# COMPUTER ALGEBRA DERIVATION OF THE BIAS OF LINEAR ESTIMATORS OF AUTOREGRESSIVE MODELS

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Abstract. A symbolic method is discussed which can be used to obtain the asymptotic bias and variance coefficients to order O(1/n) for estimators in stationary time series. Using this method the large sample bias of the Burg estimator in the AR (p) for p=1,2,3 is shown to be equal to that of the least squares estimators in both the known and unknown mean cases. Previous researchers have only been able to obtain simulation results for the Burg estimator's bias because this problem is too intractable without using computer algebra. The asymptotic bias coefficient to O(1/n) of Yule-Walker as well as least squares estimates is also derived in AR(3) models. Our asymptotic results show that for the AR (3), just as in the AR (2), the Yule-Walker estimates have a large bias when the parameters are near the non-stationary boundary. The least squares and Burg are much better in this situation. Simulation results confirm our findings.

**Keywords.** Asymptotic bias and variance; autoregression; autoregressive spectral analysis; symbolic computation.

# 1. INTRODUCTION AND SUMMARY

Tjøstheim and Paulsen (1983, Correction 1984) showed that the Yule-Walker estimates had very large mean-square errors in strongly autocorrelated AR(2) models and that this inflated mean square error was due to bias. This result was demonstrated by Tjøstheim and Paulsen (1983) in simulation experiments as well as by deriving the theoretical bias to order O(1/n). It was also mentioned by Tjøstheim and Paulsen (1983,

p.397, §5) that the bias results from simulation experiments for the Burg estimates were similar to those obtained for least squares estimates but that they had not been able to obtain the theoretical bias term. For the AR (p) with p=1,2,3 we are now able to symbolically compute the theoretical bias for Burg estimates as well as the least squares and Yule-Walker estimates. It is found that the order  $n^{-1}$  bias coefficient of the Burg estimator is equal to that of the least squares estimator while the Yule-Walker estimator has the largest bias. For strongly autocorrelated AR(p) models with p>2, Tjøstheim and Paulsen (1983, p.393, §3) suggested that the bias for the Yule-Walk estimator is at least as bad as that for the AR(2) case. The theoretical large sample bias obtained using our computer algebra methods confirms that this is the case.

As pointed out by Lysne and Tjøstheim (1987), the Burg estimators have an important advantage over the least squares estimates for autoregressive spectral estimation since Burg estimates always lie in the admissible parameter space whereas the least squares estimates do not. Burg estimators are now frequently used in autoregressive spectral estimation (Percival and Walden, 1993, §9.5) since they provide better resolution of sharp spectral peaks. As the Yule-Walker estimators, the Burg estimators may be efficiently computed using the Durbin-Levinson recursion. Our result provides further justification for the recommendation to use the Burg estimator for autoregressive spectral density estimation as well as for other autoregressive estimation applications.

It has been shown that symbolic algebra could greatly simplify derivations of asymptotic expansions in the IID case (Andrews and Stafford, 1993). Symbolic computation is a powerful tool for handling complicated algebraic problems that arise with expansions of various types of statistics and estimators (Andrews and Stafford, 2000) as well as for exact maximum likelihood computation (Currie, 1995; Rose and Smith, 2000). Cook and Broemeling (1995) show how symbolic computation can be used in Bayesian time series analysis. Smith and Field (2001) described a symbolic operator which calculates the joint cumulants of the linear combinations of products of discrete Fourier transforms. A symbolic computational approach to mathematical statistics is discussed by Rose and Smith (2002). In the following sections, through deriving the order  $n^{-1}$  bias coefficient of the Burg estimator in AR(2) models, we develop a symbolic computation method that can be used to solve a wide variety of problems involving linear time series estimators for stationary time series. Using our symbolic method, we also perform an asymptotic bias comparison of the Burg, least squares and Yule Walker estimators in AR(3) models.

# 2. ASYMPTOTIC EXPECTATIONS AND COVARIANCES

Consider n consecutive observations from a stationary time series,  $z_t, t = 1, ..., n$ , with mean  $\mu = E(z_t)$  and autocovariance function  $\gamma_k = \text{Cov}(z_t, z_{t-k})$ . If the mean is known, it may, without loss of generality be taken to be zero. Then one of the unbiased estimators of autocovariance  $\gamma(m-k)$  may be written as

$$S_{m,k,i} = \frac{1}{n+1-i} \sum_{t=i}^{n} z_{t-m} z_{t-k}, \tag{1}$$

where m, k and i are non-negative integers with  $\max(m, k) < i \le n$ . If the mean is unknown, a biased estimator of  $\gamma(m-k)$  may be written as

$$\overline{S}_{m,k,i} = \frac{1}{n} \sum_{t=i}^{n} (z_{t-m} - \overline{z}_n)(z_{t-k} - \overline{z}_n), \tag{2}$$

where  $\overline{z}_n$  is the sample mean.

THEOREM 1. Let the time series  $z_t$  be the two-sided moving average,

$$z_t = \sum_{j=-\infty}^{\infty} \alpha_j e_{t-j},\tag{3}$$

where the sequence  $\{\alpha_j\}$  is absolutely summable and the  $e_t$  are independent  $N(0, \sigma^2)$  random variables. Then for  $i \leq j$ ,

$$\lim_{n \to \infty} n \operatorname{Cov} \left( \mathcal{S}_{m,k,i}, \mathcal{S}_{f,g,j} \right) = \sum_{h = -\infty}^{\infty} T_h, \tag{4}$$

where

$$T_h = \gamma(g-k+i-j+h)\gamma(f-m+i-j+h) + \gamma(f-k+i-j+h)\gamma(g-m+i-j+h).$$

THEOREM 2. Let a time series  $\{z_t\}$  satisfy the assumptions of Theorem 1. Then

$$\lim_{n \to \infty} n \, \mathrm{E}\left(\overline{\mathcal{S}}_{m,k,i} - \gamma(m-k)\right) = -|i-1|\gamma(m-k) - \sum_{k=-\infty}^{\infty} \gamma(k)$$
 (5)

and

$$\lim_{n \to \infty} n \operatorname{Cov}(\overline{\mathcal{S}}_{m,k,i}, \overline{\mathcal{S}}_{f,g,j}) = \sum_{h=-\infty}^{\infty} T_h,$$
(6)

where

$$T_h = \gamma(g-k+i-j+h)\gamma(f-m+i-j+h) + \gamma(f-k+i-j+h)\gamma(g-m+i-j+h).$$

These two theorems may be considered as the extensions of Theorem 6.2.1 and Theorem 6.2.2 of Fuller (1996). Letting p = m - k and q = f - g,

the left side of (4) or (6) can be simplified,

$$\sum_{h=-\infty}^{\infty} T_h = \sum_{h=-\infty}^{\infty} \gamma(h)\gamma(h-p+q) + \gamma(h+q)\gamma(h-p). \tag{7}$$

There is a wide variety of estimators which can be written as a function of the autocovariance estimators,  $S_{m,k,i}$  or  $\overline{S}_{m,k,i}$ , such as, autocorrelation estimator, least squares estimator, Yule-Walker estimator, Burg estimator, etc. The asymptotic bias and variance may be obtained by the Taylor expansion. Unfortunately, in the most cases, those expansions include a large number of expectations and covariances of the autocovariance estimators. It is too intractable manually. Theorems 1 and 2 provide the basis for a general approach to the symbolic computation of the asymptotic bias and variance to order O(1/n) for those estimators. The definition of (1) or (2) allows an index set  $\{m, k, i\}$  to represent an estimator so that Theorem 1 or 2 can be easily implemented symbolically.

### 3. BIAS OF BURG ESTIMATORS IN AR(2)

The stationary second-order autoregressive model may be written as  $z_t = \phi_1 z_{t-1} + \phi_2 z_{t-2} + a_t$ , where  $a_t$  are normal and independently distributed with mean zero and variance  $\sigma^2$  and parameters  $\phi_1$  and  $\phi_2$  are in the admissible region,  $|\phi_2| < 1$ ,  $\phi_1 + \phi_2 < 1$  and  $\phi_2 - \phi_1 < 1$ . The Burg estimate for  $\phi_2$  may be obtained directly from Percival and Walden (1993, eqn. 416d) and then the estimate for  $\phi_1$  may be obtained using the Durbin-Levinson algorithm. After simplification, these estimates may be written as

$$\hat{\phi}_2 = 1 - \frac{CD^2 - 2ED^2}{CD^2 + 8F^2G - 4FHD}, \hat{\phi}_1 = \frac{2F}{D}(1 - \hat{\phi}_2)$$
 (8)

where

$$C = \frac{1}{n-2} \sum_{t=3}^{n} (z_t^2 + z_{t-2}^2), D = \frac{1}{n-1} \sum_{t=2}^{n} (z_t^2 + z_{t-1}^2), E = \frac{1}{n-2} \sum_{t=3}^{n} (z_t^2 z_{t-2}^2),$$

$$F = \frac{1}{n-1} \sum_{t=2}^{n} (z_t z_{t-1}), G = \frac{1}{n-2} \sum_{t=3}^{n} z_{t-1}^2, H = \frac{1}{n-2} \sum_{t=3}^{n} (z_t z_{t-1} + z_{t-2} z_{t-1}).$$

Using a Taylor series expansion of  $\hat{\phi}_1$  and  $\hat{\phi}_2$  about  $\mu_{\mathcal{A}} = E(\mathcal{A})$ , where  $\mathcal{A} = C, D, E, F, G$  and H, the order  $n^{-1}$  bias coefficient,  $\lim_{n\to\infty} n \ E(\hat{\phi}-\phi)$ , may be expressed in terms of the order  $n^{-1}$  expectation coefficients of products and cross products involving C, D, E, F, G and H. There are six squared terms and fifteen cross product terms involved in each expansion, that is, it is required to compute and simplify for each of these twenty one expansions involving C, D, E, F, G and H. These terms may all be written in terms of the unbiased estimate of the autocovariance,  $\mathcal{S}_{m,k,i}$ . The required asymptotic expectation coefficients of each term in the expansions are obtained by Theorem 1, that is,

$$\lim_{n \to \infty} n \operatorname{Cov} \left( \mathcal{S}_{m,k,i}, \mathcal{S}_{f,g,j} \right) = \sum_{h = -\infty}^{\infty} T_h, \tag{9}$$

where  $T_h = \gamma(h)\gamma(h-p+q) + \gamma(h+q)\gamma(h-p), p = m-k, q = f-g$  and

$$\gamma(h) = \frac{\zeta_2^{1+h} - \zeta_1^2 \zeta_2^{1+h} + \zeta_1^{1+h} \left(\zeta_2^2 - 1\right)}{\left(\zeta_1^2 - 1\right) \left(\zeta_1 - \zeta_2\right) \left(\zeta_1 \zeta_2 - 1\right) \left(\zeta_2^2 - 1\right)},\tag{10}$$

where  $h \geq 0$ ,  $\zeta_1$  and  $\zeta_2$  are the roots, assumed distinct, of the polynomial  $\zeta^2 - \phi_1 \zeta - \phi_2 = 0$ . The order  $n^{-1}$  coefficient of the covariance expansion of  $\mathcal{S}_{m,k,i}$  and  $\mathcal{S}_{f,g,j}$  given in eqn. (9) may be evaluated symbolically by defining an operator of  $\mathcal{S}_{m,k,i}$  and  $\mathcal{S}_{f,g,j}$ , LCOV  $[\{m,k,i\}\{f,g,j\}]$ . To illustrate this symbolic method consider the evaluation of  $\lim_{n\to\infty} n$  Cov (2C, H) which is

one of the twenty one order  $n^{-1}$  expansion coefficients involving C, D, E, F, G and H mentioned above. It may be obtained by

$$\lim_{n \to \infty} n \operatorname{Cov} (2C, H) = 2\{ \operatorname{LCOV} [(\{0, 0, 3\} + \{2, 2, 3\})(\{0, 1, 3\} + \{2, 1, 3\})] \}$$

$$= 2\{ \operatorname{LCOV} [\{0, 0, 3\} \{0, 1, 3\}] + \operatorname{LCOV} [\{0, 0, 3\} \{2, 1, 3\}] \}$$

$$+ \operatorname{LCOV} [\{2, 2, 3\} \{0, 1, 3\}] + \operatorname{LCOV} [\{2, 2, 3\} \{2, 1, 3\}] \},$$

since  $C = \mathcal{S}_{0,0,3} + \mathcal{S}_{2,2,3}$ ,  $H = \mathcal{S}_{0,1,3} + \mathcal{S}_{2,1,3}$ , and LCOV [·] follows the linearity and the distributive law.

After algebraic simplification the order  $n^{-1}$  bias coefficients are found to be

$$\lim_{n \to \infty} n \to (\hat{\phi}_1 - \phi_1) = -(\zeta_1 + \zeta_2)$$

and

$$\lim_{n \to \infty} n \, \mathrm{E} \left( \hat{\phi}_2 - \phi_2 \right) = (3\zeta_1 \zeta_2 - 1)$$

More simply, in terms of the original parameters we have the large sample biases,

$$E\left(\hat{\phi}_1 - \phi_1\right) \doteq -\phi_1/n \tag{11}$$

and

$$E(\hat{\phi}_2 - \phi_2) \doteq -(1 + 3\phi_2)/n.$$
 (12)

We verified, using the same approach, that eqns. (11) and (12) also hold for the case of equal roots of the polynomial  $\zeta^2 - \phi_1 \zeta - \phi_2 = 0$ .

For the stationary second-order autoregressive model with an unknown mean, the Burg estimators can be written as the same ratio function of the biased estimators of the autocovariances,  $\overline{\mathcal{S}}_{m,k,i}$ , as was given in eqn. (8). The symbolic approach is similar to the known mean case, but includes one

more inner product associated with the biases of those autocovariance estimators,  $\overline{S}_{m,k,i}$ . The required asymptotic biases and covariances of  $\overline{S}_{m,k,i}$  are obtained by Theorem 2. The order  $n^{-1}$  bias coefficients are found to be

$$\lim_{n \to \infty} n \, \mathrm{E} \left( \hat{\phi}_1 - \phi_1 \right) = (\zeta_1 \zeta_2 - \zeta_1 - \zeta_2) - 1$$

and

$$\lim_{n \to \infty} n \, \mathrm{E} \left( \hat{\phi}_2 - \phi_2 \right) = (4\zeta_1 \zeta_2 - 2)$$

That is

$$E(\hat{\phi}_1 - \phi_1) \doteq -(\phi_2 + \phi_1 + 1)/n \tag{13}$$

and

$$E(\hat{\phi}_2 - \phi_2) \doteq -(2 + 4\phi_2)/n.$$
 (14)

Once an estimator of a stationary time series is written as a well defined function composed of  $S_{m,k,i}$  or  $\overline{S}_{m,k,i}$ , by expanding it by a Taylor series, the asymptotic bias and variance to order  $n^{-1}$  may be obtained by Theorem 1 or 2 with symbolic computation. This approach can be applied in the bias derivation of the Burg estimator,  $\hat{\rho}$ , in the first order autoregressive model, AR(1). In this case, our method produced  $-2\rho/n$  in the zero mean case and  $-(1+3\rho)/n$  in an unknown mean case for the large sample bias. Therefore, for both of AR(1) and AR(2) cases, the large sample biases of the Burg estimators are the same as the least squares estimators for a known mean case as well as for an unknown mean case. These results are consistent with the simulation study reported by Tjøstheim and Paulsen (1983).

# 4. BIAS OF BURG AND OTHER COMMONLY USED LINEAR ESTIMATORS IN AR(3)

For the generality, we discuss the unknown mean case. The stationary third-order autoregressive model may be written as  $z_t - \mu = \phi_1(z_{t-1} - \mu) + \phi_2(z_{t-2} - \mu) + \phi_3(z_{t-3} - \mu) + a_t$ , where  $a_t$  are normal and independently distributed with mean  $\mu$  and variance  $\sigma^2$  and parameters  $\phi_1$ ,  $\phi_2$  and  $\phi_2$  are in the admissible region,  $|\phi_3| < 1$ ,  $\phi_1 + \phi_2 + \phi_3 < 1$ ,  $-\phi_1 + \phi_2 - \phi_3 < 1$  and  $\phi_3(\phi_3 - \phi_1) - \phi_2 < 1$ . The Burg estimates for  $\phi_i$ , i = 1, 2, 3 may be obtained from Percival and Walden (1993, eqn. 416d). The explicit forms for the Burg estimates are much more complicated in AR(3) models than in AR(2) models. For example, the Burg estimate  $\hat{\phi}_3$  for the unknown mean case may be written as

$$\hat{\phi}_3 = \frac{N}{D},\tag{15}$$

where

$$N = 2(\overline{S}_{3,0,4} - \phi_{12}(\overline{S}_{2,0,4} + \overline{S}_{3,1,4} - \overline{S}_{2,1,4}\phi_{12})$$
$$-(\overline{S}_{1,0,4} + \overline{S}_{3,2,4} - (\overline{S}_{1,1,4} + \overline{S}_{2,2,4})\phi_{12})\phi_{22} + \overline{S}_{2,1,4}\phi_{22}^{2})$$

and

$$D = \overline{S}_{0,0,4} + \overline{S}_{3,3,4} + \phi_{12}(-2(\overline{S}_{1,0,4} + \overline{S}_{3,2,4}) + (\overline{S}_{1,1,4} + \overline{S}_{2,2,4})\phi_{12})$$
$$-2(\overline{S}_{2,0,4} + \overline{S}_{3,1,4} - 2\overline{S}_{2,1,4}\phi_{12})\phi_{22} + (\overline{S}_{1,1,4} + \overline{S}_{2,2,4})\phi_{22}^{2}.$$

Using eqn. (8),  $\phi_{12}$  and  $\phi_{22}$  may be written as,

$$\phi_{22} = 1 - \frac{\overline{S}_{0,0,3} - 2\overline{S}_{2,0,3} + \overline{S}_{2,2,3}}{\overline{S}_{0,0,3} + \overline{S}_{2,2,3} - 2\phi_{11}(\overline{S}_{1,0,3} + \overline{S}_{2,1,3} - \overline{S}_{1,1,3}\phi_{11})},$$

$$\phi_{12} = \frac{(\overline{S}_{0,0,3} - 2\overline{S}_{2,0,3} + \overline{S}_{2,2,3})\phi_{11}}{\overline{S}_{0,0,3} + \overline{S}_{2,2,3} - 2\phi_{11}(\overline{S}_{1,0,3} + \overline{S}_{2,1,3} - \overline{S}_{1,1,3}\phi_{11})}$$

where

$$\phi_{11} = \frac{2\overline{\mathcal{S}}_{1,0,2}}{\overline{\mathcal{S}}_{0,0,2} + \overline{\mathcal{S}}_{1,1,2}}.$$

After the simplification,  $\hat{\phi}_3$  includes 856 indivisible subexpressions in terms of  $\overline{\mathcal{S}}_{m,k,i}$ . The order  $n^{-1}$  bias coefficient may be obtained by Theorem 2 through defining

$$\gamma(h) = A_1 \zeta_1^h + A_2 \zeta_2^h + A_3 \zeta_3^h \tag{16}$$

where

$$A_{1} = -\frac{\zeta_{1}^{2}}{(\zeta_{1}^{2} - 1)(\zeta_{1} - \zeta_{2})(\zeta_{1}\zeta_{2} - 1)(\zeta_{1} - \zeta_{3})(\zeta_{1}\zeta_{3} - 1)}$$

$$A_{2} = \frac{\zeta_{2}}{(\zeta_{1} - \zeta_{2})(\zeta_{1}\zeta_{2} - 1)(\zeta_{2}^{2} - 1)(\zeta_{2} - \zeta_{3})(\zeta_{2}\zeta_{3} - 1)}$$

$$A_{3} = -\frac{\zeta_{3}^{2}}{(\zeta_{1} - \zeta_{3})(\zeta_{2} - \zeta_{3})(\zeta_{1}\zeta_{3} - 1)(\zeta_{2}\zeta_{3} - 1)(\zeta_{3}^{2} - 1)},$$

and  $h \geq 0$ ,  $\zeta_1$ ,  $\zeta_2$  and  $\zeta_3$  are the roots, assumed distinct, of the polynomial  $\zeta^3 - \phi_1 \zeta^2 - \phi_2 \zeta - \phi_3 = 0$ . It has turned out that the order  $n^{-1}$  bias coefficient of the Burg estimate  $\hat{\phi}_3$ ,  $\lim_{n \to \infty} n \to (\hat{\phi}_3 - \phi_3)$ , includes 1,745,350 indivisible subexpressions in terms of  $\zeta_1$ ,  $\zeta_2$  and  $\zeta_3$ . Using a similar method for  $\phi_3$ , the order  $n^{-1}$  bias coefficient of the least squares or Yule-Walker estimate,  $\lim_{n \to \infty} n \to (\phi_3^* - \phi_3)$  or  $\lim_{n \to \infty} n \to (\phi_3^* - \phi_3)$ , includes 95,457 or 77,649 indivisible subexpressions in terms of  $\zeta_1$ ,  $\zeta_2$ ,  $\zeta_3$  respectively. It is not practical to work with such formulae except by using symbolic algebra software. These formulae were evaluated numerically for selected parameter values and the results are given in Table I. The parameters in the AR (3) models were chosen using the partial autocorrelations,  $\phi_{k,k}$ , k=1,2,3 taking  $\phi_{1,1}=\phi_{2,2}=\phi_{3,3}$ .

# [Table 1 about here]

For all three autoregressive coefficients  $\phi_1$ ,  $\phi_2$  and  $\phi_3$ , results from Table I show that the large sample bias of Burg estimates is equal to that of least squares estimates while Yule-Walker's is considerably worse when the partial autocorrelation  $\phi_{3,3}$  is relatively strong; overall, the biases are getting larger when the partial autocorrelation  $\phi_{3,3}$  is becoming stronger. Simulation results confirmed the findings in Table I although for larger partial autocorrelation values the difference between theoretical and simulated results is fairly large. Tjøstheim and Paulsen (1983, p.394, §3) observed the same phenomena in deriving the theoretical bias of Yule-Walker estimates in case of AR(2) models.

#### 5. CONCLUDING REMARKS

We used our computer algebra method to verify the bias results reported by Tjøstheim & Paulsen (Correction, 1984). Since many quadratic statistics in a stationary time series can be expressed in terms of  $S_{m,k,i}$  or  $\overline{S}_{m,k,i}$ , our computer algebra approach can be applied to derive their laborious moment expansions to order O(1/n). As examples, using our method, we can easily obtain the results by Bartlett (1946), Kendall (1954), Marriott and Pope (1954), White (1961) and Tjøstheim and Paulsen (1983).

Mathematica (Wolfram, 2003) notebooks with the complete details of our derivations and simulations are available from the authors.

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Table I. Bias to order O(1/n) for Burg  $\hat{\phi}$ , least squares  $\phi^*$  and Yule-Walker  $\phi^+$  estimates of the autoregressive coefficients  $\phi_1, \phi_2$  and  $\phi_3$  in AR(3) models. The order  $n^{-1}$  bias of an estimate  $\hat{\phi}$  of  $\phi$  is defined as  $\lim_{n\to\infty} n \to \mathbb{E}(\hat{\phi}-\phi)$ . In these models we set the partial autocorrelations,  $\phi_{k,k}, k=1,2,3$ , to be all equal,  $\phi_{1,1}=\phi_{2,2}=\phi_{3,3}$ . Only one numerical entry is shown for the Burg and least squares estimates since the biases to order O(1/n) are numerically identical.

$\phi_{3,3}$	$\hat{\phi_1}, \phi_1^*$	$\phi_1^+$	$\hat{\phi_2}, \phi_2^*$	$\phi_2^+$	$\hat{\phi_3}, \phi_3^*$	$\phi_3^+$
0.05	-1.145	-1.1749	-2.1955	-2.2865	-1.25	-1.401
0.25	-1.625	-1.3233	-2.9375	-3.2904	-2.25	-3.14
0.45	-1.945	-0.0796	-3.7595	-4.40173	-3.25	-5.6882
0.65	-2.105	5.69106	-4.8535	-6.12379	-4.25	-12.0918
0.75	-2.125	15.8827	-5.5625	-7.51594	-4.75	-22.1531
0.85	-2.105	54.7841	-6.4115	-9.86504	-5.25	-60.0761
0.90	-2.08	133.266	-6.896	-12.124	-5.5	-137.037
0.95	-2.045	568.435	-7.4245	-17.7786	-5.75	-567.331