a \leq b$

$$\text{Prob}\left[a \leq \hat{K}_p, \ldots, \hat{K}_2, \hat{K}_1 \leq b \right] = C(p, n) \begin{vmatrix} \gamma_0 & \gamma_1 & \cdots & \gamma_{p-1} \\ \gamma_1 & \gamma_2 & \cdots & \gamma_p \\ \vdots & \vdots & & \vdots \\ \gamma_{p-1} & \gamma_p & \cdots & \gamma_{2p-2} \end{vmatrix} \tag{33}$$

where

$$\gamma_{i+j-2} \equiv \int_a^b v^{n-p+i+j-2}\, e^{-v}\, dv \quad , \quad (i, j = 1, 2, \ldots, p) \tag{34}$$

Equation (33) gives a closed form expression for the probability that all the eigenvalues of a random Hermitian matrix A distributed $W_c(I; n, p)$ with $n \geq p$ will be between prescribed limits a and b. Equivalently, one may regard (33) as giving the probability that all the random eigenvalues of a sample spectral density matrix $\hat{\Sigma}$ will be between prescribed limits for the case when the true spectral density matrix $\Sigma = I$. Confidence band results pertaining to general spectral density matrices are derivable from Thm. 2, so that the condition that $\Sigma = I$ is not as restrictive as might appear at first glance.

Let A^* denote a random Hermitian matrix distributed $W_c(I; n, p)$ where $n \geq p$. Let $ch_{min}(A^*)$ denote the minimum eigenvalue of A^* and $ch_{max}(A^*)$ denote the maximum eigenvalue of A^*. Let Σ denote a general nonsingular $(p \times p)$ spectral density matrix. From Thm. 2 for a chosen $0 < e < 1$ one may obtain constants ℓ^* and u^* such that

$$1 - e = \text{Prob}\left[\ell^* \leq ch_{min}(A^*),\ ch_{max}(A^*) \leq u^*\right] \tag{35}$$

The probability statement (35) is equivalent to

$$1 - e = \text{Prob}\left[\ell^* \leq \frac{\bar{a}'A^*a}{\bar{a}'a} \leq u^*,\ \text{for } \underline{\text{all}} \text{ nonzero complex } (p \times 1) \text{ vectors } a\right] \tag{36}$$

Now, there exists a nonsingular $(p \times p)$ matrix M such that

$$\overline{M}'\,M = \Sigma \tag{37}$$

Let

$$a = Mb \tag{38}$$

and

$$A = \overline{M}' A^* M \tag{39}$$

The Hermitian positive definite matrix A is distributed $W_c(\Sigma;\, n, p)$. Upon substituting (38) in (36) and using (37) and (39) one obtains

$$1 - \epsilon = \text{Prob}\left[\ell^* \leq \frac{\overline{b}' A b}{\overline{b}' \Sigma b} \leq u^* \;, \quad \text{for } \underline{\text{all}} \text{ nonzero complex } (p \times 1) \text{ vectors } b\right] \tag{40}$$

Using (30) one may state (40) in the form

$$1 - \epsilon = \text{Prob}\left[\frac{\ell^*}{n} \leq \frac{\overline{b}' \widehat{\Sigma} b}{\overline{b}' \Sigma b} \leq \frac{u^*}{n} \;, \quad \text{for all nonzero complex } (p \times 1) \text{ vectors } b\right] \tag{41}$$

From (41) one obtains the <u>simultaneous confidence band</u> result:

$$1 - \epsilon = \text{Prob}\left[\frac{n}{u^*}\, \overline{b}' \widehat{\Sigma} b \leq \overline{b}' \Sigma b \leq \frac{n}{\ell^*}\, \overline{b}' \widehat{\Sigma} b \;, \quad \begin{array}{l}\text{simultaneously} \\ \text{for all complex } (p \times 1) \text{ vectors } b\end{array}\right] \tag{42}$$

The vectors b may be freely chosen in (42) with <u>all</u> bounds on the resulting linear combinations of the elements of Σ holding simultaneously with probability $1 - \epsilon$. From simultaneous confidence bounds on suitably chosen linear combinations of the elements of Σ one may obtain, for example, simultaneous confidence bounds on <u>all</u> the spectra, co-spectra, and quadrature-spectra of Σ. One may also view (42) as giving simultaneous confidence bands for values of an Hermitian quadratic form where Σ is the matrix of the quadratic form. Equation (42) also yields

$$1 - \epsilon = \mathrm{Prob}\left[\frac{n}{u^*}\, ch_{min}(\hat{\Sigma}) \leq \lambda_p, \ldots, \lambda_2, \lambda_1 \leq \frac{n}{\ell^*}\, ch_{max}(\hat{\Sigma})\right] \tag{43}$$

where $ch_{min}(\hat{\Sigma})$ denotes the minimum eigenvalue of the sample spectral density matrix $\hat{\Sigma}$ and $ch_{max}(\hat{\Sigma})$ denotes the maximum eigenvalue. Equation (43) is a confidence bound for all the eigenvalues of the true spectral density matrix Σ.

From (35) one also obtains

$$1 - \epsilon = \mathrm{Prob}\left[\frac{\ell^*}{n}\, \bar{c}'\, \hat{\Sigma}^{-1}\, c \leq \bar{c}'\, \Sigma^{-1}\, c \leq \frac{u^*}{n}\, \bar{c}'\, \hat{\Sigma}^{-1}\, c\ , \quad \begin{array}{l}\text{simultaneously for all}\\ \text{complex } (p \times 1) \text{ vectors } c\end{array}\right] \tag{44}$$

The simultaneous confidence band statement (44) yields confidence bound results pertaining to Σ^{-1} directly analogous to those for Σ described above. Viewing (44) as giving simultaneous confidence bands for values of an Hermitian quadratic form where Σ^{-1} is the matrix of the quadratic form may be especially important. Such quadratic forms occur in quadratic signal detection methods.

In conclusion it is noted that both (42) and (44) are derived from (35) and hold simultaneously, i. e.

$$1 - \epsilon = \text{Prob}\left[\begin{array}{ll} \frac{n}{u^*}\,\bar{b}'\,\hat{\Sigma} b \leq \bar{b}'\,\Sigma b \leq \frac{n}{\ell^*}\,\bar{b}'\,\hat{\Sigma} b\ , & \text{simultaneously for all} \\ & \text{complex (p x 1) vectors } b \\ & \\ \frac{\ell^*}{n}\,\bar{c}'\,\hat{\Sigma}^{-1} c \leq \bar{c}'\,\Sigma^{-1} c \leq \frac{u^*}{n}\,\bar{c}'\,\hat{\Sigma}^{-1} c\ , & \text{simultaneously for all} \\ & \text{complex (p x 1) vectors } c \end{array}\right]$$

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