Periodic Correlation in Stratospheric Ozone Data

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Abstract. A fifty-year time series of monthly stratospheric ozone readings from Arosa, Switzerland is analyzed. The time series exhibits the properties of a periodically correlated (PC) random sequence with annual periodicities. Spectral properties of PC random sequences are reviewed and a test to detect periodic correlation is presented. An ARMA model with periodically varying coefficients (PARMA) is fit to the data in two stages. First, a periodic autoregressive model (PAR) is fit to the data. This fit yields residuals that are stationary, but non-white. Next, a stationary ARMA model is fit to the residuals and the two models are combined to produce a larger model for the data. The combined model is shown to be a PARMA model and yields residuals that have the correlation properties of white noise.

Keywords: Periodic correlation, spectral analysis, coherence statistic, ARMA model, PARMA model, Yule-Walker estimation.

1. INTRODUCTION

Many real valued random sequences show nonstationarity in the form of periodic correlation. A random sequence $\{X_n\}$ with finite second moments is called periodically correlated (PC) with period T if $\mu(n) = \mathsf{E}[X_n]$ and $C(m,n) = \mathsf{C}ov(X_m, X_n)$ are periodic with period T:

$$\mu(n+T) = \mu(n) \quad \text{and} \quad C(m+T, n+T) = C(m,n). \tag{1.1}$$

To avoid ambiguity, the period T is taken as the smallest positive integer such that (1.1) holds. When $T = 1$, $\{X_n\}$ is covariance stationary and will be referred to as stationary for short. One can always assume that $\mu(n) \equiv 0$ by examining $\{X_n - \mu(n)\}$; in practice, the periodic sample mean is subtracted from the data.

This paper is concerned with modeling the correlation structure of stratospheric ozone data. A model is developed for a data set, plotted in Figure 1, that contains 50 years of monthly observations from Arosa, Switzerland. The development of adequate models for ozone data is important in the prediction of future values and in the analysis of possible trends (Hill *et al.*, 1986). A natural choice for the period is $T = 12$; this choice will be statistically justified by a test presented in Section 3. Figures 2a and 2b, which plot the monthly sample mean and standard deviation of the data set in Dobson units, clearly indicate that the data are nonstationary.

Section 2 briefly reviews frequency domain theory for PC random sequences. Section 3 discusses spectral estimation and presents a test for detecting the presence of periodic correlation. Section 4 introduces a class of models for PC random sequences and discusses estimation of model parameters. In Section 5, these ideas are applied in the development of a model for the Arosa data. The goodness of model fit is evaluated by examining the correlation properties of its residuals. Section 6 summarizes the paper.

2. FREQUENCY DOMAIN THEORY

Suppose $\{X_n\}$ is PC with period T. The frequency domain approach to the study of PC time series is based on the fact that $\{X_n\}$ is harmonizable in the sense of Loève (1978, §37.4); that is, $\{X_n\}$ has the spectral representation

$$X_n = \int_0^{2\pi} e^{in\lambda} dZ(\lambda), \tag{2.1}$$

where $\{Z(\lambda),\ 0 \leq \lambda < 2\pi\}$ is a mean zero complex valued random process. The second order structure of $\{Z(\lambda),\ 0 \leq \lambda < 2\pi\}$ is described by the complex valued bivariate signed measure R with increments

$$R(d\lambda_1, d\lambda_2) = \mathsf{E}[dZ(\lambda_1)\overline{dZ(\lambda_2)}], \qquad (\lambda_1, \lambda_2) \in [0, 2\pi)\text{x}[0, 2\pi). \tag{2.2}$$

If $\{X_n\}$ is stationary, then $Z(\lambda)$ has orthogonal increments: $\mathsf{E}[dZ(\lambda_1)\overline{dZ(\lambda_2)}] = 0$ if $\lambda_1 \neq \lambda_2$. In this case, R is supported on the main diagonal $\lambda_1 = \lambda_2$. If $\{X_n\}$ is PC with period T, then $Z(\lambda)$ has periodically correlated increments: $\mathsf{E}[dZ(\lambda_1)\overline{dZ(\lambda_2)}] = 0$ unless $\lambda_2 = \lambda_1 + \frac{2\pi k}{T}$ for some $k \in \{0, \pm 1, \ldots, \pm(T-1)\}$ (Gladyšhev, 1961). In this case, R is supported on the $2T-1$ parallel diagonal lines $\lambda_2 = \lambda_1 + \frac{2\pi k}{T}$, $k = 0, \pm 1, \ldots, \pm(T-1)$ restricted to the bifrequency square $[0, 2\pi)$x$[0, 2\pi)$. Figure 3 graphically describes this support set.

Let $\{X_n\}$ be PC with period T and let $G_\psi(d\lambda)$ be the differential of R along the diagonal line $\lambda_2 = \lambda_1 + \psi$:

$$G_\psi(d\lambda) = \mathsf{E}[dZ(\lambda)\overline{dZ(\lambda+\psi)}], \qquad \lambda \in [0, 2\pi),\ \psi \in (-2\pi, 2\pi), \tag{2.3}$$

where $\lambda + \psi$ is taken modulo 2π if necessary. The main diagonal component of R has the same interpretation as the spectrum of a stationary sequence: $G_0(d\lambda) = R(d\lambda, d\lambda) = \mathsf{E}[\,|dZ(\lambda)|^2]$. We assume that G_0 has the density $G_0(d\lambda) = g_0(\lambda)d\lambda$. Then the remaining components also have densities: $G_\psi(d\lambda) = g_\psi(\lambda)d\lambda$ (Hurd and Bloomfield, 1992). The periodic diagonal nature of the support set of R (see Figure 3) implies that $g_\psi(\lambda) \equiv 0$ unless $\psi \in \{0, \pm\frac{2\pi}{T}, \pm\frac{4\pi}{T}, \ldots, \pm\frac{2(T-1)\pi}{T}\}$. A test to detect periodic correlation based on this principle is discussed in Section 3.

There is a relationship between the correlation structure of $\{X_n\}$ and the spectra $g_\psi(\lambda)$: set $B(n,\tau) = Cov(X_n, X_{n+\tau})$. For each fixed τ, $B(n,\tau)$ is a periodic function in n with period T. Thus, $B(n,\tau)$ has the Fourier representation

$$B(n,\tau) = \sum_{k=0}^{T-1} B_k(\tau)e^{2\pi i n k/T}. \tag{2.4}$$

Hurd (1989) shows that $B_k(\tau)$ is related to $g_{-2\pi k/T}(\lambda)$ by

$$B_k(\tau) = \int_0^{2\pi} e^{i\lambda\tau} g_{-2\pi k/T}(\lambda) d\lambda, \tag{2.5}$$

The symmetry relationship $g_\psi(\lambda) = \overline{g_{-\psi}(\lambda + \psi)}$ follows from (2.3); hence, it is sufficient to consider $g_\psi(\lambda)$ for $\psi \in [0,2\pi)$ only. The main diagonal spectrum, $g_0(\lambda)$, like the spectrum of a stationary sequence, is real valued and nonnegative. In general, the other spectra are complex valued, but satisfy the Cauchy-Schwarz inequality

$$| g_\psi(\lambda) |^2 \leq g_0(\lambda) g_0(\lambda + \psi). \tag{2.6}$$

3. FREQUENCY DOMAIN ESTIMATION

Suppose $\{X_1, X_2, \ldots, X_N\}$ is a sample from a mean zero PC time series with period T. To avoid complexities later, assume that the data record contains d full years, that is, assume $d = N/T$ is an integer. The discrete Fourier transform of the data sample is defined at the Fourier frequency $\lambda_j = 2\pi j/N$ by

$$I_N(\lambda_j) = \frac{1}{\sqrt{2\pi N}} \sum_{n=1}^{N} X_n e^{-i(n-1)\lambda_j} \quad (j = 0, 1, \ldots, N-1). \tag{3.1}$$

The bifrequency periodogram is computed at each Fourier frequency pair (λ_j, λ_k) in $[0, 2\pi)$x$[0, 2\pi)$ via

$$r(\lambda_j, \lambda_k) = I_N(\lambda_j) \overline{I_N(\lambda_k)}. \tag{3.2}$$

In the context of spectral estimation from a data sequence of length N, let $g_h(\cdot)$ be shorthand notation for $g_{\lambda_h}(\cdot) = g_{2\pi h/N}(\cdot)$, $h \in \{0, \pm 1, \ldots, \pm(N-1)\}$. An estimate of $g_h(\lambda_j)$ is $\hat{g}_h(\lambda_j) = r(\lambda_j, \lambda_{j+h})$. Assuming only that the density $g_h(\lambda)$ exists, one can show that $\hat{g}_h(\lambda)$ is asymptotically unbiased:

$$\lim_{N \to \infty} \mathsf{E}[\hat{g}_h(\lambda)] = g_h(\lambda) \tag{3.3}$$

(Hurd and Bloomfield, 1992). However, as with stationary spectral estimation, $\hat{g}_h(\lambda)$ is not a consistent estimator of $g_h(\lambda)$; consistency is obtained by smoothing $\hat{g}_h(\lambda)$. Hurd and Bloomfield (1992) show that if $\{X_n\}$ is a Gaussian time series, then a consistent estimate of $g_h(\lambda)$ is obtained if the smoothing bandwidth b_N satisfies $b_N \to 0$ and $Nb_N \to \infty$ as $N \to \infty$.

An M point one-sided uniform smoothing of $\hat{g}_h(\lambda_j)$ is

$$\hat{g}_{h,M}(\lambda_j) = \frac{1}{M}\sum_{m=0}^{M-1} \hat{g}_h(\lambda_{j+m}) = \frac{1}{M}\sum_{m=0}^{M-1} I_N(\lambda_{j+m})\overline{I_N(\lambda_{j+h+m})}. \tag{3.4}$$

We recommend a centered smoothing for estimating the density $g_h(\lambda)$; however, our interest lies with finding correlations in the discrete Fourier transform; hence, the computationally convenient one-sided smoothing in (3.4) will be used in the ensuing coherence calculations. The discrete Fourier transform is extended in the usual periodic manner of

$$I_N(\lambda_{N+j}) = I_N(\lambda_j) \tag{3.5}$$

when a frequency of 2π or more is encountered in (3.4).

A test for detecting periodic correlation in $\{X_n\}$ against the stationary null hypothesis was recently presented by Hurd and Gerr (1991). A variant of this test will be used in our numerical work that follows. The test is based upon the following fact: if $\{X_n\}$ is stationary, then $g_h(\lambda) \equiv 0$ for all $h \neq 0$; if $\{X_n\}$ is PC with period T, then $g_h(\lambda) \equiv 0$ except when h is an integer multiple of $d = N/T$. The idea is made more precise by defining

$$\left|\gamma_{h,M}(\lambda_j)\right|^2 = \frac{\left|\hat{g}_{h,M}(\lambda_j)\right|^2}{\hat{g}_{0,M}(\lambda_j)\hat{g}_{0,M}(\lambda_{j+h})} = \frac{\left|\sum_{m=0}^{M-1} I_N(\lambda_{j+m})\overline{I_N(\lambda_{j+h+m})}\right|^2}{\sum_{m=0}^{M-1}\left|I_N(\lambda_{j+m})\right|^2 \sum_{m=0}^{M-1}\left|I_N(\lambda_{j+h+m})\right|^2}. \tag{3.6}$$

The quantity $|\gamma_{h,M}(\lambda_j)|^2$ is called Goodman's squared coherence statistic (Goodman, 1965) and takes values in the interval [0,1] only. The squared coherence statistic is symmetric about the line $\lambda_1 = \lambda_2$:

$$|\gamma_{h,M}(\lambda_j)|^2 = |\gamma_{-h,M}(\lambda_{j+h})|^2, \tag{3.7}$$

in view of which it is sufficient to consider $|\gamma_{h,M}(\lambda_j)|^2$ for $h \geq 0$. Note that $\hat{g}_{0,M}(\lambda_j)$ is real valued and that $|\gamma_{0,M}(\lambda_j)|^2 = 1$.

To detect periodic correlation in $\{X_n\}$, Goodman's squared coherence statistic is computed for all $h \in \{1, 2, \ldots, N-1\}$ and λ_j such that $0 \leq \lambda_j < 2\pi$. When a frequency of 2π or more is encountered in the computations, (3.5) is used. Next, the percentage of squared coherence statistics exceeding a preset threshold is computed along each diagonal line $h \geq 1$. The exceedance percentage is plotted against the diagonal line index h. *If $\{X_n\}$ is PC with period T, then the exceedance percentage should be small whenever h is not a multiple of d and should be large for some h's that are multiples of d. Thus, this diagonal exceedance percentage plot should reveal large values at some multiples of d.* If $\{X_n\}$ is stationary, no large values should appear in the diagonal exceedance percentage plot.

To determine the preset squared coherence threshold, the distribution of $|\gamma_{h,M}(\lambda_j)|^2$ must be known under the null hypothesis that $\{X_n\}$ is stationary. The squared coherence distribution is known explicitly only for the case where $\{X_n\}$ is mean zero Gaussian white noise and $h \neq 0$:

$$\mathbf{P}[\,|\gamma_{h,M}(\lambda_j)|^2 > x\,] = (1-x)^{M-1}, \quad 0 \leq x \leq 1, \tag{3.8}$$

(Goodman, 1965). One can justify the beta type distribution in (3.8) as an asymptotic distribution of the squared coherence statistic under a wide variety of departures of $\{X_n\}$ from both normality and white noise. This robustness essentially follows from the asymptotic normality of $I_N(\lambda_j)$ (see Brockwell and Davis, 1987, §10.3) and the uncorrelated nature of $I_N(\lambda_j)$ and $\overline{I_N(\lambda_k)}$ when $\lambda_j \neq \lambda_k$. A simulation study by Hurd and Lund (1991) has shown that the distribution in (3.8) is very robust against departures from both normality and white noise even for small values of N. Hence, the threshold $1-(.05)^{\frac{1}{M-1}}$ provides an approximate 95% degree of statistical confidence. See Hurd and Gerr (1991) for remarks on the selection of M.

Figure 4 displays the diagonal exceedance percentage plot of the Arosa data with the periodic sample mean removed and $M = 8$. The plot clearly indicates a large exceedance percentage at $h = 50$ indicating that $d = 50$, or equivalently, that $T = 12$. The squared coherence statistic exceeds the 95% threshold of .348 at 41.0% of the frequencies along the line $h = 50$, much larger than the approximate 5% expected under the null hypothesis of stationarity. When (3.5) is used, the diagonal exceedance percentage plot is symmetric about $h = 300$; thus, one need only plot the exceeding percentage for $1 \le h \le 300$.

4. MODELS FOR PERIODICALLY CORRELATED RANDOM SEQUENCES

PARMA Models

Periodic correlation can be introduced into an ARMA model when the coefficients of the model are allowed to vary periodically with time. This leads us to the class of periodic autoregressive moving average (PARMA) models.

For clarity, the notation of Vecchia (1985a) is adopted and $\{X_l\}$ is indexed by year and season: $X_{nT+\nu}$ refers to the time series during the νth season of year $n \ge 0$. The total number of seasons per year is T and the seasonal index ν satisfies $1 \le \nu \le T$. The random sequence $\{X_l\}$ is said to follow a PARMA model if

$$X_{nT+\nu} - \sum_{k=1}^{p(\nu)} \phi_k(\nu) X_{nT+\nu-k} = \sum_{k=0}^{q(\nu)} \theta_k(\nu) \epsilon_{nT+\nu-k}, \tag{4.1}$$

where $\{\epsilon_l\}$ is mean zero white noise with $Var(\epsilon_l) \equiv 1$. The coefficients $\phi_k(\nu)$ and $\theta_k(\nu)$, and the orders $p(\nu)$ and $q(\nu)$ can vary with the season and are extended periodically in the variable ν to all integers.

Some ARMA difference equations do not have stationary solutions; likewise, (4.1) may not have a solution that is PC with period T. Necessary and sufficient conditions guaranteeing the existence of a solution to (4.1) that is PC with period T, to our knowledge, have not yet been found. When $\{X_l\}$ is blocked into "yearly" vectors of dimension T, an ARMA difference equation for the yearly vectors can be derived. Stationarity results for multivariate ARMA sequences can be used to produce sufficient conditions guaranteeing the existence of a solution to (4.1) that is PC with period T. The reader is referred to Vecchia (1985a) for more details.

Model 4.1 has a total of $T + \sum_1^T \{p(\nu) + q(\nu)\}$ parameters. In the analysis of the Arosa data, the simple first order periodic autoregressive PAR(1) model

$$X_{nT+\nu} = \phi(\nu) X_{nT+\nu-1} + \sigma(\nu) \epsilon_{nT+\nu} \tag{4.2}$$

is used. Here, $\{\epsilon_l\}$ is mean zero white noise with $Var(\epsilon_l) \equiv 1$. Model 4.2 has $p(\nu) \equiv 1$, $q(\nu) \equiv 0$, $\phi_1(\nu) = \phi(\nu)$, $\theta_0(\nu) = \sigma(\nu)$, and a total of $2T$ parameters. A special case of model 4.2 with a constant $\phi(\nu) \equiv \phi$ was used to analyze ozone data by Reinsel and Tiao (1987).

Suppose $\{X_l\}$ is a PC random sequence with period T. For notation, let

$$\gamma_\nu(\tau) = E[X_{nT+\nu} X_{nT+\nu-\tau}] = B(\nu, -\tau) \qquad (\tau \geq 0 \quad \text{and} \quad \nu = 1, 2, \ldots, T) \tag{4.3}$$

be the correlation function for season ν. The PC nature of $\{X_l\}$ causes one to extend $\gamma_\nu(\tau)$ periodically: $\gamma_{nT+\nu}(\tau) = \gamma_\nu(\tau)$. Also, $\gamma_\nu(-\tau)$ for $\tau > 0$ is evaluated with $\gamma_\nu(-\tau) = \gamma_{\nu+\tau}(\tau)$.

Theorem 1 establishes the correlation properties of model 4.2; the proof is in the appendix. A product over an empty set of indices is interpreted as unity in parts (b) and (c).

Theorem 1 *Suppose $\{X_l\}$ has bounded second moments and satisfies the assumptions of model* 4.2.

(a) *Then $\{X_l\}$ is PC with period T if $|\phi(1)\phi(2)\ldots\phi(T)| < 1$.*

(b) *If $|\phi(1)\phi(2)\ldots\phi(T)| < 1$, then*

$$Var(X_{nT+\nu}) = \sum_{k=1}^{\nu} \sigma^2(k)\left(\prod_{l=k+1}^{\nu}\phi(l)\right)^2 + \frac{r_\nu^2}{1-r_T^2}\left\{\sum_{k=1}^{T}\sigma^2(k)\left(\prod_{l=k+1}^{T}\phi(l)\right)^2\right\}$$

where $r_\nu = \phi(1)\phi(2)\ldots\phi(\nu)$ for $\nu = 1, 2, \ldots, T$.

(c) *If $|\phi(1)\phi(2)\ldots\phi(T)| < 1$, then* $\gamma_\nu(\tau) = \left(\prod_{i=0}^{\tau-1}\phi(\nu-i)\right)Var(X_{nT+\nu-\tau})$

for $\tau \geq 0$ and $\nu = 1, 2, \ldots, T$. □

Now consider model 4.2 with a mean zero, unit variance, stationary error sequence $\{\epsilon_l\}$. Theorem 2 establishes two properties of this model. Again, the proof can be found in the appendix.

Theorem 2 *Suppose $\{X_l\}$ has bounded second moments and satisfies the assumptions of model* 4.2 *except that $\{\epsilon_l\}$ is a mean zero, unit variance, stationary random sequence.*

(a) *Then $\{X_l\}$ is PC with period T if $|\phi(1)\phi(2)\ldots\phi(T)| < 1$.*

(b) *If $\{\epsilon_l\}$ follows the stationary ARMA equation* $\epsilon_n - \sum_{k=1}^{p}\gamma_k\epsilon_{n-k} = \sum_{k=0}^{q}\beta_k\omega_{n-k}$,

where $\{\omega_l\}$ is mean zero white noise and $\beta_0 = 1$, then $\{X_l\}$ follows the PARMA model 4.1 *with*

$p(\nu) \equiv p+1$; $q(\nu) \equiv q$; $\theta_k(\nu) = \beta_k\sigma(\nu)$, $1 \leq k \leq q$; $\phi_1(\nu) = \phi(\nu) + \dfrac{\gamma_1\sigma(\nu)}{\sigma(\nu-1)}$;

$\phi_k(\nu) = \sigma(\nu)\left\{\dfrac{\gamma_k}{\sigma(\nu-k)} - \dfrac{\gamma_{k-1}\phi(\nu-k+1)}{\sigma(\nu-k+1)}\right\}$, $2 \leq k \leq p$; $\phi_{p+1}(\nu) = \dfrac{-\sigma(\nu)\gamma_p\phi(\nu-p)}{\sigma(\nu-p)}$,

and the same white noise sequence $\{\omega_l\}$. □

Part (b) of Theorem 2 suggests building models for PC data sets in stages: first, determine a simple PAR model that leaves stationary residuals. Next, fit a stationary ARMA model to the residuals. Finally, combine the models with equations similar to those found in part (b) of Theorem 2. This procedure is illustrated with the Arosa data in Section 5.

Parameter Estimation for Model 4.2

An algorithm to compute approximate maximum likelihood parameter estimates for the general PARMA model is in Vecchia (1985b); Yule-Walker moment estimates for the general PAR model are computed in Vecchia (1985a). For the Arosa data, it will be sufficient to estimate parameters for the PAR(1) model 4.2.

Yule-Walker moment estimators for model 4.2 are obtained by equating sample correlations to theoretical correlations. Multiply (4.2) by $X_{nT+\nu-j}$ for $j = 0,\ 1$ and take expectations to obtain

$$\gamma_\nu(0) = \phi(\nu)\gamma_\nu(1) + \sigma^2(\nu) \qquad \text{and} \qquad \gamma_\nu(1) = \phi(\nu)\gamma_{\nu-1}(0). \tag{4.4}$$

The relationship $\mathsf{E}[X_{nT+\nu-j}\epsilon_{nT+\nu}] = \sigma(\nu)\mathbf{I}_{\{0\}}(j)$ used in the derivation of (4.4) is easily justified from the causal relationship (A.5) established in the appendix during the proof of Theorem 1. A moment estimator of $\gamma_\nu(j)$ is

$$\hat{\gamma}_\nu(j) = \frac{1}{d}\sum_{n=0}^{d-1} X_{nT+\nu}X_{nT+\nu-j} \qquad (\nu = 1,\ 2,\ \ldots,\ T), \tag{4.5}$$

where $d = N/T$ is the number of years of data and $X_i = 0$ for $i \le 0$. The Yule-Walker parameter estimates are obtained from (4.4) by substituting $\hat{\gamma}_\nu(j)$ in for $\gamma_\nu(j)$:

$$\hat{\phi}(\nu) = \frac{\hat{\gamma}_\nu(1)}{\hat{\gamma}_{\nu-1}(0)} \qquad \text{and} \qquad \hat{\sigma}^2(\nu) = \hat{\gamma}_\nu(0) - \hat{\phi}(\nu)\hat{\gamma}_\nu(1) \qquad (\nu = 1,\ 2,\ \ldots,\ T). \tag{4.6}$$

Recall that $\hat{\gamma}_\nu(j)$ is interpreted periodically in the variable ν. The Yule-Walker estimates are easy to compute and have many desirable properties. Troutman (1979) has shown that $\hat{\sigma}^2(\nu) > 0$ and $|\hat{\phi}(1)\hat{\phi}(2)\ .\ .\ .\ \hat{\phi}(T)| < 1$ when the data is seasonally non-constant. Hence, the fitted model is PC with period T. Pagano (1978) has shown that the Yule-Walker parameter estimates are asymptotically most efficient when the error sequence $\{\epsilon_t\}$ is normally distributed.

Approximate maximum likelihood parameter estimates can also be obtained for model 4.2 under the assumption of a normally distributed error sequence $\{\epsilon_t\}$. The approximation arises by setting $X_0 = 0$. For notation, let $\vec{\epsilon} = \{\epsilon_1, \epsilon_2, \ldots, \epsilon_N\}'$ and $\vec{X} = \{X_1, X_2, \ldots, X_N\}'$. One can use the governing difference equation (4.2) to obtain

$$A\vec{X} = \Sigma\vec{\epsilon}, \tag{4.7}$$

where Σ is a NxN diagonal matrix with $\Sigma_{nT+\nu,nT+\nu} = \sigma(\nu)$ for $n = 0, 1, \ldots, d-1$ and $\nu = 1, 2, \ldots, T$, and A is an invertible NxN unit diagonal matrix whose only other nonzero entries are $A_{nT+\nu,nT+\nu-1} = -\phi(\nu)$ for $n = 0, 1, \ldots, d-1$; $\nu = 1, 2, \ldots, T$; and $nT + \nu \geq 2$. Thus, $\vec{X}$ has an N-variate normal distribution with mean zero and covariance matrix $A^{-1}\Sigma^2(A^{-1})'$.

Let $L(\vec{X}; \vec{\sigma},\vec{\phi})$ denote the approximate likelihood function evaluated at the data vector $\vec{X}$ when the parameter vectors are $\vec{\phi} = (\phi(1), \phi(2), \ldots, \phi(T))'$ and $\vec{\sigma} = (\sigma(1), \sigma(2), \ldots, \sigma(T))'$ respectively. Using $\det(A) = 1$ and the form of the multivariate normal probability density function, one obtains

$$L(\vec{X}; \vec{\phi},\vec{\sigma}) = (2\pi)^{-N/2}\{\det(\Sigma^2)\}^{-1/2}\exp\left\{-\tfrac{1}{2}(A\vec{X})'\Sigma^{-2}(A\vec{X})\right\}. \tag{4.8}$$

Taking the logarithm of (4.8) and using the form of Σ produces

$$-\log\Big\{L(\vec{X};\,\vec{\phi},\vec{\sigma})\Big\} = \frac{N}{2}\log(2\pi) + d\sum_{\nu=1}^{T}\log\{\sigma(\nu)\} + \frac{1}{2}\sum_{n=0}^{d-1}\sum_{\nu=1}^{T}\left(\frac{X_{nT+\nu}-\phi(\nu)X_{nT+\nu-1}}{\sigma(\nu)}\right)^2. \quad (4.9)$$

Explicitly minimizing (4.9) via differentiation produces the maximum likelihood estimates

$$\widehat{\phi}(\nu) = \frac{\widehat{\gamma}_\nu(1)}{\widehat{\gamma}_{\nu-1}(0)} \quad \text{and} \quad \widehat{\sigma}^2(\nu) = \widehat{\gamma}_\nu(0) - \widehat{\phi}(\nu)\widehat{\gamma}_\nu(1) \qquad (\nu = 1, 2, \ldots, T) \qquad (4.10)$$

which are the same as the Yule-Walker estimates. One advantage with the maximum likelihood approach occurs when restrictions exist between the parameters, for example, suppose $\phi(\nu) = c_0 + c_1\nu$. Then it is not clear how to modify the moment estimates in (4.5) while, one could always minimize the negative log likelihood in (4.9) numerically over the variables of interest. This issue will surface again in Section 5 when the total number of parameters modeling the Arosa data set is reduced.

To evaluate the exact likelihood function, the covariance matrix of $\vec{X}$ must be computed explicitly. In principle, this covariance matrix can be obtained from parts (b) and (c) of Theorem 1; in practice, one would still have to invert the NxN covariance matrix to evaluate the approximate negative log likelihood function in (4.8). We note that this drawback is completely bypassed with the approximation $X_0 = 0$.

5. MODEL DEVELOPMENT FOR THE AROSA DATA

Figure 5 plots the model 4.2 parameter estimates for the mean subtracted Arosa data as computed with (4.6) and\or (4.10). An approximate negative log likelihood of 2408.535 was obtained. This 24-parameter model will be called the full model. Figure 5 shows that both $\widehat{\phi}(\nu)$ and $\widehat{\sigma}(\nu)$ vary from month to month, with $\widehat{\sigma}(\nu)$ following an approximate sinusoidal shape. To evaluate the fit of the full model, the residuals

$$\widehat{\epsilon}_{nT+\nu} = \frac{X_{nT+\nu} - \widehat{\phi}(\nu)X_{nT+\nu-1}}{\widehat{\sigma}(\nu)} \qquad (5.1)$$

with $\hat{\epsilon}_1 = X_1/\hat{\sigma}(1)$ are examined. If the full model fit is good, the residuals should have correlation properties similar to those of white noise.

Figure 6 displays the diagonal exceedance percentage plot of the residuals with $M = 8$. The plot shows that the large exceedance percentage in Figure 4 at $h = 50$ has been removed; this provides statistical evidence that the residuals are from a stationary sequence. Figure 7 plots $\hat{g}_0(\lambda)$, the unsmoothed periodogram of these residuals. The periodogram has a U-shaped feature indicating that the residuals may not be white noise. To test this hypothesis statistically, the portmanteau test (see Brockwell and Davis, 1987, pg. 300) is applied to the residuals over the first 25 lags. The test statistic for the Portmanteau test is N times the sum of the square of the residual's sample correlation function over the first 25 lags. Under the null hypothesis that the residuals are white noise, one anticipates a small test statistic. In this case, the value of the portmanteau test statistic was 68.823 which produces a p-value of 5.75x10^{-6} when compared to a chi-squared random variable with 25 degrees of freedom (the approximate null hypothesis distribution). Thus, there is statistical evidence that the full model has removed the periodic correlation in the data and that the error terms belong to a stationary, but non-white random sequence.

One can attempt to reduce the total number of parameters in the full model by parametrizing $\phi(\nu)$ and $\sigma(\nu)$ as a short Fourier series (Jones and Brelsford, 1967). Parametrize $\phi(\nu)$ and $\sigma(\nu)$ via

$$\phi(\nu) = \alpha_1\left\{1 + \alpha_2\cos\left(\frac{2\pi(\nu - \alpha_3)}{12}\right)\right\}, \qquad \sigma^2(\nu) = \alpha_4\left\{1 + \alpha_5\cos\left(\frac{2\pi(\nu - \alpha_6)}{12}\right)\right\}. \tag{5.2}$$

The α_i's for this six-parameter reduced model can be selected by minimizing the approximate negative log likelihood in (4.9). This was numerically performed and produced $\hat{\alpha}_1 = .314 \pm .042$, $\hat{\alpha}_2 = .282 \pm .169$, $\hat{\alpha}_3 = -2.001 \pm 1.207$, $\hat{\alpha}_4 = 230.797 \pm 14.141$, $\hat{\alpha}_5 = .788 \pm .020$, $\hat{\alpha}_6 = 1.792 \pm .160$, and an approximate negative log likelihood of 2419.790. Uncertainties are one standard error and were calculated from an approximation to the observed information matrix. The estimates of $\phi(\nu)$ and $\sigma(\nu)$ for the six-parameter reduced model are plotted in Figure 5.

Twice the difference between the approximate negative log likelihoods of the full model and the six-parameter reduced model is 22.51. This produces a p-value of .210 when compared to a chi-squared random variable with 18 degrees of freedom; hence, we prefer the six-parameter reduced model over the 24-parameter full model. The parameter estimates for the six-parameter reduced model and their standard errors indicate that α_2 may not be significantly different from zero. Hence, let us parametrize $\phi(\nu)$ and $\sigma(\nu)$ with

$$\phi(\nu) \equiv \phi, \qquad \sigma^2(\nu) = \alpha_4\left\{1 + \alpha_5 \cos\left(\frac{2\pi(\nu - \alpha_6)}{12}\right)\right\}. \tag{5.3}$$

This model will be called the four-parameter reduced model. The approximate maximum likelihood estimates of the parameters in (5.3) and their approximate standard errors are $\widehat{\phi} = .293 \pm .038$, $\widehat{\alpha}_4 = 231.579 \pm 14.603$, $\widehat{\alpha}_5 = 0.787 \pm .031$, and $\widehat{\alpha}_6 = 1.786 \pm .160$. The four-parameter reduced model produced an approximate negative log likelihood of 2421.057. Twice the difference between the approximate negative log likelihoods of the six-parameter reduced model and the four-parameter reduced model is 2.534. This produces a p-value of .282 when compared to a chi-squared random variable with two degrees of freedom; hence, we prefer the four-parameter reduced model over the six-parameter reduced model. The estimates of $\phi(\nu)$ and $\sigma(\nu)$ for the four-parameter reduced model are plotted in Figure 5.

Figure 8 presents the diagonal exceedance percentage plot of the residuals for the four-parameter reduced model with $M = 8$. Again, the large exceedance percentage at $h = 50$ is absent. Figure 9 plots $\widehat{g}_0(\lambda)$, the unsmoothed periodogram of the four-parameter reduced model's residuals. This periodogram displays the same U-shaped feature encountered with the full model's residuals. Applying the portmanteau test to these residuals over the first 25 lags produces a test statistic of

67.756. The p-value of this test is $8.25\text{x}10^{-6}$. Thus, there is statistical evidence that the four-parameter reduced model's residuals are stationary, but not white noise.

The full model and the four-parameter reduced model both produced stationary, non-white residuals. We proceed with the four-parameter reduced model because of its fewer total parameters. As suggested in Section 4, a stationary ARMA model is fit to the residuals of the four-parameter reduced model. The optimal ARMA model for these residuals as selected by both the AIC and BIC criterions (Brockwell and Davis, 1987) is the ARMA(2,1) model

$$\hat{\epsilon}_l - \gamma_1 \hat{\epsilon}_{l-1} - \gamma_2 \hat{\epsilon}_{l-2} = \omega_l + \beta_1 \omega_{l-1}. \tag{5.4}$$

The maximum likelihood estimates of the parameters in (5.4) are $\hat{\gamma}_1 = .644 \pm .080$, $\hat{\gamma}_2 = .206 \pm .042$, and $\hat{\beta}_1 = -.738 \pm .077$. The estimated white noise variance of $\{\omega_l\}$ is 0.943. The model fitted in (5.4) yields $\mathsf{E}[\hat{\epsilon}_l^2] \equiv 1.0004$ which is roughly consistent with the model 4.2 assumption that $\mathsf{E}[\epsilon_l^2] \equiv 1$. The ARMA model in (5.4) and the PAR(1) four-parameter reduced model can be combined with part (b) of Theorem 2 to produce a PARMA model with the seasonal orders $p(\nu) \equiv 3$ and $q(\nu) \equiv 1$. We omit the listing of the PARMA model's coefficients.

As a final check, the residuals of the combined PARMA model are analyzed. These residuals are computed recursively via

$$\hat{\omega}_{nT+\nu} = \frac{X_{nT+\nu} - \sum_{k=1}^{p(\nu)} \hat{\phi}_k(\nu) X_{nT+\nu-k} - \sum_{k=1}^{q(\nu)} \hat{\theta}_k(\nu) \hat{\omega}_{nT+\nu-k}}{\hat{\theta}_0(\nu)}, \tag{5.5}$$

where $X_i = 0$ and $\hat{\omega}_i = 0$ for $i \leq 0$.

Figure 11 displays the diagonal exceedance percentage plot of the combined model's residuals when $M = 8$. The plot shows no large exceedance percentages; hence, the combined model has removed the periodic correlation in the data. Figure 12 plots $\hat{g}_0(\lambda)$, the unsmoothed periodogram of the combined model's residuals. This periodogram does not appear to deviate sharply from a white spectrum. Applying the portmanteau test over the first 25 lags to the combined model's residuals produces a test statistic of 22.728. The p-value of this test is .593. Thus, there is statistical evidence that the combined model's residuals are white noise. Hence, the combined model appears to fit the data well.

At this point, a few remarks are in order. First, one can check that $|\hat{\phi}(1)\hat{\phi}(2)\ldots\hat{\phi}(T)| < 1$ for both the full and the four-parameter reduced models. Part (a) of Theorem 2 allows us to infer that the combined fitted PARMA model is PC with period T.

The second remark concerns a drawback of the staged model building procedure. The approximate negative log likelihood in (4.9) was derived under the assumption of an uncorrelated error sequence $\{\epsilon_l\}$. When $\{\epsilon_l\}$ is stationary, the approximation in (4.9) may not be as accurate as in the case where $\{\epsilon_l\}$ is uncorrelated. One can derive an analogous likelihood for (4.9) that includes the covariance structure of $\{\epsilon_l\}$, but the calculation is very cumbersome. Since the model fit diagnostics gave no indication of any inconsistencies, this calculation will not be performed.

6. SUMMARY

A PARMA model was developed for a data set containing 50 years of monthly stratospheric ozone readings. The data set tested positive for periodic correlation with a period of 12 months. A model for the data was built up in two stages: a PAR(1) model was first fit to the mean adjusted data. The number of parameters in the PAR(1) model was reduced by expressing the seasonal parameters as a short Fourier series. The PAR(1) model fit yielded residuals that were stationary, but non-white. Next, a stationary ARMA model was fit to the residuals of the PAR(1) model. Finally, the PAR(1) model and the ARMA model were combined to produce a PARMA model for the data. The combined PARMA model was judged to be adequate from an analysis of its residuals.

APPENDIX

Proof of Theorem 1

Let $\{\vec{Y}_n\}$ be the T dimensional random vector containing the data from the nth year, that is, the νth component of $\vec{Y}_n$ is $X_{nT+\nu}$ for $\nu = 1, 2, \ldots, T$. To prove (a), assume that $|r_T| < 1$, and note that it is sufficient to establish the multivariate stationarity of $\{\vec{Y}_n\}$ (Gladyšhev, 1961). From the governing difference equation of model 4.2, one can show that $\{\vec{Y}_n\}$ follows the T dimensional AR(1) model

$$\vec{Y}_n = \Phi\vec{Y}_{n-1} + \vec{Z}_n, \tag{A.1}$$

where Φ is a TxT matrix whose only nonzero entries are $\Phi_{\nu,T} = r_\nu = \phi(1)\phi(2) \ldots \phi(\nu)$ for $\nu = 1, 2, \ldots, T$ and $\{\vec{Z}_n\}$ is T dimensional mean zero white noise whose covariance matrix Γ has the form

$$\Gamma_{i,j} = \sum_{k=1}^{\min(i,j)} \sigma^2(k)\left(\prod_{l=k+1}^{i}\phi(l)\right)\left(\prod_{l=k+1}^{j}\phi(l)\right) \quad (i,\ j = 1,\ 2,\ \ldots,\ T). \tag{A.2}$$

Recursing (A.1) provides

$$\vec{Y}_n - \sum_{j=0}^{k}\Phi^j\vec{Z}_{n-j} = r_T^k\Phi\vec{Y}_{n-k-1} \qquad \text{for } k \geq 0. \tag{A.3}$$

when the relationship $\Phi^{k+1} = r_T^k\Phi$, $k \geq 0$ is applied. Define the mean squared norm on the T dimensional random vector $\vec{V}$ by $\|\vec{V}\|^2 = \text{trace}\left(\mathbf{E}[\vec{V}\vec{V}']\right)$. Then (A.3) yields

$$\left\|\vec{Y}_n - \sum_{j=0}^{k}\Phi^j\vec{Z}_{n-j}\right\|^2 = r_T^{2k}\ \text{trace}\left(\Phi\mathbf{E}[\ \vec{Y}_{n-k-1}\vec{Y}'_{n-k-1}\ ]\Phi'\right). \tag{A.4}$$

The right hand side of (A.4) goes to zero as $k \to \infty$ because $|r_T| < 1$ and $\{X_n\}$ has bounded second moments. From this, one obtains the causal mean square representation

$$\vec{Y}_n = \sum_{j=0}^{\infty} \Phi^j \vec{Z}_{n-j}. \tag{A.5}$$

From (A.5), one can verify that $\{\vec{Y}_n\}$ is a mean zero T dimensional stationary random sequence with

$$E[\vec{Y}_{n+h}\vec{Y}'_n] = \begin{cases} \sum_{j=0}^{\infty} \Phi^{j+h}\Gamma(\Phi^j)' & \text{for } h \geq 0 \\ \sum_{j=0}^{\infty} \Phi^{j}\Gamma(\Phi^{j-h})' & \text{for } h < 0 \end{cases}. \tag{A.6}$$

This proves (a). Use (A.6) with $h = 0$, $\Phi^{k+1} = r_T^k\Phi$ for $k \geq 0$, and sum a geometric series to obtain

$$E[\vec{Y}_n\vec{Y}'_n] = \Gamma + \frac{1}{1-r_T^2}\Phi\Gamma\Phi'. \tag{A.7}$$

With (A.2), the diagonal of the matrix on the right hand side of (A.7) can be evaluated as

$$Var(X_{nT+\nu}) = \sum_{k=1}^{\nu} \sigma^2(k)\left(\prod_{l=k+1}^{\nu}\phi(l)\right)^2 + \frac{r_\nu^2}{1-r_T^2}\left\{\sum_{k=1}^{T}\sigma^2(k)\left(\prod_{l=k+1}^{T}\phi(l)\right)^2\right\}. \tag{A.8}$$

A product over an empty set of indices is interpreted as unity in (A.8). This proves (b). Recursing (4.2), using the causal relationship in (A.5), and taking expectations produces

$$\gamma_\nu(\tau) = \left(\prod_{i=0}^{\tau-1}\phi(\nu-i)\right)Var(X_{nT+\nu-\tau}) \quad (\tau \geq 0 \quad \text{and} \quad \nu = 1, 2, \ldots, T). \tag{A.9}$$

which proves (c). □

Proof of Theorem 2

Notice that (A.1) and (A.5) still hold, but now $\{\vec{Z}_n\}$ is a stationary T dimensional random sequence with the covariance matrix function $\Gamma(h) = E[\vec{Z}_{n+h}\vec{Z}'_n]$ say. When $|r_T| < 1$, Fubini's Theorem yields

$$\mathsf{E}[\,\vec{Y}_{n+h}\vec{Y}'_n\,] = \sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\Phi^j\Gamma(h-j+k)(\Phi^k)'. \tag{A.10}$$

Hence, $\{\vec{Y}_n\}$ is a T dimensional stationary random sequence and Gladyšhev's result (Gladyšhev, 1961) stipulates that $\{X_l\}$ is PC with period T. This proves (a) and (b) follows from simple algebraic manipulation. □

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Figure 1: The Arosa Data

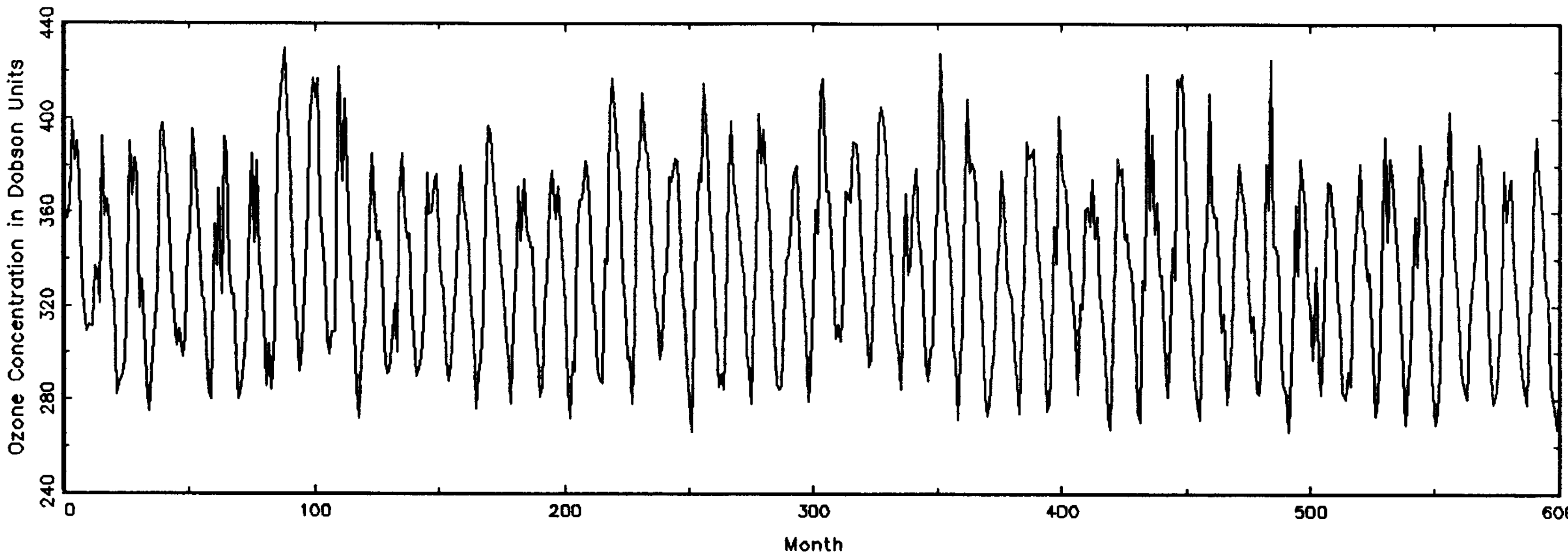


Figure 2a: Monthly Mean of the Data

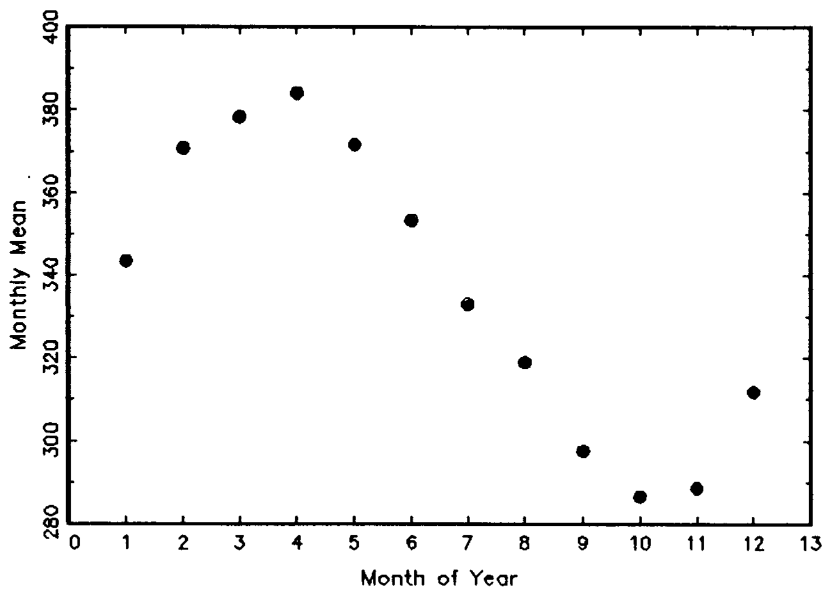


Figure 2b: Monthly Standard Deviation of the Data

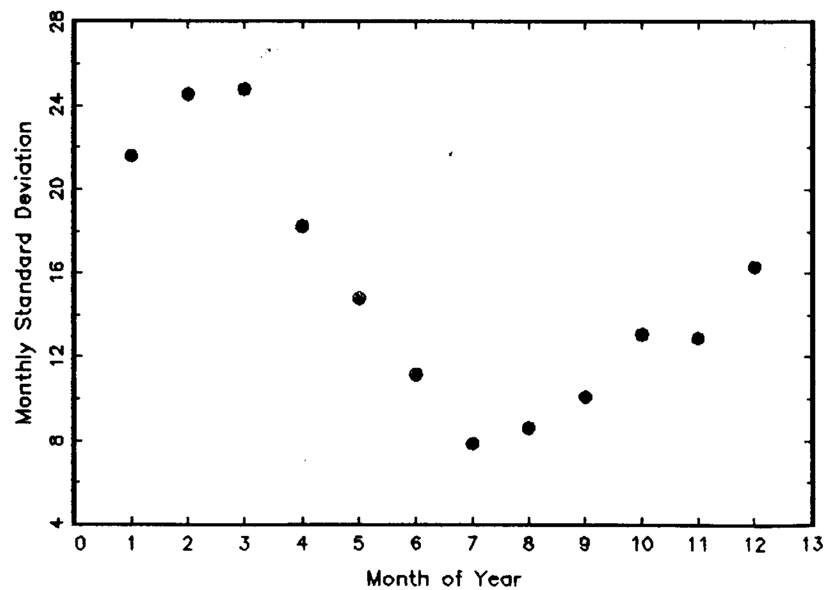


Figure 3: Support Set of a PC Random Sequence

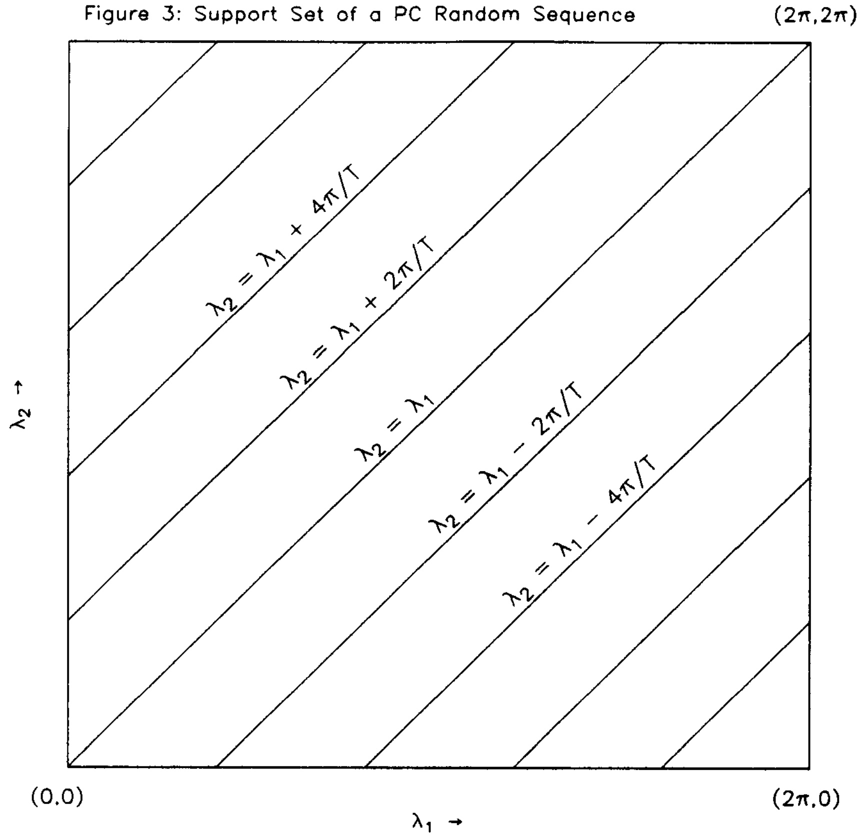
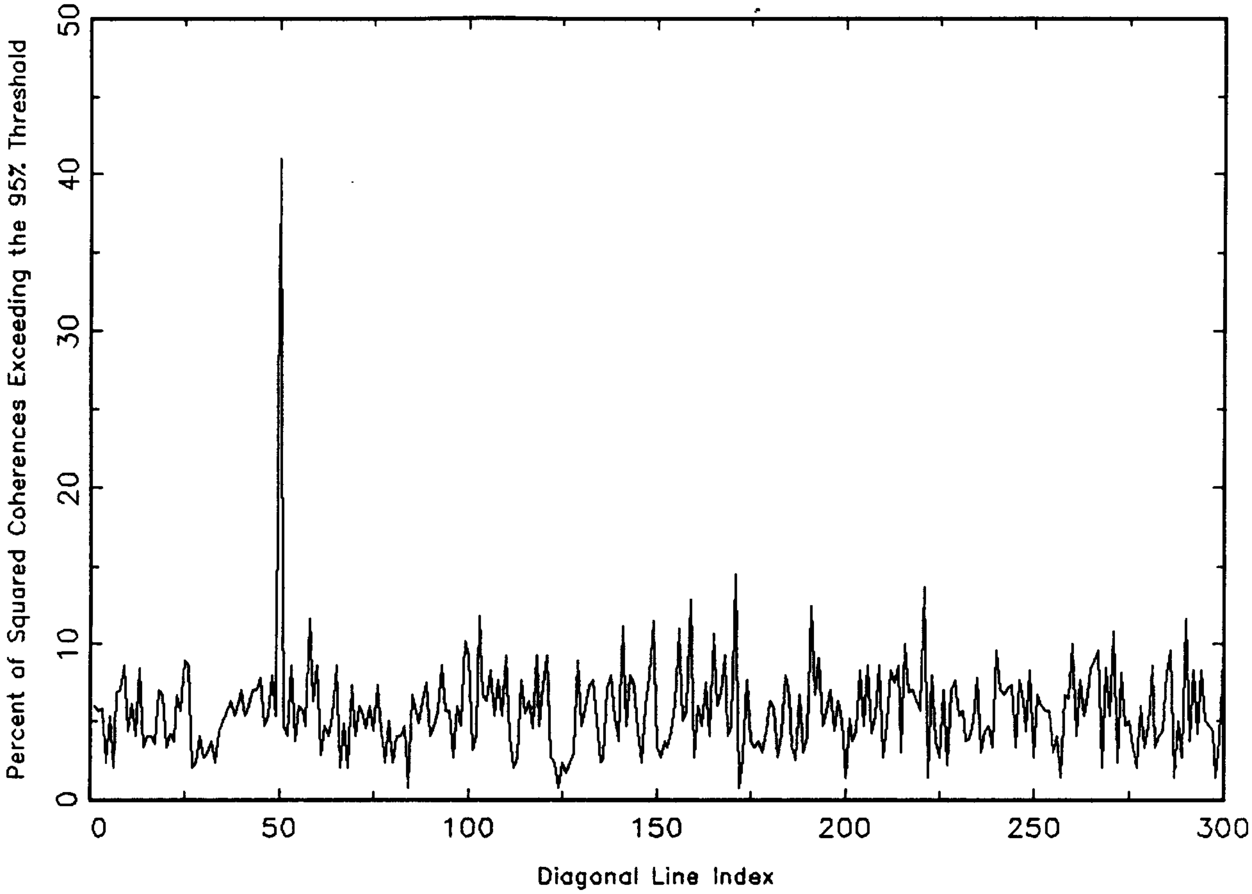


Figure 4: Diagonal Exceedance Percentage Plot of the Arosa Data



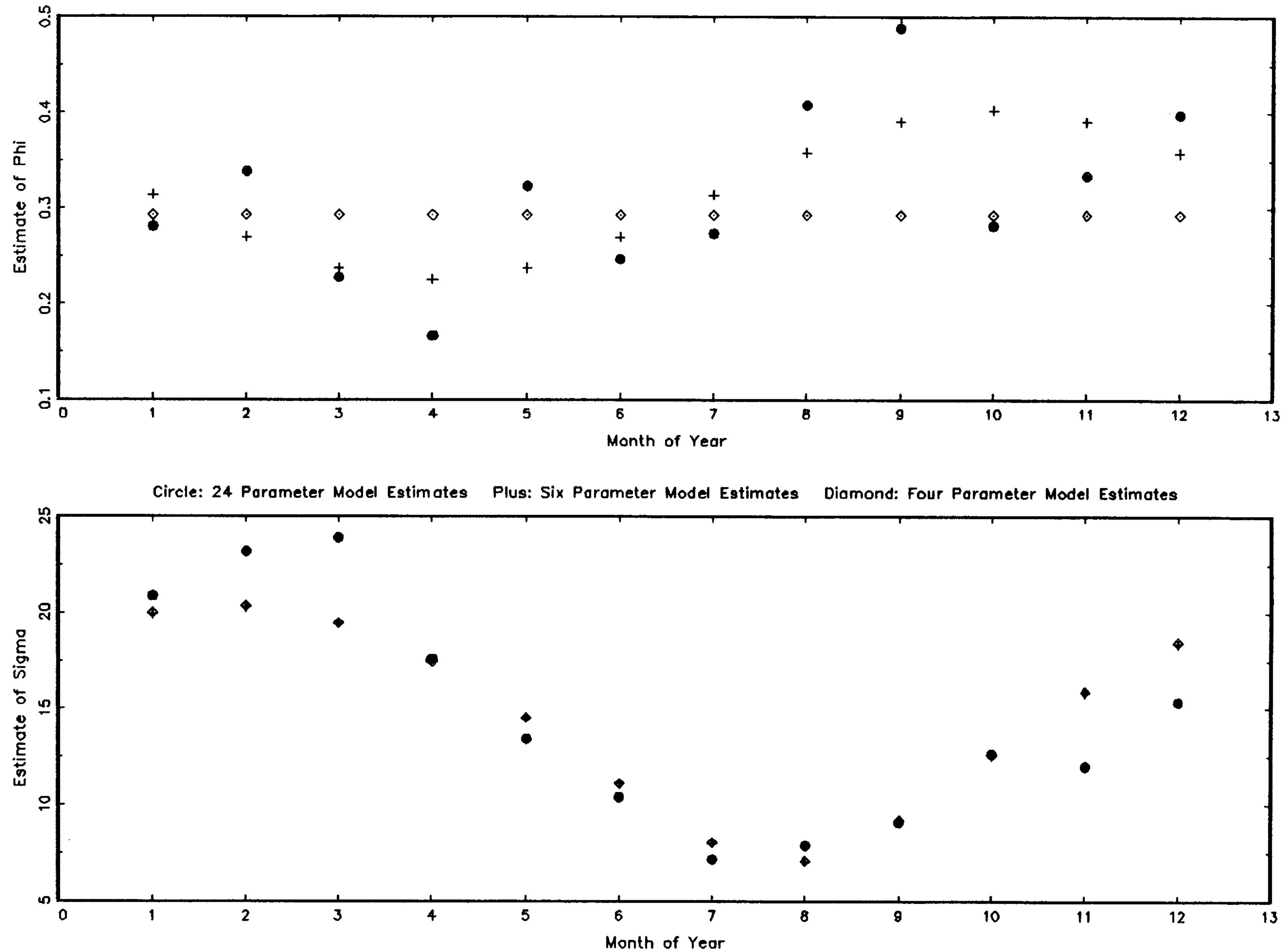


Figure 5: Estimates of Phi and Sigma

Figure 6: Diagonal Exceedance Percentage Plot of the Full Model's Residuals

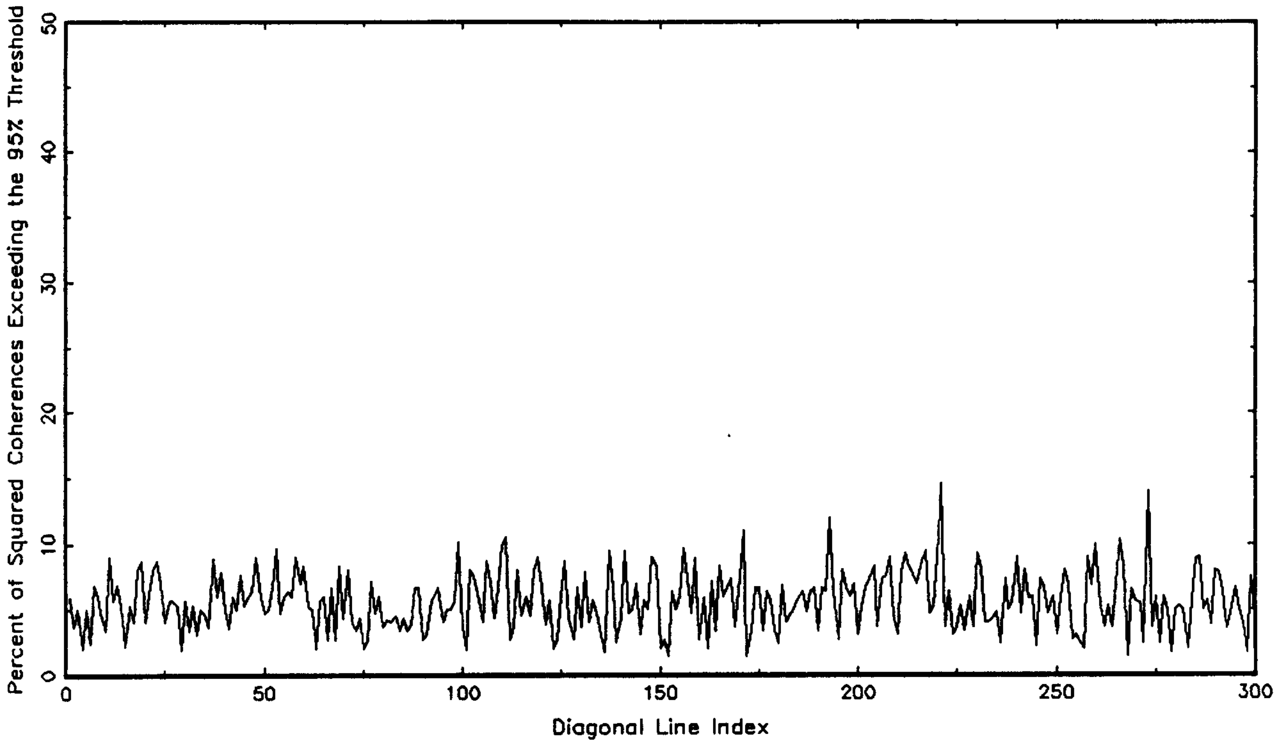


Figure 7: Main Diagonal Periodogram of the Full Model's Residuals

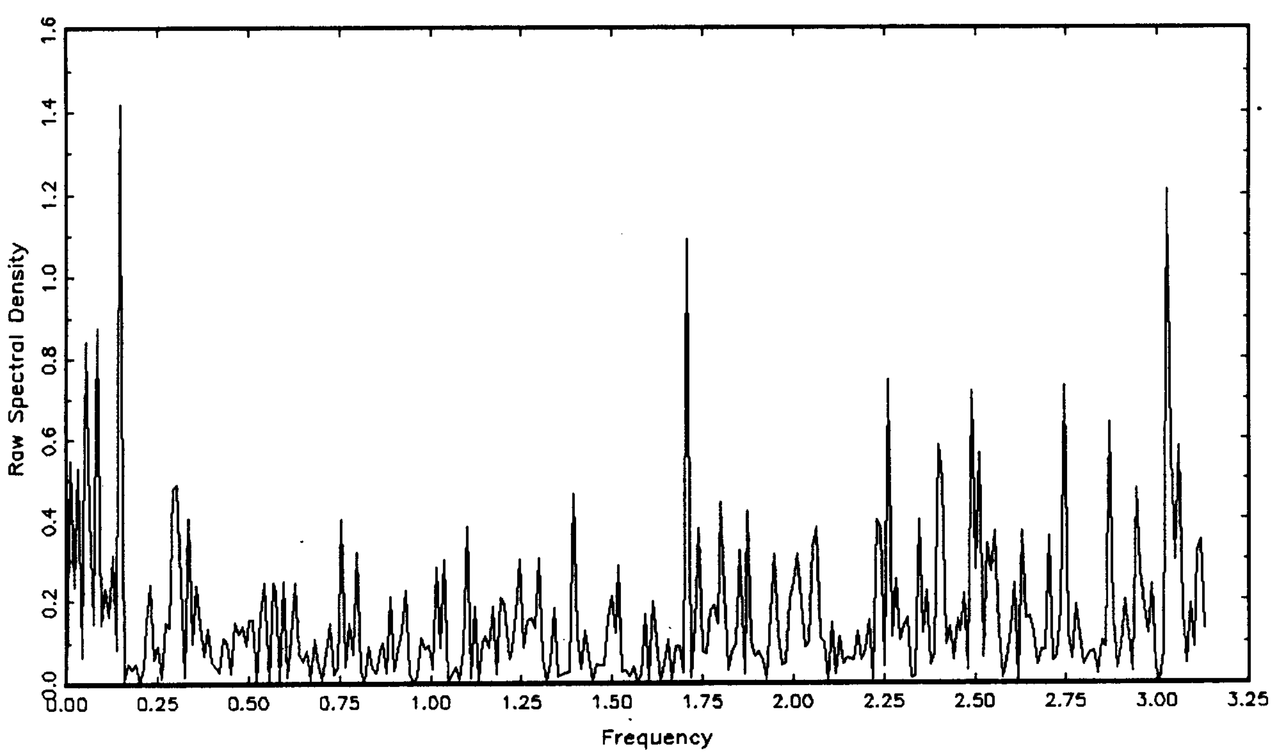


Figure 8: Diagonal Exceedance Percentage Plot of the Four-parameter Reduced Model's Residuals

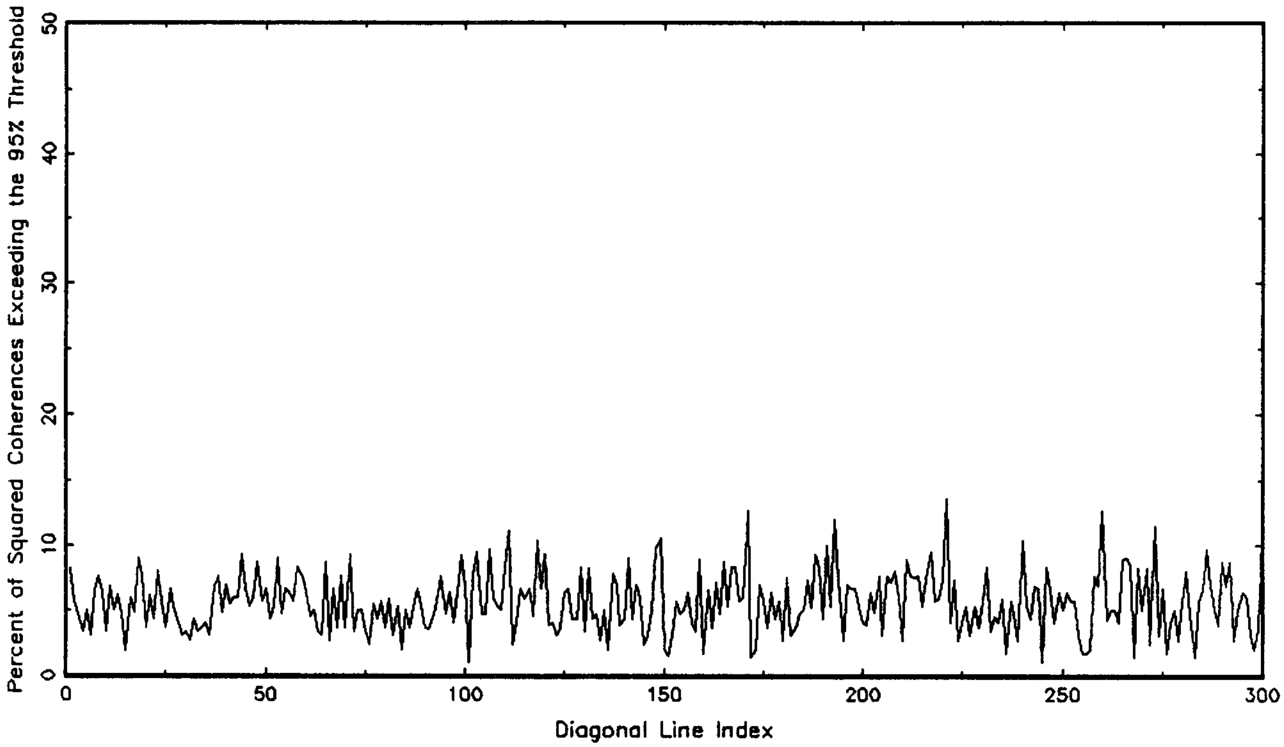


Figure 9: Main Diagonal Periodogram of the Four-parameter Reduced Model's Residuals

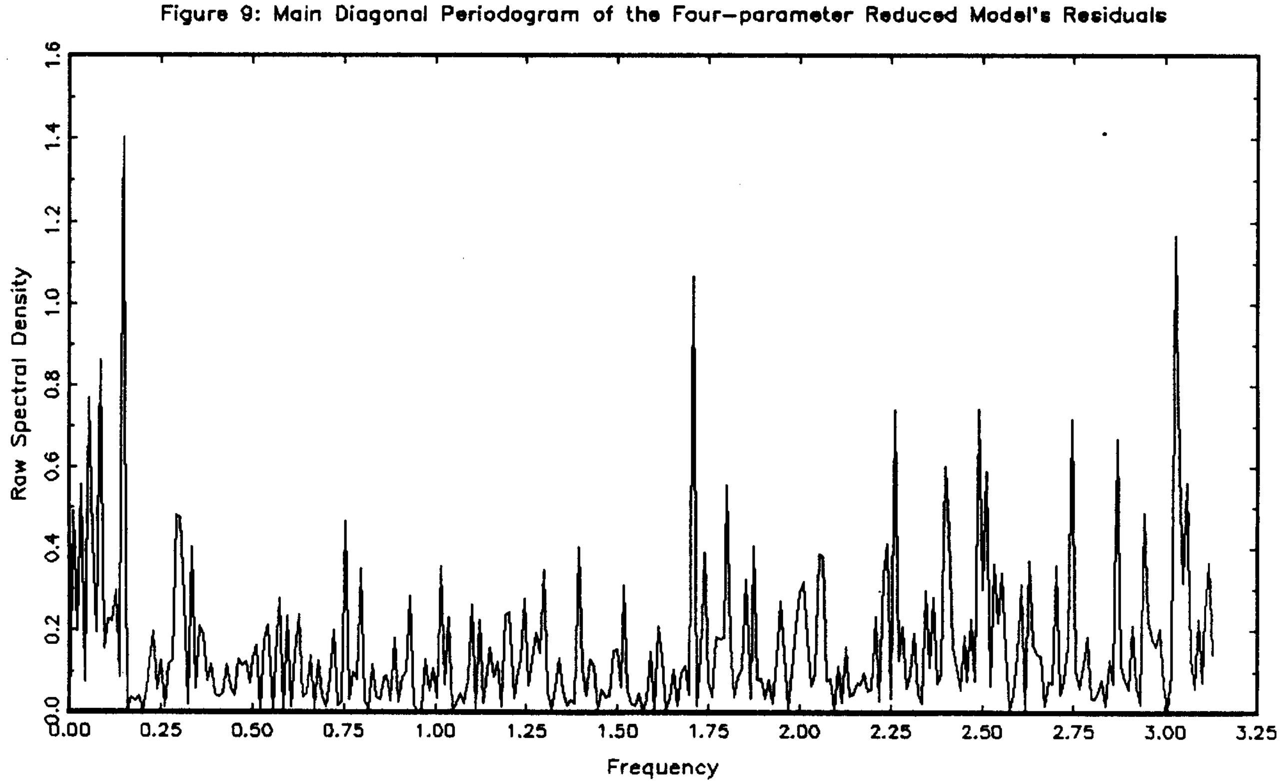


Figure 10: Diagonal Exceedance Percentage Plot of the Combined Model's Residuals

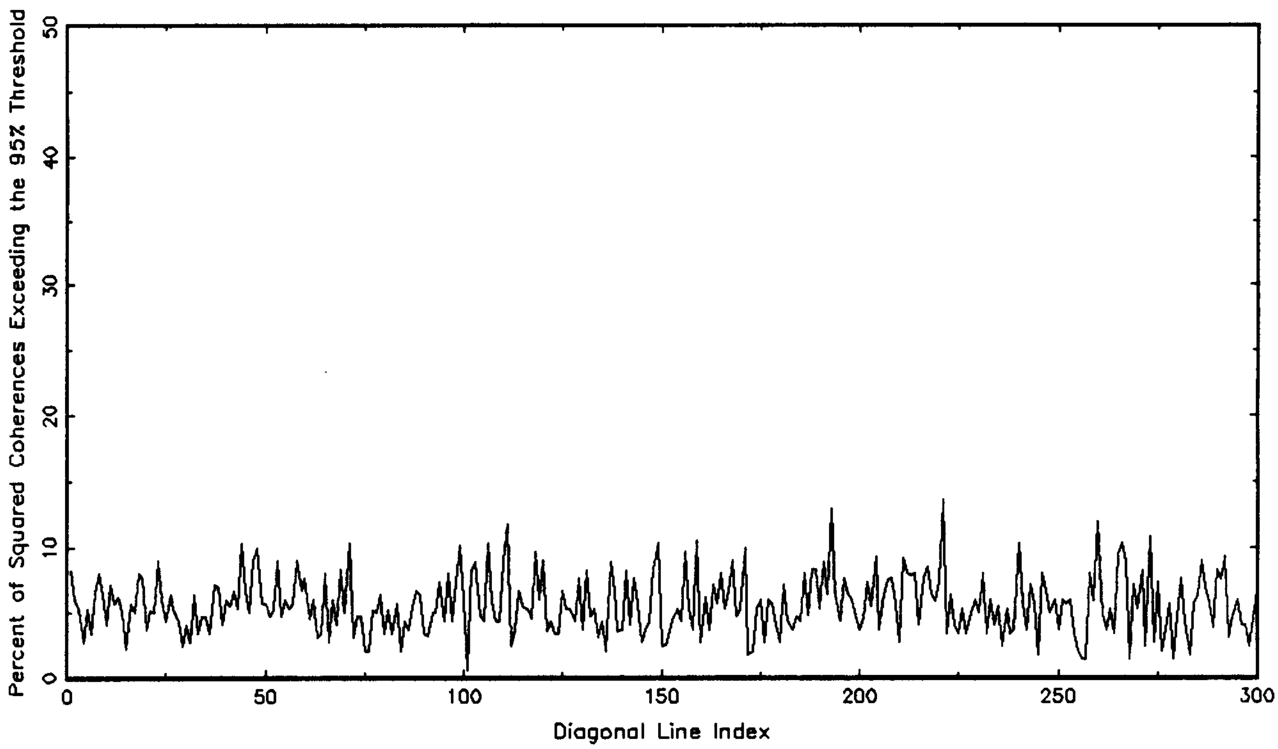
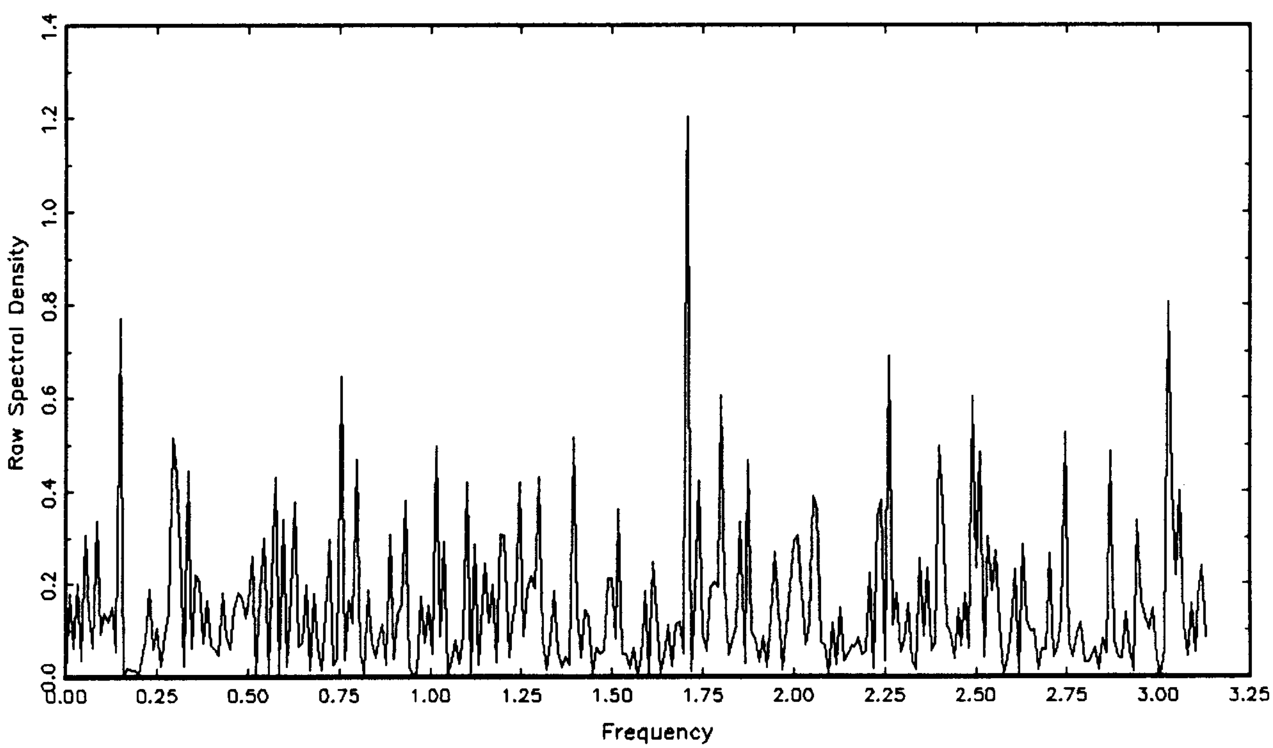


Figure 11: Main Diagonal Periodogram of the Combined Model's Residuals



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