

# Automatic Estimation of Multivariate Spectra via Smoothing Splines

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## SUMMARY

The classical method for estimating the spectral density of a multivariate time series is to first calculate the periodogram, and then smooth it to obtain a consistent estimator. Typically, to ensure the estimate is positive definite, all the elements of the periodogram are smoothed the same way. There are, however, many situations for which different components of the spectral matrix have different degrees of smoothness, and hence require different smoothing parameters in order to obtain optimal estimates. We suggest a Bayesian approach that uses Markov chain Monte Carlo techniques to fit smoothing splines to each component—real and imaginary—of the Cholesky decomposition of the the periodogram matrix. The spectral estimate is then obtained by reconstructing the spectral estimator from the smoothed Cholesky decomposition components. Our technique allows for automatic smoothing of the different components of the spectral density matrix. In addition, because our procedure produces a sample from the posterior distribution of all the parameters, credible intervals are easily obtained.

*Some key words:* Coherency; Cholesky decomposition; DNA nucleotide sequence; MCMC; Multivariate spectral density, Smoothing splines; Spectral analysis; Spectral envelope.

## 1 INTRODUCTION

The classical method for estimating the spectral density of a multivariate time series is to first calculate the periodogram, and then smooth it to obtain a consistent estimator; for example, see Brillinger (2001, Ch. 5) or Shumway & Stoffer (2000, Ch. 3). A major difficulty is to guarantee that the final estimate is positive definite while allowing optimal smoothing for each element of the spectral matrix. Typically, to ensure the estimate is positive definite, all the elements of the periodogram are smoothed the same way. Pawitan (1996) proposed a penalized likelihood estimator for the cross-spectrum of a bivariate time series. The smoothing parameters for the real and imaginary parts can be chosen objectively from the data. Thus the real and imaginary parts can have different smoothness. With an implicit restriction on the estimation procedure to make the coherence less than or equal to one, the estimator is positive semidefinite. Extension of this method beyond bivariate time series is difficult because estimating the cross-spectra one at a time cannot guarantee that the final multivariate spectral estimate is positive semidefinite. Another difficulty is in constructing confidence intervals for the spectrum. In the univariate setting, Franke & Härdle (1992) proposed a bootstrap procedure for constructing confidence intervals. It is, however, difficult to generalize this method to the multivariate setting. As pointed out in Dai & Guo (2004), there are many situations for which different components of the spectral matrix have different degrees of smoothness, and hence require different smoothing parameters in order to obtain optimal estimates.

Dai & Guo (2004) overcame these problems by smoothing the Cholesky decomposition of a multitaper spectral estimate and then reconstructing the spectral estimate from the smoothed Cholesky components. Given data from a stationary, vector-valued, time series, their estimation and inference procedure consisted of the following steps: (i) compute the periodogram of the data; (ii) smooth the periodogram using a multitaper spectral estimator (Thomson, 1982); (iii) perform the Cholesky decomposition on the multitaper estimator; (iv) smooth each of the Cholesky decomposition components with its own smoothing parameter; (v) reconstruct the spectral estimator from the smoothed Cholesky decomposition components, and (vi) use a bootstrap method to obtain pointwise confidence intervals.

In this paper we take a Bayesian approach that uses Markov chain Monte Carlo (MCMC) techniques to fit smoothing splines to each component—real and imaginary—of the Cholesky decomposition of the the periodogram matrix. The spectral estimate is then obtained by reconstructing the spectral estimator from the smoothed Cholesky decomposition components. The advantage of our technique is that it allows for automatic smoothing of the components but avoids having to pre-smooth the periodogram by calculating a multitaper estimate. In addition, because our procedure produces a sample from the posterior distribution of all the parameters, credible intervals are easily obtained.

We describe the details of our procedure in the next section. Throughout, we assume that we have a sufficiently large number,  $n$ , of observations from a  $p$ -dimensional stationary time series,  $\mathbf{x}_t$ , whose  $p \times p$  autocovariance matrix,  $\Gamma(h) = \{\gamma_{jk}(h)\}$ , satisfies  $\sum_{h=-\infty}^{\infty} |\gamma_{jk}(h)| < \infty$  for all  $j, k = 1, \dots, p$ . The  $p \times p$  spectral density matrix is given by

$$f(\nu) = \sum_{h=-\infty}^{\infty} \Gamma(h) e^{-2\pi i \nu h}, \quad -1/2 \leq \nu \leq 1/2,$$

where  $f(\nu) = \{f_{jk}(\nu)\}$ , for  $j, k = 1, \dots, p$ , and frequency,  $\nu$ , is measured in cycles per time; note that  $f(\nu) = f^*(\nu)$ , where  $*$  denotes the conjugate transpose. Finally, we assume  $f(\nu)$  is positive definite.

## 2 THE MODEL AND PRIOR SPECIFICATION

Given a realization  $\mathbf{x}_1, \dots, \mathbf{x}_n$  from a multivariate stationary time series, the discrete Fourier transform (DFT) of the data is given by

$$\mathbf{y}(\nu_k) = n^{-1/2} \sum_{t=1}^n \mathbf{x}_t e^{-2\pi i \nu_k t}$$

for  $k = 0, 1, \dots, n-1$ , where  $\nu_k = k/n$  are the Fourier frequencies. The DFTs,  $\mathbf{y}(\nu_k)$ ,  $k = 0, \dots, n-1$ , of a zero-mean stationary multivariate time series are approximately independent complex multivariate normal random variables. Let  $\mathbf{y}_k \equiv \mathbf{y}(\nu_k)$  and  $f_k \equiv f(\nu_k)$ ,  $k = 0, \dots, n-1$ . The approximate likelihood is given by

$$L(\mathbf{y}_0, \dots, \mathbf{y}_{n-1}; f_0, \dots, f_{n-1}) \approx \prod_{k=0}^{n-1} |f_k|^{-1} \exp(-\mathbf{y}_k^* f_k^{-1} \mathbf{y}_k), \quad (1)$$

where  $|\cdot|$  denotes determinant. Equation (1) is an extension of the Whittle likelihood (Whittle, 1957) to the multivariate case. Note that since the spectral matrix and the DFT are even functions of  $\nu$ , there are only  $\lfloor n/2 \rfloor$  distinct observations.

Our goal is to obtain smooth estimates of the elements of  $f$  as a function of  $\nu$  while satisfying the constraint that  $f$  is positive definite. To this end, we express the inverse of the spectral matrix at frequency  $\nu_k$  as the modified complex Cholesky factorization

$$f_k^{-1} = T_k^* D_k^{-1} T_k, \quad (2)$$

where  $T_k$  is a complex unit lower triangular matrix, and  $D_k$  is a diagonal matrix. More specifically,

$$T_k = \begin{pmatrix} 1 & & & & \\ -\theta_{21}^{(k)} & 1 & & & \\ -\theta_{31}^{(k)} & -\theta_{32}^{(k)} & 1 & & \\ \vdots & \vdots & & \ddots & \\ -\theta_{p1}^{(k)} & -\theta_{p2}^{(k)} & \dots & -\theta_{p,p-1}^{(k)} & 1 \end{pmatrix}$$

and  $D_k = \text{diag}(\delta_{1k}^2, \dots, \delta_{pk}^2)$ . Note that in general, the  $\theta_{il}^{(k)}$ 's are complex valued. The real modified Cholesky decomposition has been used to model covariance matrices; see, for example, Pourahmadi (1999), Pourahmadi (2000), Daniels & Pourahmadi (2002), Pourahmadi & Daniels (2002), and Wu & Pourahmadi (2003).

We note that Dai & Guo (2004) worked directly with the complex Cholesky decomposition of  $f_k$ , say  $f_k = L_k L_k^*$ , where  $L_k$  is lower triangular. In particular, they obtained smoothed estimates of the elements of  $L_k$ . In our case, we use the modified decomposition of  $f_k^{-1}$  given in (2) because it appears naturally in the likelihood, (1). As previously stated, modeling the elements of the spectral matrix directly is difficult due to the constraint that the spectral matrix must be positive definite at each frequency. In the factorization (2), the  $\theta_{il}^{(k)}$ 's are unconstrained and the  $\delta_{jk}^2$ 's are positive. Thus, modeling these parameters rather than the elements of the spectral matrix is a much easier task. Once  $T_k$  and  $D_k$  have been estimated, the resulting estimate of  $f_k$  is automatically positive definite.

To facilitate the estimation of the  $\theta_{il}^{(k)}$ 's and the  $\delta_{jk}^2$ 's and thereby the estimation of the spectral matrix, we use the likelihood (1) in combination with the factorization (2).

We first rewrite the likelihood (1) as a function of the  $\theta_{il}^{(k)}$ 's and the  $\delta_{jk}^2$ 's. Let  $N=[n/2]$ ,  $\boldsymbol{\theta}_k$  be the  $p(p-1)/2$ -dimensional vector  $(\theta_{21}^{(k)}, \theta_{31}^{(k)}, \theta_{32}^{(k)}, \dots, \theta_{p,p-1}^{(k)})'$ ,  $\Theta = (\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_N)$ ,  $\Delta = \{\delta_{1k}^2, \dots, \delta_{pk}^2\}_{k=1}^N$  and  $Y = (\mathbf{y}_1, \dots, \mathbf{y}_N)$ . From (1) and (2) it follows that the likelihood can be expressed as

$$L(Y; \Delta, \Theta) \propto \prod_{k=1}^N \prod_{j=1}^p \delta_{jk}^{-2} \exp\{(\mathbf{y}_k - Z_k \boldsymbol{\theta}_k)' D_k^{-1} (\mathbf{y}_k - Z_k \boldsymbol{\theta}_k)\}, \quad (3)$$

where  $Z_k$  is a  $p \times p(p-1)/2$  design matrix given by

$$Z_k = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ y_{1k} & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & y_{1k} & y_{2k} & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & y_{1k} & y_{2k} & y_{3k} & 0 & \dots & 0 \\ \vdots & & & & & & & & \\ 0 & & \dots & & \dots & 0 & y_{1k} & y_{2k} & \dots & y_{p-1,k} \end{pmatrix}$$

with  $y_{ik}$  denoting the  $i$ th entry of  $\mathbf{y}_k$ . Note that in (3) we have ignored the endpoint involving  $\mathbf{y}_0$ . Next, we place linear smoothing splines priors on the  $\theta_{il}^{(k)}$ 's and the  $\delta_{jk}^2$ 's. Dai & Guo (2004) used cubic smoothing splines. In our experience, linear smoothing splines are better suited for estimating the spectral matrix, as they can better accommodate narrowband peaks. In particular, each of the  $\log \delta_{jk}^2$ 's and the real and imaginary parts of each of the negative  $\theta_{il}^{(k)}$ 's are expressed as follows

$$\alpha_0 + \alpha_1 \nu_k + \sum_{s=1}^N \psi_s(\nu_k) \beta_s, \quad (4)$$

where  $\psi_s(\nu_k) = \sqrt{2} \cos((s-1)\pi\nu_k)$ . The  $\psi_s(\cdot)$ 's are the Demmler-Reinsch basis functions for linear smoothing splines (see Eubank, 1999). Let  $X_\beta$  be the matrix whose columns are the basis functions  $\psi_s(\cdot)$  evaluated at  $\nu_1, \dots, \nu_N$ , and  $X_\alpha$  a matrix whose columns are the unit vector and  $(\nu_1, \dots, \nu_N)'$ . Let  $X = (X_\alpha | X_\beta)$ , i.e., the matrix formed by binding  $X_\alpha$  and  $X_\beta$  columnwise,  $\boldsymbol{\gamma}_j = (\boldsymbol{\alpha}'_j, \boldsymbol{\beta}'_j)'$ ,  $\boldsymbol{\Delta}_j = (\delta_{j1}^2, \dots, \delta_{jN}^2)'$  and  $\boldsymbol{\theta}_{il} = (\theta_{il}^{(1)}, \dots, \theta_{il}^{(N)})'$ , then

$$\log \boldsymbol{\Delta}_j = X \boldsymbol{\gamma}_j, \quad -\Re(\boldsymbol{\theta}_{il}) = X \boldsymbol{\gamma}_{il(re)}, \quad -\Im(\boldsymbol{\theta}_{il}) = X \boldsymbol{\gamma}_{il(im)}, \quad (5)$$

for  $j = 1, \dots, p$ ,  $i = 2, \dots, p$ , and  $l = 1, \dots, i-1$ , where  $\Re(\cdot)$  and  $\Im(\cdot)$  denote the real part and the imaginary part, respectively. Corresponding to (5), the priors on  $\boldsymbol{\alpha}_j$ ,  $\boldsymbol{\alpha}_{il(re)}$  and  $\boldsymbol{\alpha}_{il(im)}$

are taken to be  $N(\mathbf{0}, \sigma_\alpha^2 I_2)$ , and those on  $\boldsymbol{\beta}_j$ ,  $\boldsymbol{\beta}_{il(re)}$  and  $\boldsymbol{\beta}_{il(im)}$  are taken to be  $N(\mathbf{0}, \tau_j^2 I_N)$ ,  $N(\mathbf{0}, \tau_{il(re)}^2 I_N)$  and  $N(\mathbf{0}, \tau_{il(im)}^2 I_N)$ , respectively. Viewing the  $\theta_{il}^{(k)}$ 's and the  $\delta_{jk}^2$ 's as functions of  $\nu$ , the parameters  $\tau_j^2$ ,  $\tau_{il(re)}^2$  and  $\tau_{il(im)}^2$  are smoothing parameters, governing the amount of smoothing of each of these functions. A zero value of a smoothing parameter means a linear fit, while a value tending to infinity results in an interpolating linear spline. The priors on the smoothing parameters are  $p(\tau_j^2) \propto 1/\tau_j^2$ ,  $p(\tau_{il(re)}^2) \propto 1/\tau_{il(re)}^2$  and  $p(\tau_{il(im)}^2) \propto 1/\tau_{il(im)}^2$ . We estimate the spectral matrix by its posterior mean using MCMC methods to perform the required multidimensional integration.

### 3 THE SAMPLING SCHEME

Let  $\mathbf{u}_k = \mathbf{y}_k - Z_k \boldsymbol{\theta}_k$ . Plugging the expression for  $\log \boldsymbol{\Delta}_j$  in (5) into the likelihood (3) and incorporating the priors, the conditional distribution of  $\boldsymbol{\gamma}_j$ ,  $j = 1, \dots, p$  is given by

$$p(\boldsymbol{\gamma}_j \mid \Theta, Y) \propto \exp \left\{ - \sum_{k=1}^N (\mathbf{x}'_k \boldsymbol{\gamma}_j + |u_{jk}|^2 \exp(-\mathbf{x}'_k \boldsymbol{\gamma}_j)) - \frac{1}{2\sigma_\alpha^2} \boldsymbol{\alpha}'_j \boldsymbol{\alpha}_j - \frac{1}{2\tau_j^2} \boldsymbol{\beta}'_j \boldsymbol{\beta}_j \right\}, \quad (6)$$

where  $u_{jk}$  is the  $j$ th element of  $\mathbf{u}_k$ ,  $|\cdot|$  denotes the complex modulus and  $\mathbf{x}_k$  is the  $k$ th row of  $X$ . Since this is not a standard distribution, we use a Metropolis-Hastings step to sample from it. The conditional distributions of the corresponding smoothing parameters are  $\text{IG}(N/2, \frac{1}{2} \boldsymbol{\beta}'_j \boldsymbol{\beta}_j)$  for  $j = 1, \dots, p$ . The conditional distributions of  $\boldsymbol{\gamma}_{il(re)}$  and  $\boldsymbol{\gamma}_{il(im)}$  for  $i = 2, \dots, p$  and  $j = 1, \dots, i-1$ , are multivariate normal, and the conditional distributions of the corresponding smoothing parameters are  $\text{IG}(N/2, \frac{1}{2} \boldsymbol{\beta}'_{il(re)} \boldsymbol{\beta}_{il(re)})$  and  $\text{IG}(N/2, \frac{1}{2} \boldsymbol{\beta}'_{il(im)} \boldsymbol{\beta}_{il(im)})$ , where IG denotes the inverse gamma distribution. In principle, for smoothing splines, the knots are at the abscissa values of the data points. Thus, in our case, there are  $N$  basis functions. In practice, however, not all the  $N$  basis functions are necessary; in fact, only about  $N/10$  are usually sufficient. More details of the sampling scheme are given in the appendix.

## 4 EXAMPLES

We illustrate our methodology with three examples. First, to test the viability of our approach, we consider simulated data from a bivariate time series. The second example is a bivariate time series consisting of monthly measurements of the Southern Oscillation Index and the associated number of new fish in the Pacific Ocean. This example is taken from Shumway & Stoffer (2000), who used the data to explore the El Niño cycle. In the third example, we use the method to estimate the spectral envelope (Stoffer et al., 1993) of a DNA sequence. Further details on the spectral envelope will be given in the subsection corresponding to the analysis. For each example, the MCMC procedure was run for a total of 2000 iterations with a burn-in period of 1000 iterations.

### 4.1 Simulated data

We simulated  $n = 1024$  observations from the bivariate times series,  $\mathbf{x}_t = (x_{1t}, x_{2t})'$ ,

$$\mathbf{x}_t = \Phi_1 \mathbf{x}_{t-1} + \Phi_2 \mathbf{x}_{t-2} + \mathbf{z}_t,$$

where

$$\Phi_1 = \begin{pmatrix} 0.5 & 0 \\ 0 & -0.3 \end{pmatrix}, \Phi_2 = \begin{pmatrix} 0 & 0 \\ 0 & -0.5 \end{pmatrix} \quad \text{and} \quad \mathbf{z}_t \sim N\left(\mathbf{0}, \Sigma = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}\right);$$

The  $\mathbf{z}_t$  were generated independently. The  $2 \times 2$  spectral matrix of the process is (see Shumway & Stoffer, 2000, Ch. 3)

$$f(\nu) = \Phi^{-1}(\nu) \Sigma \Phi^{*-1}(\nu)$$

where

$$\Phi(\nu) = I - \Phi_1 \exp(-2\pi i\nu) - \Phi_2 \exp(-4\pi i\nu).$$

From this fact, we may calculate the elements of the spectral matrix of this process:

$$f_{11}(\nu) = [1.25 - \cos(2\pi\nu)]^{-1},$$

$$f_{22}(\nu) = [1.34 + 0.9 \cos(2\pi\nu) + \cos(4\pi\nu)]^{-1},$$

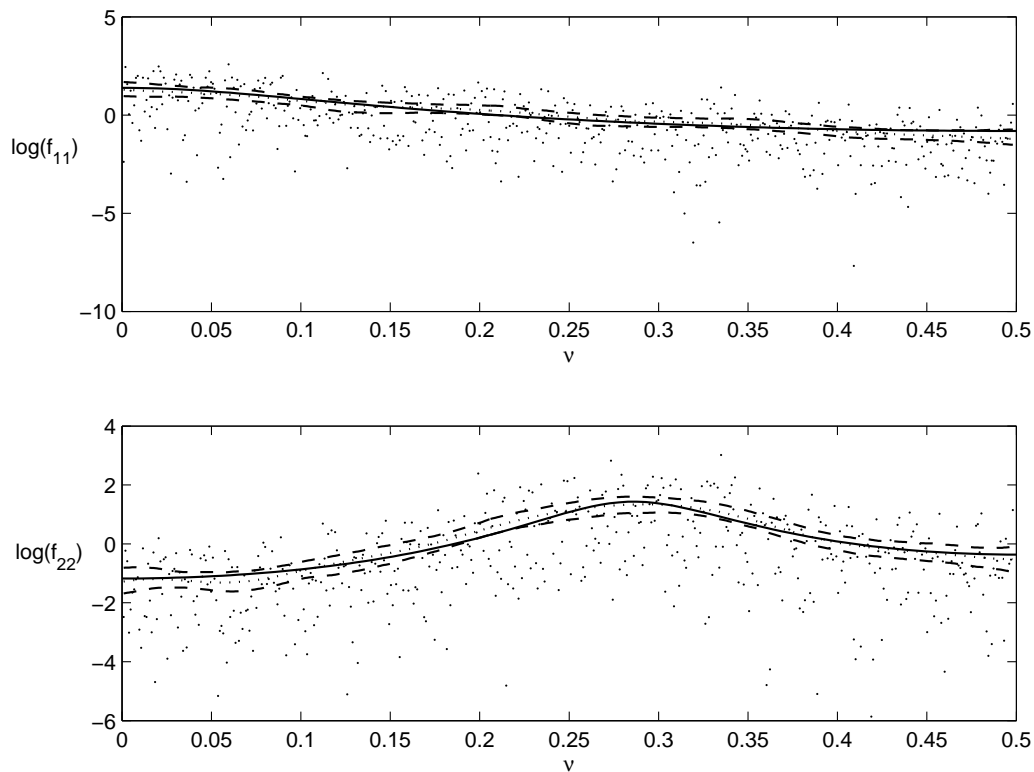


Figure 1: The periodograms, true spectra (solid), estimates (dotted) and 99% credible intervals (dashdotted), all on a log scale.

$$f_{12}(\nu) = 0.9\{0.85 - 0.45 \cos(2\pi\nu) + 0.5 \cos(4\pi\nu) + i[0.5 \sin(4\pi\nu) + 0.55 \sin(2\pi\nu)]\}^{-1}$$

and  $f_{21}(\nu) = f_{12}^*(\nu)$ . In addition, the squared coherency between the component processes is constant,

$$\rho_{12}^2(\nu) = \frac{|f_{12}(\nu)|^2}{f_{11}(\nu)f_{22}(\nu)} = .81.$$

Figure 1 displays the periodogram ordinates of the simulated series, the true spectral components,  $f_{11}(\nu)$  and  $f_{22}(\nu)$ , and the corresponding estimated spectra along with 99% pointwise credible intervals, all on a log scale. These intervals are obtained as the 0.005 and 0.995 empirical percentiles of the MCMC iterates, after the burn-in period, of  $X\gamma_1$  and  $X\gamma_2$  at each  $\nu_k$ . In addition, the estimated squared coherency (not shown) is approximately a straight line around the true squared coherency,  $\rho_{12}^2(\nu) = .81$ . This example demonstrates that our technique is a viable approach for obtaining smoothed spectral estimates of multi-



variate processes.

Finally, some comments are in order. First, we note that the spectral density of the second component,  $f_{22}(\nu)$ , has a fairly sharp peak around  $\nu = .28$ . This fact is obscured in Figure 1 because, to improve the visual impact, the spectra are plotted on a log scale, and in landscape mode (spectra are typically plotted this way). Second, because changing the order of the time series will change the Cholesky decomposition of the spectral matrix, we investigated the possibility that the ordering matters. In particular, we repeated this simulation with the components reversed, that is, with  $\mathbf{x}_t = (x_{2t}, x_{1t})'$ , instead of  $\mathbf{x}_t = (x_{1t}, x_{2t})'$ . Although the components of the Cholesky decomposition were changed, the final estimates of the spectra and cross-spectra did not change. Finally, to monitor convergence, we ran four chains with dispersed random starting points. We then looked at iteration plots, i.e., the iterates from the four chains for a given parameter as a function of the iteration number. In all the plots, following the warm-up period, the within-chain variation was in close agreement with the between-chain variation, i.e., the four chains were almost indistinguishable.

## 4.2 *El Niño Cycle*

Throughout Shumway & Stoffer (2006), two simultaneously recorded series are used to explore the El Niño cycle. Figure 2 shows these series, which are monthly values of the Southern Oscillation Index (SOI) and associated Recruitment (number of new fish) for a period of 453 months ranging over the years 1950–1987. The SOI measures changes in air pressure related to sea surface temperatures in the central Pacific Ocean. The central Pacific Ocean warms every three to seven years due to the El Niño effect. Both series exhibit regularly repeating cycles. The two series are related because the fish spawn in colder waters.

Figure 3 presents the estimated spectra (the diagonal elements of the estimated spectral matrix) as a function of frequency. Both spectra have peaks at about the same frequencies. One is at  $\nu = 1/12$  cycles per month which is the obvious yearly cycle. The other peak at about  $\nu = 1/48$  represents a possible El Niño effect. The yearly cycle has more power in the SOI series. In addition, both spectra show small peaks at the harmonic frequencies of the

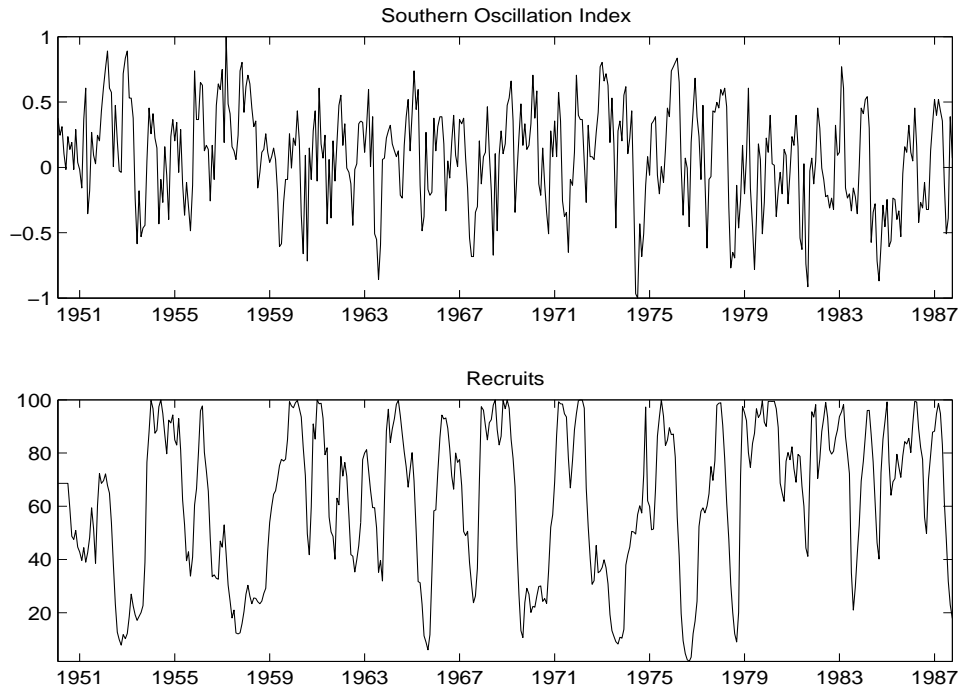


Figure 2: Monthly SOI and Recruitment series over the years 1950–1987.

yearly cycle.

To examine how the two series are related, we also plotted the estimated squared coherency in Figure 4. This plot shows that the El Niño and yearly cycles are strongly coherent. Other frequencies are also coherent but this is less meaningful, because they are harmonics of the yearly cycle and the power spectra at the harmonics (see Figure 3) are small.

### 4.3 Spectral envelope and DNA sequences

In some applications, an investigator may be more interested in a function of the components of a spectral matrix, such as coherency, described in the previous subsections. We now investigate the case of estimating eigenvalues and eigenvectors of the spectral matrix. In particular, we focus on estimating the spectral envelope (an eigenvalue) and the corresponding scaling (an eigenvector) of a DNA nucleotide sequence. In this case, the data are a sequence of multivariate  $3 \times 1$  indicator vectors that correspond to the sequence of nucleotides. For

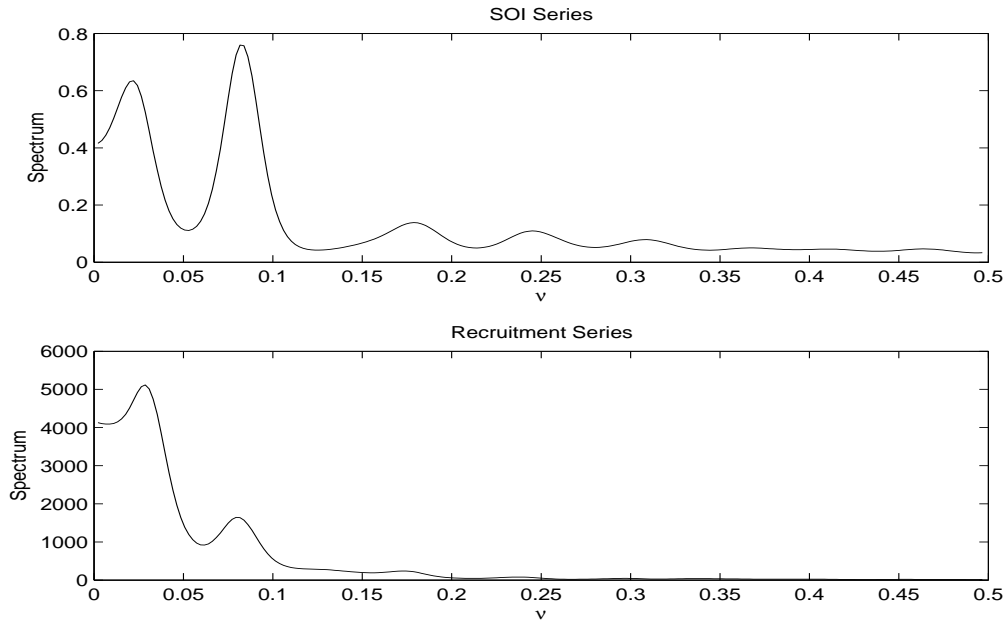


Figure 3: Individual estimated spectra of the SOI and Recruitment series.

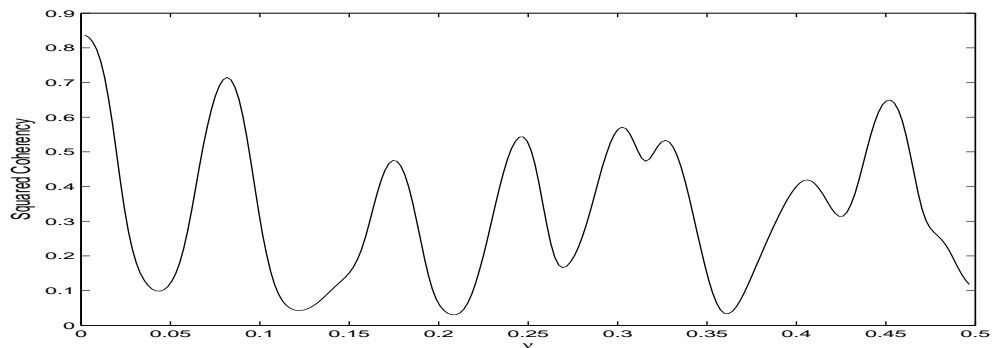


Figure 4: Squared coherency function relating SOI to Recruitment.

brevity, we do not include a discussion of the spectral envelope and we refer the reader to Stoffer et al. (1993) or Shumway & Stoffer (2006, Ch §7.9) for details.

In this example, we analyze part of the BNRF1 gene in Herpesvirus saimiri (HVS); the data are taken from GenBank. This particular coding sequence occurs from bp 6821 to 10561. As in Stoffer (2002), we estimate the spectral envelope for 1000 bps starting at bp 8820 of the CDS. Figure 5 displays the estimated spectral envelope corresponding to this subset of the HVS sequence. The spectral envelope picks up a signal at one cycle every three

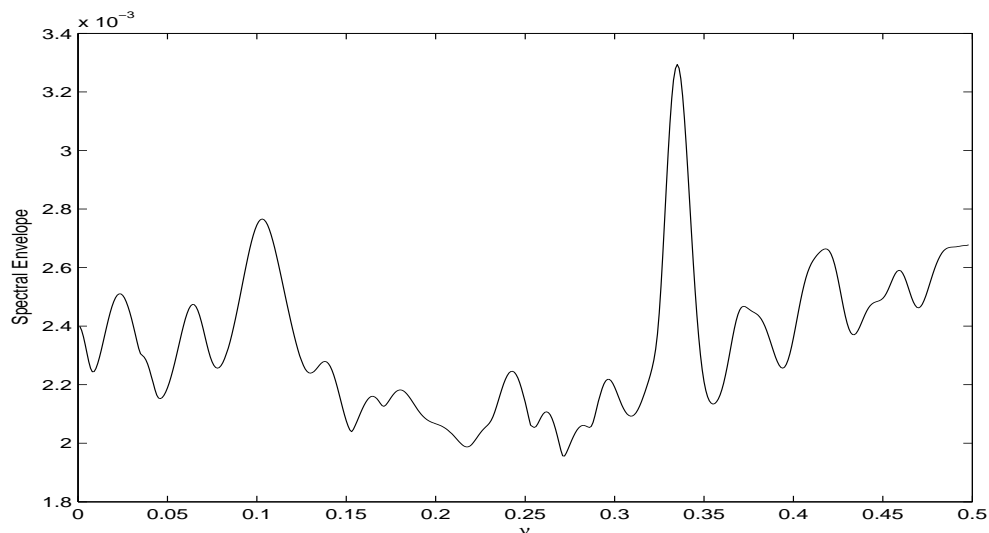


Figure 5: Spectral envelope for part of a coding sequence in *Herpesvirus saimiri*.

bp, which occurs often in CDS we have analyzed. There is another peak in the spectral envelope indicating a signal at one cycle every ten bp. This signal is particularly interesting because, while the double helix makes one turn about every 10 bp, the 10 bp signal is rarely seen and the importance of this twisting is not clear.

Finally, it is worthwhile to look at the scalings corresponding to each peak. For  $\nu = 1/10$ , the scalings are  $A = 2.12$ ,  $C = 1.93$ ,  $G = 0.17$ ,  $T = 0$ . This suggests that the signal is attributed to the M-K alphabet, where  $M = A$  or  $C$  and  $K = G$  or  $T$  is the complement of  $M$ . This structure itself is of interest. The relationship between  $A$  and  $C$  is that both have aMino (hence the M) groups at the ring position most distant from the point of attachment to the sugar and the relationship between guanine and thymine is that both have Keto (hence the K) groups at the corresponding position. For  $\nu = 1/3$ , the scalings are  $A = 2.28$ ,  $C = 0.89$ ,  $G = 2.16$ ,  $T = 0$ . This suggests that the signal may be attributed to the common RYY alphabet, where R denotes a puRine ( $A$  or  $G$ ) and Y denotes a pYrimidine ( $C$  or  $T$ ).

## ACKNOWLEDGMENTS

This work was supported, in part, by a grant from the National Science Foundation. We thank the reviewers for their valuable suggestions for improvement.

## APPENDIX: DETAILS OF THE SAMPLING SCHEME

In this appendix we give more details about the conditional distributions of  $\gamma_{il(re)}$  and  $\gamma_{il(im)}$ ,  $i = 2, \dots, p$ ,  $l = 1, \dots, i - 1$  used for performing the Gibbs sampler. We use the notation established in §2 and §3.

### A.1 *Bivariate time series*

Let

$$\begin{aligned} \mathbf{v}_{21(re)} &= \sum_{k=1}^N \delta_{2k}^{-2} (y_{2k}^* y_{1k} + y_{1k}^* y_{2k}) \mathbf{x}_k, \\ \mathbf{v}_{21(im)} &= \sum_{k=1}^N \delta_{2k}^{-2} i (y_{2k}^* y_{1k} - y_{1k}^* y_{2k}) \mathbf{x}_k, \\ A_{21(\cdot)} &= \text{diag} \left\{ \frac{1}{2} (\sigma_\alpha^{-2}, \sigma_\alpha^{-2}, \tau_{21(\cdot)}^{-2}, \dots, \tau_{21(\cdot)}^{-2}) \right\}, \end{aligned}$$

for  $\cdot = re, im$ , and

$$B_{21} = \sum_{k=1}^N \delta_{2k}^{-2} |y_{1k}|^2 \mathbf{x}_k \mathbf{x}_k',$$

where  $y_{jk}$  denotes the complex conjugate of  $y_{jk}$  and  $i = \sqrt{-1}$ . Then

$$p(\gamma_{21(re)} | \gamma_2, \tau_{21(re)}^2, Y) \sim N(\boldsymbol{\mu}_{21(re)}, \Sigma_{21(re)}) \tag{A.1}$$

and

$$p(\gamma_{21(im)} | \gamma_2, \tau_{21(im)}^2, Y) \sim N(\boldsymbol{\mu}_{21(im)}, \Sigma_{21(im)}), \tag{A.2}$$

where  $\Sigma_{21(\cdot)} = \frac{1}{2} (A_{21(\cdot)} + B_{21})^{-1}$  and  $\boldsymbol{\mu}_{21(\cdot)} = \Sigma_{21(\cdot)} \mathbf{v}_{21(\cdot)}$ , for  $\cdot = re, im$ .

The conditional distribution for drawing  $\gamma_j$ ,  $j = 1, 2$  is given in (6). To draw from it, we use a Metropolis-Hastings step with a multivariate normal proposal distribution. The mean and variance-covariance of this multivariate normal distribution are the maximizer

of (6) with respect to  $\gamma_j$ , and the inverse of the negative hessian of (6) evaluated at this maximizer, respectively. The sampling scheme, thus, consists of

1. Drawing  $\gamma_j$  from (6), for  $j = 1, 2$ .
2. Drawing  $\gamma_{21(re)}$  and  $\gamma_{21(im)}$  from (A.1) and (A.2), respectively.
3. Drawing  $\tau_j^2$ ,  $j = 1, 2$ ,  $\tau_{21(re)}^2$  and  $\tau_{21(im)}^2$  from the inverse Gamma distributions described in Section 3.

### A.2 Trivariate time series

The vectors  $\gamma_{21(re)}$  and  $\gamma_{21(im)}$  are drawn according to (A.1) and (A.2), respectively. Let

$$\begin{aligned} \mathbf{v}_{31(re)} &= \sum_{k=1}^N \delta_{3k}^{-2} [y_{3k}^* y_{1k} + y_{3k} y_{1k}^* - \mathbf{x}'_k \gamma_{32(re)} (y_{1k}^* y_{2k} + y_{2k}^* y_{1k})] \mathbf{x}_k, \\ \mathbf{v}_{31(im)} &= \sum_{k=1}^N \delta_{3k}^{-2} [i(y_{3k}^* y_{1k} - y_{3k} y_{1k}^*) - \mathbf{x}'_k \gamma_{32(im)} (y_{1k}^* y_{2k} + y_{2k}^* y_{1k})] \mathbf{x}_k, \\ B_{31} &= \sum_{k=1}^N \delta_{3k}^{-2} |y_{1k}|^2 \mathbf{x}_k \mathbf{x}'_k, \\ \mathbf{v}_{32(re)} &= \sum_{k=1}^N \delta_{3k}^{-2} [y_{3k}^* y_{2k} + y_{3k} y_{2k}^* - \mathbf{x}'_k \gamma_{31(re)} (y_{1k}^* y_{2k} + y_{2k}^* y_{1k})] \mathbf{x}_k, \\ \mathbf{v}_{32(im)} &= \sum_{k=1}^N \delta_{3k}^{-2} [i(y_{3k}^* y_{2k} - y_{3k} y_{2k}^*) - \mathbf{x}'_k \gamma_{31(im)} (y_{1k}^* y_{2k} + y_{2k}^* y_{1k})] \mathbf{x}_k, \\ B_{32} &= \sum_{k=1}^N \delta_{3k}^{-2} |y_{2k}|^2 \mathbf{x}_k \mathbf{x}'_k. \end{aligned}$$

For  $i = 3$ ,  $l = 1, 2$  and  $\cdot = re, im$ , let  $A_{il(\cdot)} = \text{diag} \left\{ \frac{1}{2}(\sigma_\alpha^{-2}, \sigma_\alpha^{-2}, \tau_{il(\cdot)}^{-2}, \dots, \tau_{il(\cdot)}^{-2}) \right\}$ , then

$$p(\gamma_{31(re)} | \gamma_{32(re)}, \gamma_3, \tau_{31(re)}^2, Y) \sim N(\boldsymbol{\mu}_{31(re)}, \Sigma_{31(re)}), \quad (\text{A.3})$$

$$p(\gamma_{31(im)} | \gamma_{32(im)}, \gamma_3, \tau_{31(im)}^2, Y) \sim N(\boldsymbol{\mu}_{31(im)}, \Sigma_{31(im)}), \quad (\text{A.4})$$

$$p(\gamma_{32(re)} | \gamma_{31(re)}, \gamma_3, \tau_{32(re)}^2, Y) \sim N(\boldsymbol{\mu}_{32(re)}, \Sigma_{32(re)}) \quad (\text{A.5})$$

and

$$p(\boldsymbol{\gamma}_{32(im)} | \boldsymbol{\gamma}_{31(im)}, \boldsymbol{\gamma}_3, \tau_{32(im)}^2, Y) \sim N(\boldsymbol{\mu}_{32(im)}, \boldsymbol{\Sigma}_{32(im)}) , \quad (\text{A.6})$$

where  $\boldsymbol{\Sigma}_{il(\cdot)} = \frac{1}{2}(A_{il(\cdot)} + B_{il})^{-1}$  and  $\boldsymbol{\mu}_{il(\cdot)} = \boldsymbol{\Sigma}_{il(\cdot)}\boldsymbol{v}_{il(\cdot)}$ , for  $i = 3, l = 1, 2$  and  $\cdot = re, im$ . The different parameters are drawn in an analogous fashion to that described in Section A.1.

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