

Diagnostic checking of time series models

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Abstract

Diagnostic checks have become a standard tool for identification of models before forecasting the data. The overall test for lack of fit for autoregressive moving average models proposed by Box and Pierce (1970) and a measure of lack of fit in time series models proposed by Ljung and Box (1978) are considered. In this paper, a modification is made and it is shown that a substantially improved approximation results from a simple improvement of this test. Cumulative periodogram check is also given.

Keywords: Time series, ARMA, ARIMA, forecasting.

General

Extensive literature is available on diagnostic checks for ARMA models (Jenkins & Watts, 1969; Hokstad, 1983; Box *et al.*, 1994). McLeod and Li (1983) proposed the diagnostic checks using residual autocorrelation. McLeod (1994) obtained new results on the distribution of residual autocorrelation and derived suitable diagnostic checks and illustrated them with an application of Fraser river time series. Ljung (1986) examined the properties of Portmanteau statistic for testing the adequacy of the model for various choices of m where m is the number of autocorrelations. Some of the commonly applied diagnostic checks are discussed subsequently.

To justify the modified diagnostic checking introduced the monthly rainfall data of Chennai city from the month of January 1984 to December 1994 is analyzed.

Overfitting

One class of diagnostic checks is devised to test adequacy by over fitting. Over fitting involves fitting a more elaborate model, than the one estimated to see, if the inclusion of one or more parameters greatly improves the fit. Extra parameters should be estimated for the more complex model, only where it is feared that the simpler model may require more parameters. However, the method of overfitting by extending the model in a particular direction assumes that model discrepancies are known in advance, which may not be possible in most of the cases. Procedures, less dependent upon such knowledge are based on the analysis of the residuals.

The graph of the residuals

If the fitted model is appropriate, then the graph of $\{\hat{a}_t, t = 1, 2, \dots, n\}$ should resemble that of a white noise process. While it is difficult to identify the correlation structure of $\{\hat{a}_t\}$ from its graph, deviation of the mean from zero is sometimes clearly indicated by a trend or cyclic component and inconsistency of the variance by

fluctuations in $\{\hat{a}_t\}$ whose magnitude depends strongly on t .

The next step is to check that the sample autocorrelation function of $\hat{a}_1, \hat{a}_2, \dots, \hat{a}_n$ behaves as it should, under the assumption that the fitted model is appropriate.

Autocorrelation check

Brockwell and Davis (1991) have proved that the sample autocorrelations of an identically and independently distributed (i.i.d) sequence $\{z_1, z_2, \dots, z_n\}$ with $E(z_t^2) < \infty$ for large n are approximately i.i.d with distribution $N(0, 1/\sqrt{n})$. Assuming, therefore, that an appropriate ARMA model is generated by a white noise sequence, the same approximation should be valid for the sample autocorrelation function (ACF) of $\{\hat{a}_t/t = 1, 2, \dots, N\}$ defined by

$$r_k(\hat{a}) = \frac{\sum_{t=1}^{n-k} (\hat{a}_t - \bar{a})(\hat{a}_{t+k} - \bar{a})}{\sum_{t=1}^n (\hat{a}_t - \bar{a})^2} \quad (1.1)$$

where $k = 1, 2, \dots$ and $\bar{a} = n^{-1} \sum_{t=1}^{n-k} \hat{a}_t$

However, because each \hat{a}_t is a function of the maximum likelihood estimator $(\hat{\varphi}, \hat{\theta}, \hat{a}_1, \hat{a}_2, \dots, \hat{a}_n)$ is not an i.i.d sequence and the distribution of $r_k(\hat{a})$ is not quite the same as in the i.i.d case. In certain cases, recognizable patterns in the estimated ACF of \hat{a}_t could point to appropriate modifications in the model. Supposing the form of the model were correct and the true values of AR and MA parameters, namely, φ, θ are known exactly, then by Bartlett's approximation (Bartlett, 1946) to the standard error of ACF, and as illustrated by

Anderson (1941), the estimated autocorrelations $r_k(\hat{a})$ of the \hat{a}_t 's would be uncorrelated and distributed normally about mean zero and variance $1/n$ and hence with a standard error of $n^{-1/2}$. Using these results, the significance of the apparent departure of these autocorrelations from zero may be analyzed. In practical applications to real time data, the true values of the parameters are not known and only the estimated values are available for analysis. The autocorrelations $r_k(\hat{a})$ and \hat{a}_t 's may yield valuable evidence concerning lack of fit and the nature of model inadequacy.

However, Durbin (1960) pointed out that it might be dangerous to assess the statistical significance of apparent discrepancies of these autocorrelations $r_k(\hat{a})$ from their theoretical zero values on the basis of a standard error of $n^{-1/2}$, appropriate to the $r_k(\hat{a})$'s. Subsequently Box and Pierce (1970) have shown that, while in all cases, a reduction in variance can occur for low lags and that at these low lags, the autocorrelations $r_k(\hat{a})$ can be highly correlated and these effects usually disappear rather quickly at higher lags. Thus, the use of $n^{-1/2}$ as the standard error for $r_k(\hat{a})$ would underestimate the statistical significance of apparent departures from zero of the autocorrelation at low lags, but could usually be employed for moderate or higher lags. Hence, except at moderate lags, $n^{-1/2}$ must be regarded as supplying an upper level for the standard errors of the $r_k(\hat{a})$'s rather than the standard errors themselves.

Ljung and Box (1978) made a simple modification of the test of Box and Pierce (1970) which substantially improved approximation that should be adequate for most practical purposes. Godfrey (1979) examined both the above tests and proposed a new approach and some Monte Carlo results on the finite sample size for testing the adequacy of a time series model.

Cumulative periodogram

In some applications, particularly in the fitting of seasonal time series, it may be feared that the model has not adequately taken into account, the periodic characteristics of the available data. Therefore, one must be on the lookout for the periodic behaviour of the residuals. In such cases, the ACF will not be a sensitive indicator of such departures from randomness because periodic effects will typically dilute themselves among several autocorrelations. The periodogram, on the other hand, is specifically designed for the periodic patterns in a background of white noise. The periodogram of a time series $\{a_t, t = 1, 2, \dots, n\}$ is defined as

$$I(f_i) = \frac{2}{n} \left[\left(\sum_{t=1}^n a_t \cos 2\pi f_i t \right)^2 + \left(\sum_{t=1}^n a_t \sin 2\pi f_i t \right)^2 \right] \quad i = 1, 2, \dots \quad (1.2)$$

where $f_i = \frac{i}{n}$ is the frequency.

Thus, it is a device for correlating the a_t with sine and cosine waves of different frequencies. A pattern with frequency f_i in the residual is reinforced when correlated with a sine and cosine wave at that same frequency and so produces a large value of $I(f_i)$. It has been shown by Bartlett (1946) that the cumulative periodogram provides an effective means for the detection of non-randomness. Jenkins and Watts (1968) have also discussed in detail the applications of the cumulative periodogram.

The power spectrum $P(f)$ for white noise has a constant value $2\sigma_a^2$ over the frequency 0-0.5 cycles. Consequently, the cumulative spectrum for white noise, namely

$$P(f) = \int_0^f p(a) da$$

plotted against f is a straight line running from $(0, 0)$ to $(0.5, \sigma_a^2)$, that is $P(f)/\sigma_a^2$ is a straight line running from $(0,0)$ to $(0.5, 1)$. $I(f)$ produces an estimate of the power spectrum at frequency f . In fact, for white noise $E\{I(f)\} = 2\sigma_a^2$ and hence the estimate is unbiased. It follows that

$\frac{1}{n} \sum_{i=1}^j I(f_i)$ provides an unbiased estimate of the integrated spectrum $P(f_j)$ and

$$C(f_j) = \frac{\sum_{i=1}^j I(f_i)}{n \hat{\sigma}_a^2} \quad (1.3)$$

is an estimate of $P(f_j)/\hat{\sigma}_a^2$ where $\hat{\sigma}_a^2$ is an estimate of σ_a^2 . $C(f_j)$ is called the cumulative periodogram.

Now if the models were adequate and the parameters known exactly, the a_t 's could be computed from the data and would yield a white noise series. For a white noise series, the plot of $C(f_j)$ against f_j would be scattered about a straight line, joining the points $(0, 0)$ and $(0.5, 1)$. On the other hand, non-randomness would produce non-random a_t 's whose cumulative periodogram could show systematic deviations from the line. In particular, periodicities in the a_t 's would tend to produce a series of neighbouring values of $I(f_i)$, which are large. These large ordinates would reinforce each other in $C(f_j)$, and form a lump on the expected straight line.

Box and Jenkins (1976) have used approximate probability limits for cumulative periodogram using Kolmogorov-Smirnov test. The limits lines are drawn about the theoretical line which are such that, if the $\{a_t\}$ series were white noise, then the cumulative periodogram would deviate from the straight line, sufficiently to cross the limits, only with stated property. The limit lines are such that for a true random series, they would be crossed by a proportion of the time. They are drawn at distances $\pm K_\epsilon / \sqrt{q}$ above and below the theoretical line, where $q = (n-2)/2$ for n even and $q = (n-1)/2$ for n odd where ϵ is the

level of significance. Approximate values of K_ϵ are given in Table 1. With the availability of computer packages for diagnostic checking, the entire process reduces to the selection of the appropriate test depending on the parameters used.

Table 1. Coefficient for calculating approximate probability limits for cumulative periodogram test.

$\epsilon\{\text{PRIVATE}\}$	K_ϵ
0.01	1.63
0.05	1.36
0.10	1.22
0.25	1.02

Portmanteau statistic

1.6.1. Portmanteau lack of fit test

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

$$\varphi(B) w_t = \theta(B) a_t, \text{ where } w_t = \nabla^d z_t$$

Where d is an integer or any real number and $\{z_t\}$ is any time series.

$$\begin{aligned} \varphi(B) &= 1 - \phi_1 B - \dots - \phi_p B^p \\ \theta(B) &= 1 - \theta_1 B - \dots - \theta_q B^q \end{aligned}$$

Here w_t 's can in general represent the d th difference or some other suitable transformation of a non-stationary series $\{z_t\}$. After a model of this form has been fitted to a series w_1, w_2, \dots, w_n , it is useful to study the adequacy of the fit by examining the residuals $\hat{a}_1, \dots, \hat{a}_n$ and in particular their autocorrelations

$$r_k(\hat{a}) = \frac{\sum_{t=k+1}^n \hat{a}_t \hat{a}_{t+k}}{\sum_{t=1}^n \hat{a}_t^2}, \quad k = 1, 2, \dots$$

A graphical analysis of these quantities combined with overfitting procedure given by Box and Jenkins (1976) usually prove to be most effective in detecting possible deficiencies in the model. Box and Pierce (1970) suggested that if the models were appropriate and parameters were known, the quantity

$$Q_2(r) = n(n+2) \sum_{k=1}^m \frac{r_k^2(a)}{(n-k)}, \text{ where } r_k(a) = \frac{\sum_{t=k+1}^n a_t a_{t-k}}{\sum_{t=1}^n a_t^2}$$

Would for large n be distributed as χ_m^2 since the limiting distribution of $r = (r_1, \dots, r_m)'$ is multivariate normal with mean zero (Ljung & Box, 1978).

$$\text{Var}(r_k(a)) = \frac{n-k}{n(n+2)}$$

$$\text{cov}(r_k(a), r_l(a)) = 0 \quad (k \neq l)$$

Using further approximation,

$$\text{var}(r_k(a)) = 1/n$$

Box and Pierce (1970) suggested that the distribution of

$$Q_1(r) = n \sum_{k=1}^m r_k^2(a)$$

Could be approximated by that of χ_m^2 . Further, they showed that when $p+q$ parameters of an appropriate model are estimated and the $r_k(\hat{a})$'s replace the $r_k(a)$'s, then

$$Q_1(\hat{r}) = n \sum_{k=1}^m r_k^2(\hat{a})$$

would for large n be distributed as χ_{m-p-q}^2

A modified test based on the criterion $Q_2(\hat{r}) = n(n+2)$

$$\sum_{k=1}^m \frac{r_k^2(\hat{a})}{(n-k)}$$

Was recommended by Ljung and Box (1978). The modified test provides an improved approximation that should be adequate for most practical purposes. It is also noted by Davies *et al.* (1977) that the variance of $Q_2(\hat{r})$ exceeds that of the ψ_{m-p-q}^2 distribution. The above criterion is further modified in this study to facilitate better approximation to the distribution and in turn to give better identification of the models.

The proposed Q statistics are

$$Q_3(r) = n \sum_{k=1}^m \frac{n-k}{(n+k)} r_k^2(\hat{a}) \text{ and}$$

$$Q_4(r) = n(n+2) \sum_{k=1}^m \frac{r_k^2(\hat{a})}{(n+k)}$$

1.6.2. Mean and variance of Portmanteau statistics

The residual autocorrelation r_k of the process is written in the form

$$r_k(a) = \frac{\sum_{t=k+1}^n a_t a_{t-k}}{\sum_{t=1}^n a_t^2}, \quad k = 1, 2, \dots$$

Then

$$E(r_k(a)) = E \frac{\sum_{t=k+1}^n a_t a_{t-k}}{\sum_{t=1}^n a_t^2} = \frac{1}{n^2 \sigma^2} E \sum_{t=k+1}^n a_t a_{t-k} = 0$$

$$\text{var}(r_k(a)) = E(r_k^2(a)) = \frac{1}{n^2 \sigma^2} E \sum_{t=k+1}^n a_t a_{t-k}$$

$$= \frac{1}{n^2 \sigma^2} (a_{k+1} a_1 + a_{k+1} a_2 + \dots + a_n a_{n-k})^2$$

$$= \frac{n-k}{n^2} \rightarrow \frac{1}{n} \text{ for large } n$$

It is found that (Davies *et al.*, 1977),

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

$$\text{cov}(r_k^2(a), r_l^2(a)) = \frac{(n-k)(n-l)+4(n-l)+8(n-k-l)}{n(n+2)(n+4)(n+6)} - \frac{(n-k)(n-l)}{n^2(n+2)^2}$$

$$+ 2n^2(n+2)^2 \sum_{k=1}^{m-1} \sum_{l=k+1}^m \frac{\text{cov}(r_k^2(a), r_l^2(a))}{(n-k)(n+l)}$$

$Q_i(r)$, $i=1, 2, 3, 4$ are asymptotically distributed as χ_m^2 and have expectation m and variance $2m$. Variance of $Q_i(r)$, $i = 1,2,3,4$ are tabulated in Table 2 for comparative study for different values of n and m .

The Q statistics and their variances of the existing ones and the proposed ones are given below

i) $Q_1(r) = n \sum_{k=1}^m r_k^2(a)$ (Box & Pierce, 1970)

$$\text{var}(Q_1(r)) = n^2 \sum_{k=1}^m \text{var}(r_k^2(a)) + 2n^2 \sum_{k=1}^{m-1} \sum_{l=k+1}^m \text{cov}(r_k^2(a), r_l^2(a))$$

ii) $Q_2(r) = n(n+2) \sum_{k=1}^m \frac{r_k^2(a)}{(n-k)}$ (Ljung & Box 1978)

$$\text{var}(Q_2(r)) = n^2(n+2)^2 \sum_{k=1}^m \frac{(r_k^2(a))}{(n-k)} + 2n^2(n+2)^2 \sum_{k=1}^{m-1} \sum_{l=k+1}^m \frac{\text{cov}(r_k^2(a), r_l^2(a))}{(n-k)(n-l)}$$

iii) $Q_3(r) = n \sum_{k=1}^m \frac{n-k}{(n+k)} r_k^2(a)$

$$\text{var}(Q_3(r)) = n^2 \sum_{k=1}^m \frac{n-k^2}{(n+k)} \text{var}(r_k^2(a)) + 2n^2 \sum_{k=1}^{m-1} \sum_{l=k+1}^m \frac{(n-k)(n-l)}{(n-k)(n+l)} \text{cov}(r_k^2(a), r_l^2(a))$$

iv) $Q_4(r) = n(n+2) \sum_{k=1}^m \frac{r_k^2(a)}{(n+k)}$

$$\text{var}(Q_4(r)) = n^2(n+2) \sum_{k=1}^m \frac{\text{var}(r_k^2(a))}{(n-k)^2}$$

Diagnostic checks have become a standard tool for assessing the adequacy of a forecasting system, since ARIMA modeling techniques (Box & Jenkins, 1976) became popular. Box and Pierce (1970) gave an overall test of fit which is based on the residual autocorrelation. Davies *et al.* (1977) suggested that there are cases in which low values of the portmanteau statistic are often found and in such cases, the true significance levels are likely to be much lower than predicted by asymptotic theory. Ljung and Box (1978) have shown that a substantially improved approximation results from a simple modification of Box and Pierce (1970) portmanteau test for transfer function-noise models. A simple statistic to check model adequacy in time series is also suggested by Abraham and Vijayan (1988). Most of the checks are available only for normal and second order stationary models. Smith (1985) has given various diagnostic checks that can be performed simply on non-normal and non-standard models. Anders Milhøj (1981) proposed a goodness of fit and flat statistic for time series models in which the asymptotic power of the tests found are compared to the empirical power of the portmanteau test.

Analysis of Chennai city rainfall data

Models are identified for the different time series using the procedure given by Box and Jenkins (1976). The best model is chosen with help of modified portmanteau lack of fit test.

Model identification

The general behaviour of the estimated autocorrelation and partial autocorrelation function of the appropriate differenced series will give the clues about the choice of the orders of p, q, P and Q for the autoregressive and moving average operators for non-stationary seasonal model to identify the multiplicative ARIMA process (Box & Jenkins, 1976). The rainfall data of the Chennai city for the period 1981 to 1994 is taken for analysis. The given series z_t is transformed by adding a constant C . The transformation of the original asymmetric periodic time series z_t into a normally distributed time series z_t is done by taking logarithms of $z_t + C$. The value of C is usually assumed to be lower bound of the series or it is chosen arbitrarily.

The autocorrelation (Table 3) and partial autocorrelation of the transformed series z_t do not render any help for model identification except that the given time series is seasonal with period 12. The seasonality in the series is removed by taking twelfth difference. The

Table 2. Mean and Variance of $Q_i(r)$, $i = 1, 2, 3, 4$.

{PRIVATE }n, m	$Q_1(r)$ Box & Pierce	$Q_2(r)$ Box & Ljung	$Q_3(r)$	$Q_4(r)$
n=150, m=15	28.240	43.022	16.408	23.605
n= 50, m=12	22.435	31.974	14.217	19.516
n=100, m=30	63.1546	91.480	37.421	51.216
n=100, m=25	52.269	71.577	33.264	43.789
n=100, m=20	41.218	53.470	28.315	25.773
n=100, m=50	110.608	147.672	71.090	91.257
n=100, m=45	48.859	128.380	65.978	82.994
n=100, m=30	63.842	76.425	48.051	56.705
n=100, m=75	169.113	223.871	109.049	138.810
n=100, m=50	109.294	132.075	80.285	95.329
n=400, m=100	227.662	300.099	147.043	186.386
n=400, m=75	167.085	205.634	118.854	143.069
n=400, m=50	107.767	124.056	85.053	96.937

Table 3. Autocorrelation of the series z_t and $(1-B^{12}) z_t$.

lag k	Autocorrelation of z_t	lag k	Autocorrelation of $(1-B^{12}) z_t$
1	0.500	1	-0.230
2	0.286	2	0.073
3	-0.070	3	-0.082
4	-0.286	4	0.067
5	-0.483	5	-0.062
6	-0.553	6	-0.068
7	-0.448	7	0.143
8	-0.354	8	-0.090
9	-0.058	9	0.066
10	-0.220	10	0.031
11	-0.537	11	0.080
12	-0.631	12	-0.499
13	-0.526	13	0.118
14	-0.255	14	0.034
15	-0.046	15	-0.049
16	-0.248	16	0.078
17	-0.456	17	-0.058
18	-0.472	18	0.110
19	-0.457	19	-0.119
20	-0.325	20	0.034
21	-0.059	21	0.015
22	-0.153	22	-0.082
23	0.509	23	0.123
24	0.576	24	0.063
25	0.467	25	-0.062
26	0.202	26	-0.136
27	-0.011	27	0.129
28	-0.257	28	-0.077
29	-0.399	29	0.017
30	-0.454	30	-0.080

autocorrelation of the differenced time series (Table 3) indicates that it has large autocorrelation only at lag 12. After trying many values for C the appropriate value of C is found to be 15.0.

In this case the additive constant is necessitated because Chennai city did not experience any amount of rain in some months. As with the non-seasonal model by equating observed autocorrelation to their expected values, approximate values can be obtained for the parameter Θ ($\theta = 0$). On substituting the estimation r_{12} in the place of ρ_{12} in the equation:

$$\rho_{12} = \frac{-\Theta}{1 + \Theta^2}$$

We obtain the initial estimate for Θ as $\Theta = 0.8013$. The ARIMA model for the rainfall data can be written in the form $\nabla_{12} z_t = (1 - \Theta B^{12}) a_t$

The value of Θ can be estimated by using either least squares estimate method or estimation by numerical derivations.

The above model can be written in the form.

$$a_{t,0} = (\Theta - \Theta_0) x_{2,t} + a_t$$

Where $x_{2,t} = \frac{-\partial a_t}{\partial \Theta}$ and Θ_0 is the assumed value of

$$a_{t,0} = [a_t / \Theta_0]$$

The derivatives are most easily computed numerically by

$$x_{2,t} = \frac{[a_t] - [a_{t,0}]}{\delta}, \delta > 0 \text{ which is very small.}$$

To obtain the first adjustment for Θ , we compute

$$\Theta - \Theta_0 = \frac{\sum_{t=0}^n [a_{t,0}]}{\sum_{t=0}^n x_t^2}, \quad n = N - sD = 156$$

The value of Θ is estimated as $\hat{\Theta} = 0.9265$ (Table 4). The model is written in the form

$$\nabla^{12} z_t = (1 - \hat{\Theta} B^{12}) a_t \quad \text{where } \hat{\Theta} = 0.9265.$$

Table 4. Iterative estimation of Θ for the rainfall data.

{PRIVATE }Iteration	Θ
1	0.9291
2	0.9268
3	0.9265
4	0.9265
5	0.9265
6	0.9265
7	0.9265
8	0.9265
9	0.9265
10	0.9265

Portmanteau lack of fit test

After identifying the model, it is customary to validate the model before forecasting the data. The proposed portmanteau criteria and the existing tests are applied and the model is then identified.

In the case of ARIMA model (Box & Jenkins, 1976), We refer $Q_3(r) = 37.0563$ to a χ^2 table with 47 degrees of freedom. The 90% and 75% for χ^2 with 47 degrees of freedom are 30.7 and 37.3 (Table 5). It shows that there is no basis for questioning this model and that it can be used for further analysis.

Table 5. Comparison of sum of the squared residuals.

{PRIVATE } $Q_i(r)$ $i=1,2,3,4$	Residual square sum	χ^2 distribution with 47 degrees of freedom	
$Q_1(1)$	47.7441	50%	25%
		45.6	55.3
$Q_2(r)$	56.4925	25%	10%
		55.3	65.1
$Q_3(r)$	37.0563	90%	75%
		30.7	37.3
$Q_4(r)$	42.9438	75%	50%
		37.3	45.6

Forecasting

Forecasting can be done from the difference equation itself. The ARIMA model for the rainfall data written in the form at lead time l where we are currently standing at time t is given by

$$\nabla_{12} z_{t+l} = (1 - \hat{\Theta} B^{12}) a_{t+l}, \text{ where } \hat{\Theta} = 0.9265.$$

$$z_{t+l} - z_{t+l-12} = a_{t+l} - \hat{\Theta} a_{t+l-12}$$

$$z_{t+l} = z_{t+l-12} - \hat{\Theta} a_{t+l-12} + a_{t+l}$$

The minimum mean square error forecast at lead time l and at origin t is given by

$$\hat{z}_{t+l} = [z_{t+l-12}] - \hat{\Theta} [a_{t+l-12}] + [a_{t+l}].$$

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