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ON A MEASURE OF LACK OF FIT IN TIME SERIES MODELS

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The overall test for lack of fit in autoregressive-moving average models proposed by Box and Pierce (1970) is considered. It is shown that a substantially improved approximation results from a simple modification of this test. Some consideration is given to the power of such tests and their robustness when the innovations are non-normal. Similar modifications in the overall tests used for transfer function-noise models are proposed.
Very many physical situations are described by a series of numbers occurring sequentially in time, the observed numbers arising from a deterministic underlying smoothly varying sequence perturbed by random errors. Typical examples are observations of the position of a vehicle or missile at successive intervals in time, and many other examples occur in connection with engineering production and business management.

Such time-series are normally analyzed, after allowing for the deterministic part, by assuming some underlying model for the process involved, the relevant model in the present work being an autoregressive moving average model described in the first paragraph of the paper. This is the model on which the Box-Jenkins technique is based.

If the parameters in a model are estimated from an experimental time-series, the next question is the adequacy of fit of the data by the model. In this connection it is useful to study the residuals and their autocorrelations $r_k$.

Box and Pierce (1970) propose an overall test for lack of fit based on approximating the distribution of $Q(\hat{r}) = n \sum_{k=1}^{m} r_k^2$ by the $\chi^2_{m-p-q}$ distribution where $n$ is the number of observations in the time series, $m$ is the number of lags, and $p + q$ is the number of parameters in the model. Recent studies have shown that this approximation is not adequate unless $n$ is large relative to $m$.

The present paper illustrates that the use of the modified test statistic $\hat{Q}(\hat{r}) = n(n+2) \sum_{k=1}^{m} (n-k)^{-1} r_k^2$ leads to a substantially improved approximation.

The power of the overall test and its robustness to non-normality of the innovations (i.e. random perturbations on the data) in the model are discussed briefly.

Some consideration is also given to testing for lack of fit in transfer function-noise models, where one has two time series, variations in one series being related to variations in the other.
ON A MEASURE OF LACK OF FIT IN TIME SERIES MODELS

G. M. Ljung and G. E. P. Box

1. INTRODUCTION

Consider a discrete time series \( \{w_t\} \) generated by a stationary autoregressive moving average model

\[
\phi(B)w_t = \theta(B)a_t
\]

(1.1)

where \( \phi(B) = 1 - \phi_1 B - \cdots - \phi_p B^p \), \( \theta(B) = 1 - \theta_1 B - \cdots - \theta_q B^q \), \( a_t \) is a sequence of independent and identically distributed \( N(0, \sigma^2) \) random deviates, and where the \( w_t \)'s can represent the \( d \)-th difference or some other suitable transformation of a nonstationary series \( \{z_t\} \).

After a model of this form has been fitted to a series \( w_1, \ldots, w_n \), it is useful to study the adequacy of the fit by examining in various ways the residuals \( \hat{a}_1, \ldots, \hat{a}_n \) and, in particular, their autocorrelations

\[
\hat{r}_k = \frac{\sum_{t=k+1}^{n} \hat{a}_t \hat{a}_{t-k}}{\sum_{t=1}^{n} \hat{a}_t^2}, \quad k = 1, 2, \ldots
\]

An informal graphical analysis of these quantities combined with overfitting [see, for example, Box and Jenkins (1970)] usually proves most effective in detecting possible deficiencies in the model. In addition, however, it is often worthwhile to look at an overall criterion of adequacy of fit. Box and Pierce (1970) noted that if the model were appropriate and the parameters were known, the quantity

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\[ Q(r) = n(n+2) \sum_{k=1}^{m} (n-k)^{-1} r_k^2, \]  
(1.2)

where

\[ r_k = \frac{\sum_{t=k+1}^{n} a_t a_{t-k}}{\sum_{t=1}^{n} a_t^2}, \]

would for large \( n \) be distributed as \( \chi^2_m \) since the limiting distribution of \( r = (r_1, \ldots, r_m) \) is multivariate normal with mean vector zero [Anderson (1942), Anderson and Walker (1964)], \( \text{Var}(r_k) = (n-k)/n(n+2) \) and \( \text{Cov}(r_k, r_l) = 0, k \neq l \). Using the further approximation \( \text{Var}(r_k) = 1/n \), Box and Pierce suggested that the distribution of

\[ Q(r) = n \sum_{k=1}^{m} r_k^2 \]  
(1.3)

could be approximated by that of \( \chi^2_m \). Furthermore, they showed that when the \( p + q \) parameters of an appropriate model are estimated and the \( r_k \)'s replace the \( r_k \)'s, then

\[ Q(\hat{r}) = n \sum_{k=1}^{m} \hat{r}_k^2 \]

would for large \( n \) be distributed as \( \chi^2_{m-p-q} \) yielding an approximate test for lack of fit.

In applications of this test, suspiciously low values of \( Q(\hat{r}) \) have sometimes been observed and studies by Ljung and Box (1976) and Davies et al. (1977) have verified that the distribution of \( Q(\hat{r}) \) can deviate from \( \chi^2_{m-p-q} \). This observation was also made by Prothero and Wallis (1976, Discussion). The observed discrepancies could be accounted for by several factors among these departures from normality of the autocorrelations. It appears, however, that the main difficulty is caused by the approximation of (1.2) by (1.3).
A modified test based on the criterion

\[ \hat{Q}(r) = n(n+2) \sum_{k=1}^{m} (n-k)^{-1} r_k^2 \]

was recommended by Ljung and Box (1976) but its usefulness was questioned by Davies et al. (1977) on the ground that the variance of \( \hat{Q}(r) \) exceeds that of the \( \chi^2_{m-p-q} \) distribution. Our studies show however that the modified test provides a substantially improved approximation that should be adequate for most practical purposes.

2. MEANS AND VARIANCES OF \( Q(r) \) AND \( \hat{Q}(r) \)

To examine the overall test, it is useful to initially consider the quantities \( Q(r) \) and \( \hat{Q}(r) \) which involve the white noise autocorrelations \( r \).

Since the limiting distribution of \( r \) is \( N(0,n^{-1}I_m) \), \( Q(r) \) and \( \hat{Q}(r) \) are asymptotically distributed as \( \chi^2_m \) and have expectation \( m \) and variance \( 2m \).

For finite values of \( n \), \( \hat{Q}(r) \) has expectation \( m \), whereas

\[ E\hat{Q}(r) = n \sum_{k=1}^{m} E(r_k^2) = \frac{mn}{n+2} \left[ 1 - \frac{m+1}{2n} \right]. \tag{2.1} \]

Clearly, unless \( n \) is large relative to \( m \), \( E\hat{Q}(r) \) can be much smaller than \( m \).

The variances are

\[ \text{Var} Q(r) = n^2 \sum_{k=1}^{m} \text{Var}(r_k^2) + 2n^2 \sum_{k=1}^{m-1} \sum_{\ell=k+1}^{m} \text{Cov}(r_k^2,r_\ell^2) \]

and

\[ \text{Var} \hat{Q}(r) = n^2(n+2)^2 \sum_{k=1}^{m} (n-k)^{-2} \text{Var}(r_k^2) \]

\[ + 2n^2(n+2)^2 \sum_{k=1}^{m-1} \sum_{\ell=k+1}^{m} (n-k)^{-1}(n-\ell)^{-1} \text{Cov}(r_k^2,r_\ell^2) \]. \tag{2.2} \]
where for fixed $n$, $\text{Cov}(r_k^2, r_k^2)$ is non-zero. The univariate and bivariate moments of the $r_k$'s needed to evaluate (2.2) can be obtained using the identity

$$E(r_k^i r_k^j) = \frac{E((\sum a_t^2 - k) \sum a_t^2)}{E(\sum a_t^2)} (i+j)$$

(2.3)

which follows from independence of the $r_k$'s and $\sum a_t^2$ [see, for example, Anderson (1971), p. 304]. Taking $\text{Var}(a_t^2) = 1$ without loss of generality, $\sum a_t^2$ is distributed as $\chi^2_n$ and $E(\sum a_t^2)^{i+j} = n(n+2) \cdots (n+2i+2j-2)$. The term in the numerator of (2.3) can be evaluated by multiplying term by term taking the expected value. Using this procedure, it can be verified that for $k \leq n/2$

$$\text{Var}(r_k^2) = \frac{6(3n-5k) + 3(n-k)^2}{n(n+2)(n+4)(n+6)} - \frac{(n-k)^2}{n^2(n+2)^2}$$

and

$$\text{Cov}(r_k^2, r_k^2) = \frac{(n-k)(n-\ell) + 4(n-\ell) + 8(n-k-\ell)}{n(n+2)(n+4)(n+6)} - \frac{(n-k)(n-\ell)}{n^2(n+2)^2}.$$  

(2.4)

The exact variances of $Q(r)$ and $\hat{Q}(r)$ are readily evaluated using (2.2) and (2.4). By ignoring terms of order higher than $1/n$ it may be shown that approximately, for $n$ large relative to $m$,

$$\text{Var}Q(r) = 2m(1 + \frac{m-10}{n})$$

and

$$\text{Var}\hat{Q}(r) = 2m(1 + \frac{2m-5}{n}).$$

The variance of $\hat{Q}(r)$ exceeds $2m$ but the absence of a location bias makes its distribution much closer to $\chi^2_m$ than that of $Q(r)$. This is illustrated in Figure 1 which compares Monte Carlo distributions of $Q(r)$.
Fig. 1. Monte Carlo distributions of $Q(r)$ and $\hat{Q}(r)$ and approximations; 1000 replications, $n = 100$ and $m = 30$; \(\chi^2_{30}\), \(\chi^2_{b}\) (\(a = 1.52, b = 19.68\)).
and \( \tilde{Q}(r) \) based on 1000 replications to the \( \chi^2_m \) distribution for \( m = 30 \) and \( n = 100 \). The means and variances of the observed distributions are

\[
\bar{Q}(r) = 24.97, \quad \overline{\tilde{Q}(r)} = 30.17, \quad s^2_Q(r) = 60.47 \quad \text{and} \quad s^2_{\tilde{Q}(r)} = 88.25
\]

and agree quite closely with the corresponding theoretical values 24.85, 30.00, 63.15 and 91.48. Also shown by dashed lines in Figure 1 is a distribution of the form \( a\chi^2_b \) for which both the mean and variance is adjusted to correspond with that of \( \tilde{Q}(r) \). It is seen that there is perhaps a somewhat better agreement in the upper tail area but the main improvement results from adjusting the mean.

3. THE TEST STATISTICS \( Q(r) \) AND \( \tilde{Q}(r) \)

Box and Pierce (1970) showed that the residual autocorrelations

\[
\hat{\xi} = (\hat{r}_1, \ldots, \hat{r}_m)'
\]

dr from a correctly identified and fitted model can to a close approximation be represented as

\[
\hat{\xi} \approx (I - D)\xi
\]

where \( I - D \) is an idempotent matrix of rank \( m-p-q \). Using this relationship, the expectation of \( Q(\hat{r}) \) is

\[
E\{Q(\hat{r})\} \approx E\{nr' (I-D)\xi\} = tr\{n(I-D)C\},
\]

where \( C \) is the exact covariance matrix of \( r \). The matrix \( D \) has its largest elements in the upper left corner with the remaining elements \( d_{ij} \) decreasing to zero as \( i \) and/or \( j \) increases. The matrix \( DC \) is therefore nearly equal to \( n^{-1}D \). Using this approximation and noting that \( E\{Q(\hat{r})\} = tr\{nC\} \), we have

\[
E\{Q(\hat{r})\} \approx E(Q(r)) - p-q
\]

Combining (2.1) and (3.2), the expected value of \( Q(\hat{r}) \) is approximately

\[
E\{Q(\hat{r})\} \approx \frac{mn}{n+2} \left\{ 1 - \frac{m+1}{2n} \right\} - p-q
\]
which indicates that the distribution of $Q(r)$ can deviate markedly from $\chi^2_{m-p-q}$ unless $n$ is large relative to $m$. However, using the same approximations it can be shown that

$$E\hat{Q}(r) = E\tilde{Q}(r) - p-q = m-p-q.$$ 

It may be expected therefore that the distribution of $\hat{Q}(r)$ might be approximated by the $\chi^2_{m-p-q}$ distribution.

The adequacy of this approximation was questioned by Davies et al. (1977) on the ground that the variance of $\hat{Q}(r)$ exceeds $2(m-p-q)$. However, results from a simulation study reported in the next section suggest that the reduction in the location bias results as before in a markedly improved approximation that should be adequate for most practical purposes. It also appears that the expression for the variance given by Davies et al., which is not exact, over-estimates the variance of $\hat{Q}(r)$. For example, for fitting a first order autoregressive model to white noise, Davies et al. obtain for $m = 20$, $n = 50$, 100 and 200, $\text{Var}Q(r) = 58.80$, 50.08 and 44.20, respectively, while our study gives $\text{Var}\hat{Q}(r) = 46.84$, 43.20 and 41.97, respectively.

4. SOME NUMERICAL RESULTS

Comparison of the Overall Tests

A Monte Carlo study was conducted by generating 4000 sets of observations $\{w_1, \ldots, w_n\}$ from the first order autoregressive model $w_t = \phi w_{t-1} + a_t$, estimating $\phi$ by the approximate maximum likelihood estimator

$$\hat{\phi} = \frac{n-2}{n-1} \times \frac{\sum_{t=2}^{n} w_t w_{t-1}}{\sum_{t=2}^{n-1} w_t^2}.$$
[Box and Jenkins (1970), p. 279], and calculating autocorrelations of the residuals \( \hat{a}_1 = (1-\phi^2)w_1 \), \( \hat{a}_t = w_t - \phi w_{t-1}, t = 2, \ldots, n \). The statistics \( \hat{Q}(\hat{r}) \) and \( \hat{Q}(\hat{r}) \) were then calculated.

Table 1 shows the proportion of \( \hat{Q}(\hat{r}) \) and \( \hat{Q}(\hat{r}) \) values exceeding the upper i) 5, ii) 10 and iii) 25 percentage points of the \( \chi^2_{m-1} \) distribution for a few combinations of \( n \) and \( m \) and for \( \phi = .5 \). The table also gives the means and variances of the observed distributions. It seems clear that although the variance of \( \hat{Q}(\hat{r}) \) exceeds 2(m-1) a test based on this statistic would for smaller sample sizes provide a considerable improvement over the previously used \( \hat{Q}(\hat{r}) \) test.

### An Alternative Test Based on \( \hat{Q}(\hat{r}) \)

The above results suggest that a closer approximation to the distribution of \( \hat{Q}(\hat{r}) \) should be obtainable by appropriately adjusting the mean of the approximating distribution. Furthermore, Table 1 shows values of \( \text{Var} \hat{Q}(\hat{r}) \) which are nearly twice the mean, suggesting the approximation

\[
\hat{Q}(\hat{r}) \sim \chi^2_{\text{EQ}(\hat{r})}
\]

with \( \text{EQ}(\hat{r}) \) given by (3.3). Empirical significance levels obtained using this approximation and the criterion \( \hat{Q}(\hat{r}) \) are compared in Table 2. The agreement is quite close.

### A Power Calculation

The two criteria \( \hat{Q}(\hat{r}) \) and \( \hat{Q}(\hat{r}) \) differ essentially in the weighting which is applied to the autocorrelations \( \hat{r}_k \), \( \hat{Q}(\hat{r}) \) giving more emphasis to later autocorrelations. This would perhaps be an advantage if serial correlation occurs at high lags \( k \). However, for large \( n \) this difference should
Table 1. Empirical means, variances and significance levels of the statistics \( Q(r) \) and \( \hat{Q}(r) \); data generated from the model \( w_t = 0.5w_{t-1} + a_t \).

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<td>67.37</td>
<td>5.9</td>
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Table 2. Empirical significance levels based on the approximations

\( Q(\hat{r}) \sim \chi^2_{E_0}(\hat{r}) \) and \( \tilde{Q}(\hat{r}) \sim \chi^2_{m-1} \); data generated from the model

\[ w_t - \phi w_{t-1} = a_t. \]

\[ Q(\hat{r}) \sim \chi^2_{E_0}(\hat{r}) \]

\[ \tilde{Q}(\hat{r}) \sim \chi^2_{m-1} \]

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<th>( n=200 )</th>
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<td>0.9</td>
<td>5.6 10.6 25.6</td>
<td>6.3 10.9 24.9</td>
<td>6.3 11.4 25.7</td>
</tr>
</tbody>
</table>

| \( m = 10 \) | \( m = 20 \) |
| 5.0 10.0 25.0 | 5.0 10.0 25.0 |

| \( \phi \) | 5.0 10.0 25.0 | 5.0 10.0 25.0 |
| 0.1 | 4.3 8.8 23.4 | 5.1 9.3 22.2 | 4.7 9.3 23.5 | 5.9 10.0 22.7 |
| 0.3 | 4.4 8.5 23.4 | 5.2 9.0 22.7 | 4.8 9.1 23.5 | 6.0 9.8 23.1 |
| 0.5 | 4.4 8.5 23.5 | 5.3 9.1 22.6 | 4.7 9.3 23.4 | 6.0 10.1 22.9 |
| 0.7 | 4.7 9.0 24.1 | 5.6 9.6 22.7 | 4.9 9.4 24.0 | 6.2 10.3 23.2 |
| 0.9 | 5.3 9.6 25.4 | 6.2 10.2 23.7 | 5.5 9.9 25.4 | 7.0 11.2 24.1 |

| \( m = 10 \) | \( m = 20 \) |
| 5.0 10.0 25.0 | 5.0 10.0 25.0 |

| \( \phi \) | 5.0 10.0 25.0 | 5.0 10.0 25.0 |
| 0.1 | 5.0 9.6 24.1 | 5.2 9.8 22.7 | 5.2 9.9 24.2 | 5.5 10.2 23.2 |
| 0.3 | 4.9 9.3 23.8 | 5.1 9.7 22.6 | 5.2 9.6 24.0 | 5.4 10.1 22.8 |
| 0.5 | 4.8 9.6 23.8 | 5.1 9.4 22.4 | 5.0 9.8 23.9 | 5.4 10.0 22.7 |
| 0.7 | 4.8 9.9 24.1 | 4.9 10.0 22.5 | 5.0 10.1 24.2 | 5.3 10.5 22.8 |
| 0.9 | 5.4 10.2 25.8 | 5.4 10.7 23.3 | 5.6 10.3 25.8 | 5.7 11.1 23.5 |
be rather small. If the type of discrepancies to be expected is known, tests specifically aimed at detecting these discrepancies should be used. Such specific tests will of course be much more powerful. This point is illustrated in Table 3 which empirically compares the power of the overall tests and the method of "overfitting" [Box and Jenkins (1970)]. The results are based on data generated from a second order autoregressive model, with a first order model being fitted to obtain $Q(\hat{r})$ and $\hat{Q}(\hat{r})$. As might be expected, the overall tests are much less powerful than overfitting which tests the hypothesis that the second order autoregressive coefficient is zero. A smaller value of $m$ improves the power of the overall tests for this particular alternative.

**Effect of nonnormality of the $a_t$'s**

In developing the overall test, the assumption is made that the innovations $a_t$ in the model are normally distributed. Circumstances occur where this assumption is not true. For example, it is known that stock price innovations often have highly leptokurtic distributions. While Anderson and Walker (1964) show that the asymptotic normality of the $r_k$'s does not require normality of the $a_t$'s, only that their variance exists, results for finite sample sizes are lacking. An empirical investigation was therefore conducted into the behavior of the statistic $\hat{Q}(\hat{r})$ when the $a_t$'s have i) a double exponential and ii) a uniform distribution. The results, which are given in Table 4, agree closely with those obtained under the normality assumption for the $a_t$'s in Table 1.

5. **EXTENSION TO TRANSFER FUNCTION-NOISE MODELS**

To check the adequacy of a fitted model of the form

$$w_t = \frac{\omega(B)}{\delta(B)} a_{t-b-1} + \frac{\theta(B)}{\phi(B)} a_t$$

-11-
Table 3. Empirical power of the overall tests and the method of overfitting for \( n = 100 \). Assumed model:

\[ w_t - \phi w_{t-1} = a_t; \text{ true model: } (1 - .7B)(1 - G_2B)w_t = a_t; \]

Nominal significance level: 5 percent.

<table>
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<th>.1</th>
<th>.3</th>
<th>.5</th>
<th>.7</th>
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<td>( \hat{Q}(r) \sim \chi^2 )</td>
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<td>58.1</td>
<td>91.7</td>
<td>99.5</td>
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Table 4. Empirical means, variances and significance levels of \( \hat{Q}(r) \) when the innovations \( a_t \) have i) a double exponential and ii) a uniform distribution; data generated from the model \( w_t - .5w_{t-1} = a_t; \)

i) \( a_t \sim \) double exponential

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<th>( m )</th>
<th>( \text{mean} )</th>
<th>( \text{variance} )</th>
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<th>( \text{variance} )</th>
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<td>72.25</td>
<td>6.6</td>
<td>11.6</td>
<td>25.3</td>
</tr>
</tbody>
</table>
where
\[
\omega(B) = \omega_0 - \omega_1 B - \ldots - \omega_u B^u
\]
\[
\delta(B) = 1 - \delta_1 B - \ldots - \delta_v B^v
\]
and \( \phi(B) \) and \( \theta(B) \) are as in (1.1), and where the input series \( \{a_t\} \)
is assumed to be white noise, it is useful to examine, in addition to the
residual autocorrelations \( \hat{r}_k \), the crosscorrelations between the residuals
and the input series
\[
\hat{r}_k^* = \frac{\sum_{t=k+1}^{n} a_{t-k} \hat{a}_t}{\left( \sum_{t=1}^{n} a_t^2 \right)^{1/2}}.
\]

Pierce (1968, 1972) and Box and Jenkins (1970) propose an overall test
for lack of fit in the transfer function \( \omega(B)/\delta(B) \) based on approximating
the distribution of
\[
S(\hat{r}^*) = n \sum_{k=0}^{m} (\hat{r}_k^*)^2
\]
by a \( \chi_{m-v-u}^2 \) distribution. However, arguing as above it appears that a
criterion of the form
\[
\tilde{S}(\hat{r}^*) = n^2 \sum_{k=0}^{m} (n-k)^{-1} (\hat{r}_k^*)^2
\]
might be more appropriate. This is suggested by the fact that the distribution
of
\[
\tilde{S}(\hat{r}^*) = n^2 \sum_{k=0}^{m} (n-k)^{-1} (\hat{r}_k^*)^2,
\]
where
\[ r_k^* = \frac{\sum_{t=k+1}^{n} a_{t-k} a_t}{\left( \sum_{t=1}^{n} a_t^2 / \sum_{t=1}^{n} a_t \right)^{1/2}} \]

is for large \( n \) approximately \( \chi^2_{m+1} \) since the \( r_k^* \)'s are asymptotically normal with mean zero, \( \text{Var}(r_k^*) = (n-k)/n^2 \) and \( \text{Cov}(r_k^*, r_\ell^*) = 0, \ell \neq k \) [Pierce (1968)].
REFERENCES


The overall test for lack of fit in autoregressive-moving average models, proposed by Box and Pierce (1970), is considered. It is shown that a substantially improved approximation results from a simple modification of this test. Some consideration is given to the power of such tests and their robustness when the innovations are non-normal. Similar modifications in the overall tests used for transfer function-noise models are proposed.