Residual diagnostic plots for checking for model mis-specification in time series regression.

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Abstract: This paper considers residuals for time series regression. Despite much literature on visual diagnostics for uncorrelated data, there is little on the autocorrelated case. In order to examine various aspects of the fitted time series regression model, three residuals are considered. The fitted regression model can be checked using *orthogonal residuals*; the time series error model can be analysed using *marginal residuals*; and the white noise error component can be tested using *conditional residuals*. When used together, these residuals allow identification of outliers, model mis-specification and mean shifts. Due to the sensitivity of conditional residuals to model mis-specification, it is suggested that the orthogonal and marginal residuals be examined first.

Keywords: autocorrelation; conditional residuals; generalised least squares; marginal residuals; mean shifts; model mis-specification; model transformation; orthogonal residuals; residual diagnostics; residual plots; time series regression.

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1 Introduction

Regression models with autocorrelated errors have received much attention in recent years. An overview of time series regression is presented by Tsay (1984). Influence diagnostics are discussed by Puterman (1988) and Hossain (1990), and outlier detection is considered by Tsay (1986) and Ledolter (1988). Haslett and Hayes (1998) and Martin (1992) establish generalised versions of residuals and diagnostics that are commonly used when performing Ordinary Least Squares (OLS) regression. However, there has been little attention given to residual diagnostic plots for time series regression.

We shall consider a linear regression model with an autoregressive (AR) error :

$$Y_t = f(\boldsymbol{X}_t) + e_t \qquad \text{where} \quad \Phi_p(B)e_t = z_t \tag{1}$$

where $\boldsymbol{X}_t$ is a vector of explanatory variables assumed to be known, the regression model is $f(\boldsymbol{X}_t) = \boldsymbol{X}_t\boldsymbol{\beta}$ where $\boldsymbol{\beta}$ is a vector of coefficients, $\Phi_p(B) = (1 - \phi_1 B - \cdots - \phi_p B^p)$ is a polynomial of order p in the backshift operator B, and z_t is a zero mean Gaussian white noise series with variance σ^2.

Model (1) can also be written as

$$\boldsymbol{Y} = \boldsymbol{X}\beta + \boldsymbol{e} \qquad \text{where} \quad \boldsymbol{e} \stackrel{d}{=} \mathrm{N}(0, \boldsymbol{\Sigma}) \tag{2}$$

where the correlated error structure is represented in the matrix $\boldsymbol{\Sigma}$ which has $(i,j)^{th}$ element $\gamma(|i-j|)$, and where γ is the autocovariance function of the time series model represented by e_t. This representation of the time series regression model allows Generalised Least Squares (GLS) to be used to estimate the parameters $\boldsymbol{\beta}$ and $\boldsymbol{\Sigma}$. The use of GLS estimation in an iterative procedure is outlined by Judge et al. (1988, p.392), and is the method used for obtaining parameter estimates for the examples presented herein.

The limitation to AR models in (1) is not particularly restrictive as any ARMA model can be approximated by a high order AR model (see Brockwell and Davis, 1991, p.91). Hence, the results presented within can be extended to regression models with ARMA time series errors.

It is a common practise with ordinary regression, where the errors are uncorrelated ($p = 0$), to plot the residuals against each of the explanatory variables. Patterns in residual plots indicate the fitted model is mis-specified. The pattern seen indicates the form of the mis-specification (e.g., a quadratic shape indicates that a quadratic term should be included in the model).

Our goal is to produce similar residual plots for models with autocorrelated errors. The

resulting residual plots should also allow other aspects of the fitted model to be assessed, such as checking the assumed properties of z_t. In Section 2, we examine a type of residual that, whilst being an intuitive diagnostic to use, is sometimes misleading when assessing the fitted regression model. In Section 3, a more suitable type of residual is derived, with its use demonstrated on examples presented in Section 4. A third type of residual examined in Section 5 provides further checking of other elements of the fitted model. When used together, these three types of residuals provide the means for assessing various aspects of the time series regression model.

2 Marginal Residuals

The marginal expectation for model (1) is $\mathrm{E}(Y_t \,|\, \boldsymbol{X}) = f(\boldsymbol{X}_t)$. Departures from the best estimate of this expectation are called *marginal residuals*, $\hat{e}_t = Y_t - \hat{f}(\boldsymbol{X}_t)$. It would seem natural to produce diagnostics plots based on the marginal residuals. This approach is used when performing OLS estimation on uncorrelated data, but its use with autocorrelated data is problematic.

Asymptotically, $\mathrm{Var}(\hat{\boldsymbol{e}}) = \boldsymbol{\Sigma}$ (following from Proposition 9.7.1 in Fuller, 1996, p.519) and so these residuals must be expected to exhibit autocorrelation which may lead to "patterns" in a residual plot. These autocorrelation-induced patterns will often interfere with other patterns that indicate mis-specification. Consequently, it is difficult to visually identify when mis-specification has occurred and what form of mis-specification is present.

An example of a plot of marginal residuals is shown in Figure 1. This plot is based on the mean shift data example which will be presented in Section 4.2. The autocorrelation in the data is evident in the residual plot, and makes it difficult to discern the existence of other patterns.

Under the hypothesis that the regression model has been correctly specified, the marginal residuals $\hat{\boldsymbol{e}}$ estimate the unobservable time series error process. It is therefore suggested that marginal residuals be plotted in time order. Other types of residuals presented herein could also be plotted against time, or against the fitted values as is the norm.

The nature of marginal residuals allows them to be treated as an observed time series, and so current time series diagnostic methods can be utilised. For example, parameter changes can be detected using techniques discussed in Bagshaw and Johnson (1977), and outliers in error models can be identified using methods such as those proposed by Ljung (1993) and Ledolter (1988).

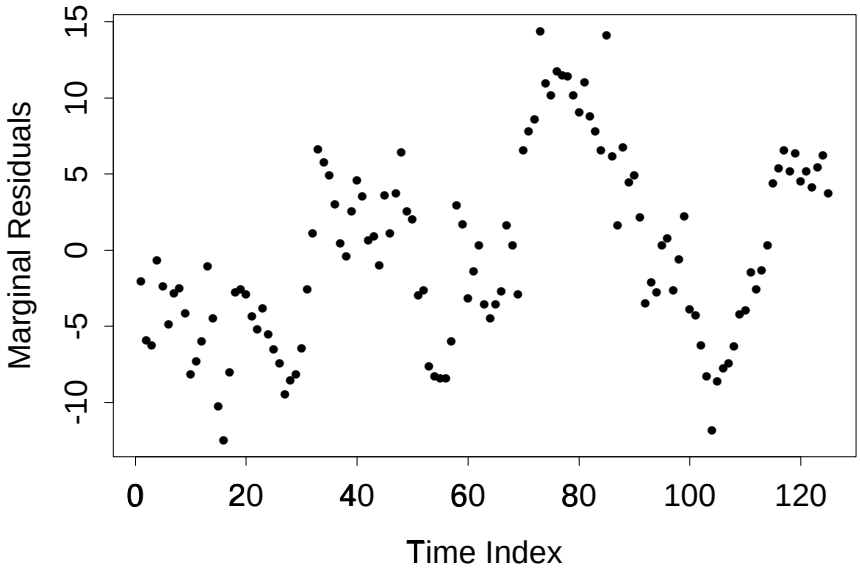

Figure 1: *An example of a plot of marginal residuals where the error model is AR(1). The pattern dominating the plot is due to autocorrelation.*

3 Residual Orthogonality

Let $\boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}$ denote the hat matrix from a linear model fitted using generalized least squares regression. For ordinary least squares, $p = 0$ and $\boldsymbol{\Sigma}^{-1} = \sigma^{-2}\boldsymbol{I}$. In this case,

$$\hat{\boldsymbol{e}}'\boldsymbol{X} = ((\boldsymbol{I} - \boldsymbol{H})\boldsymbol{Y})'\boldsymbol{X} = \boldsymbol{Y}'(\boldsymbol{I} - \boldsymbol{H})'\boldsymbol{X} = \boldsymbol{Y}'\boldsymbol{X} - \boldsymbol{Y}'\boldsymbol{H}'\boldsymbol{X} = \boldsymbol{0}. \tag{3}$$

Similarly, $\hat{\boldsymbol{e}}'\hat{\boldsymbol{Y}} = \hat{\boldsymbol{e}}'\boldsymbol{X}\hat{\beta} = \boldsymbol{0}$. Thus, the marginal residuals are orthogonal to $\hat{\boldsymbol{Y}}$ and to $\boldsymbol{X}$. We believe that this orthogonality is the essential reason why for uncorrelated observations, it 'makes sense' to plot the residuals $\hat{\boldsymbol{e}}$ against $\boldsymbol{X}$ and $\hat{\boldsymbol{Y}}$.

However, for time series regression, where $p > 0$, $\boldsymbol{H}'\boldsymbol{X} \neq \boldsymbol{X}$ and so the above orthogonality does not hold. Thus, the vector of residuals, $\hat{\boldsymbol{e}}$, is correlated with $\hat{\boldsymbol{Y}}$ and $\boldsymbol{X}$. As a result, patterns may appear in residual plots when, in fact, the residuals do not vary systematically.

A solution to finding a suitable type of residual for time series regression lies in the above orthogonality principle. In the following section, a residual orthogonal to $\hat{\boldsymbol{Y}}$ and $\boldsymbol{X}$ is presented.

3.1 The orthogonal residual

In generalized least squares regression, the normal equations are $\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{Y} = \boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X}\hat{\beta}$. Therefore

$$\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}(\boldsymbol{Y} - \boldsymbol{X}\beta) = \boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{e} = \boldsymbol{0} \tag{4}$$

and so $\boldsymbol{v} = \boldsymbol{\Sigma}^{-1}\boldsymbol{e}$ is orthogonal to $\boldsymbol{X}$ (and can also be shown to be orthogonal to $\hat{\boldsymbol{Y}} = \boldsymbol{X}\beta$).

The *orthogonal errors*, $\boldsymbol{v}$, have mean zero and their covariance matrix, $\text{Cov}(\boldsymbol{\Sigma}^{-1}\boldsymbol{e}) = \boldsymbol{\Sigma}^{-1}$, is not diagonal so they are correlated. However, the covariance has an interesting property that arises from the duality between autoregressive and moving average (MA) processes. Specifically, the inverse of the autocovariance matrix from an MA(p) process is approximately equal to the autocovariance matrix from an AR(p) process (Anderson, 1976). Murthy (1974) shows that for an AR(p) autocovariance matrix, $\boldsymbol{\Sigma}$, the inverse may be represented as

$$\boldsymbol{\Sigma}^{-1} \quad = \quad \check{\boldsymbol{\Sigma}}^{-1} + \tilde{\boldsymbol{\Sigma}}^{-1} \tag{5}$$

where $\check{\boldsymbol{\Sigma}}^{-1}$ is an MA(p) autocovariance matrix, and $\tilde{\boldsymbol{\Sigma}}^{-1}$ is a matrix of zeros except for the leading and trailing $p \times p$ submatrices.

Now, for an MA(p) process, the autocovariance function satisfies $\gamma(k) = 0$ for $k > p$. Therefore, the matrix $\check{\boldsymbol{\Sigma}}^{-1}$ consists of zeros except for the main diagonal and up to p off-diagonals either side of the main diagonal. Adding the matrix $\tilde{\boldsymbol{\Sigma}}^{-1}$ only changes some of the non-zero values in the matrix $\check{\boldsymbol{\Sigma}}^{-1}$ and so $\boldsymbol{\Sigma}^{-1}$ has the same pattern as $\check{\boldsymbol{\Sigma}}^{-1}$. Therefore, the ith orthogonal error, $\boldsymbol{v}_i$, will only be correlated with those p orthogonal errors that occur immediately before and after it. For a low order AR process (and with sufficiently large n), $\boldsymbol{\Sigma}^{-1}$ is nearly diagonal, and so the orthogonal errors have low order autocorrelation.

When estimated from sample data, the *orthogonal residuals* are defined as $\hat{\boldsymbol{v}} = \hat{\boldsymbol{\Sigma}}^{-1}\hat{\boldsymbol{e}}$. The duality property described above has an important consequence for the use of orthogonal residuals in a residual plot. As illustrated in Figure 2, low-order autocorrelation is not obvious in a scatterplot. An observer will therefore not be distracted from other patterns that may indicate mis-specification or the presence of outlying observations. Similarly for orthogonal residuals, low-order autocorrelation will not detract from the presence of other patterns or unusual residuals that exist in the plot.

The orthogonal residuals have estimated covariance matrix

$$\begin{aligned}
\text{Cov}(\hat{\boldsymbol{\Sigma}}^{-1}\hat{\boldsymbol{e}}) &= \hat{\boldsymbol{\Sigma}}^{-1}(\boldsymbol{I} - \hat{\boldsymbol{H}})\hat{\boldsymbol{\Sigma}}(\boldsymbol{I} - \hat{\boldsymbol{H}})'\hat{\boldsymbol{\Sigma}}^{-1} \\
&= \hat{\boldsymbol{\Sigma}}^{-1}(\boldsymbol{I} - \hat{\boldsymbol{H}})\hat{\boldsymbol{\Sigma}}(\boldsymbol{I} - \hat{\boldsymbol{\Sigma}}^{-1}\boldsymbol{X}(\boldsymbol{X}'\hat{\boldsymbol{\Sigma}}^{-1}\boldsymbol{X})\boldsymbol{X}')\hat{\boldsymbol{\Sigma}}^{-1}
\end{aligned}$$

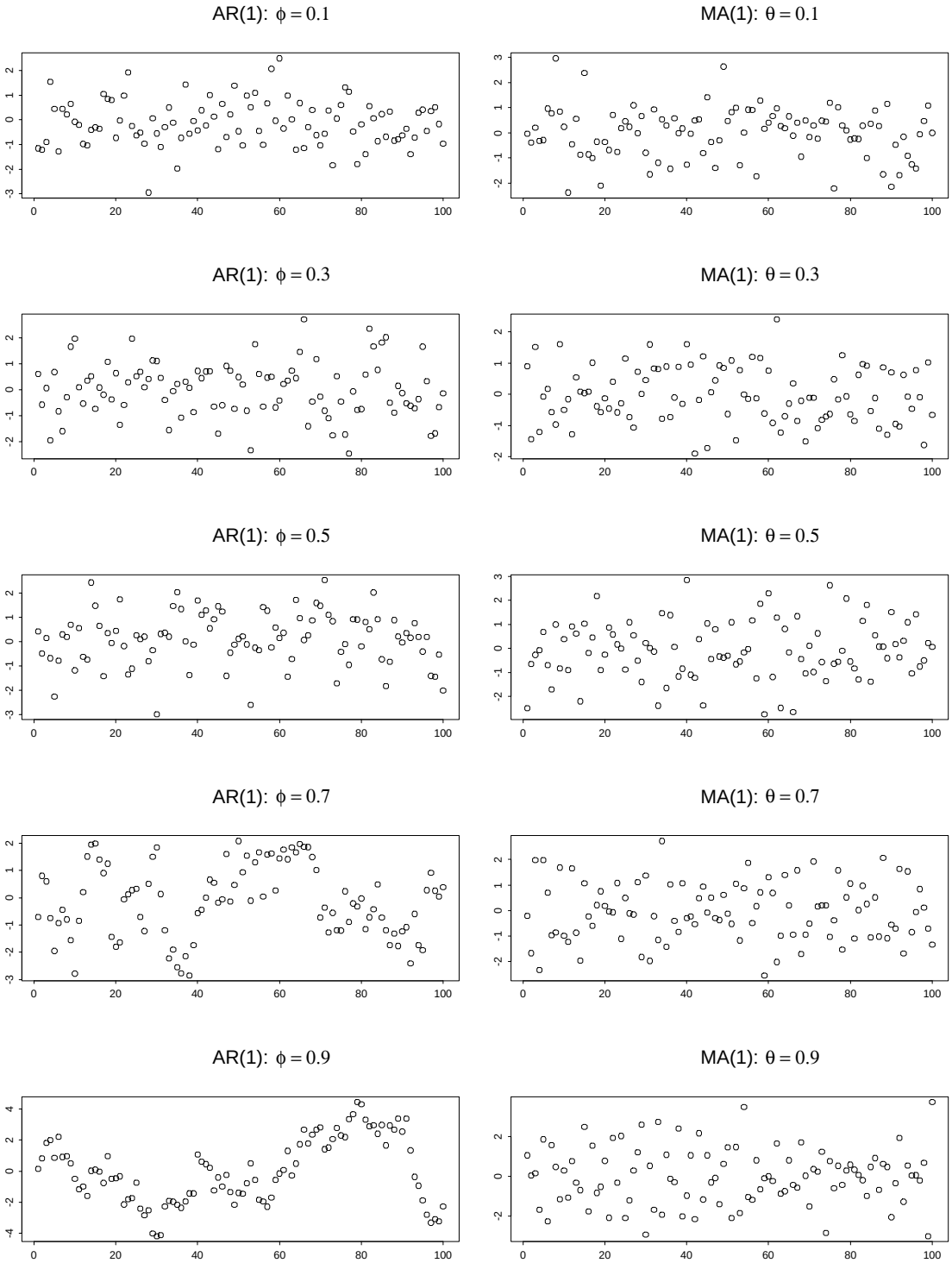

Figure 2: *Left: Simulated AR(1) series showing that the autocorrelation can be confused with mis-specification, especially with large ϕ. Right: Simulated MA(1) series showing that the lower order autocorrelation does not lead to patterns likely to be confused with mis-specification regardless of the value of θ.*

$$
\begin{aligned}
&= \hat{\boldsymbol{\Sigma}}^{-1}(\boldsymbol{I} - \hat{\boldsymbol{H}})(\hat{\boldsymbol{\Sigma}} - \boldsymbol{X}(\boldsymbol{X}'\hat{\boldsymbol{\Sigma}}^{-1}\boldsymbol{X}')\boldsymbol{X}')\hat{\boldsymbol{\Sigma}}^{-1} \\
&= \hat{\boldsymbol{\Sigma}}^{-1}(\boldsymbol{I} - \hat{\boldsymbol{H}})(\boldsymbol{I} - \hat{\boldsymbol{H}}) \\
&= \hat{\boldsymbol{\Sigma}}^{-1}(\boldsymbol{I} - \hat{\boldsymbol{H}}).
\end{aligned}
$$

Note that the hat matrix, $\hat{\boldsymbol{H}}$, is idempotent. The estimated standard deviation of $\hat{v}_i$ is therefore

$$\hat{\sigma}\sqrt{(\hat{\boldsymbol{\Sigma}}^{-1}(\boldsymbol{I} - \hat{\boldsymbol{H}}))_{ii}}. \tag{6}$$

4 Examples using Orthogonal Residuals

4.1 Lake Huron Data

Figure 3 shows a plot of the level of Lake Huron in feet, reduced by 570, as recorded over the years from 1875 to 1972. The data are listed in Brockwell and Davis (1991, p.555).

A time series regression model was fitted to the data, with the result summarised in Table 1. A linear relationship is shown to exist between lake level and time, with the errors following an AR(2) process. There is a slight downward trend in the lake level during the time in which observations were made.

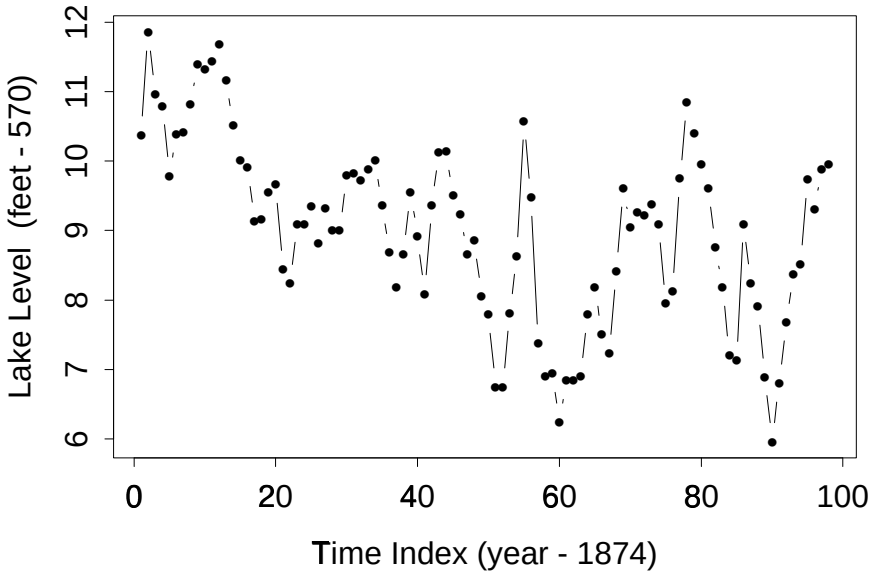

Figure 3: *Level of Lake Huron in feet from 1875 to 1972.*

Parameter	Estimate	Std.Err
Intercept	10.099	0.4601
Time Index	-0.022	0.0080
AR(2) Model		
Lag 1 Coefficient	0.977	
Lag 2 Coefficient	-0.278	
σ	0.705	

Table 1: Summary of parameter estimation for the Lake Huron data.

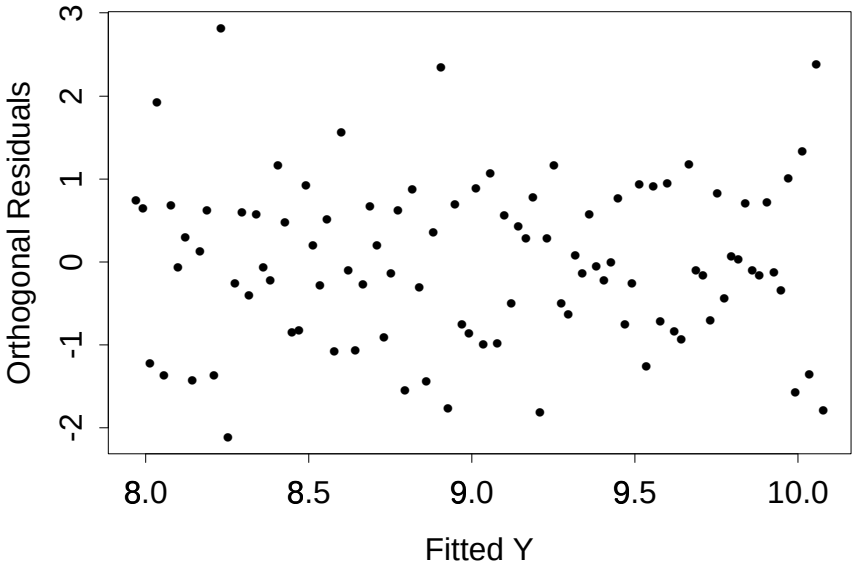

Figure 4: *Studentized orthogonal residual plot for the Lake Huron data.*

In Figure 4 the studentized orthogonal residuals (obtained by dividing $\hat{v}_i$ by (6)) are plotted against the fitted observations, $\hat{\boldsymbol{Y}}$. The marginal residuals, plotted in time order, are shown in Figure 5.

The marginal residual plot reveals systematic variation in the residuals that could be mistaken as an indication of the fitted model being inadequate. Instead, the pattern in this plot is a result of the autocorrelation in the residuals. In contrast, the plot of studentized orthogonal residuals does not indicate any such systematic variation. Apart from a few possible outliers, the orthogonal residuals indicate that the fitted time series regression model is satisfactory in explaining the level of Lake Huron over time.

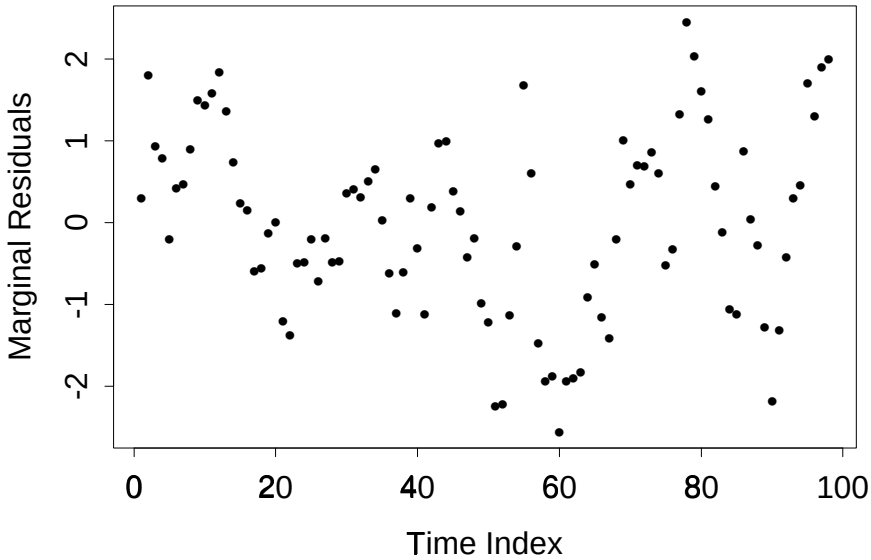

Figure 5: *Marginal residual plot for the Lake Huron data.*

4.2 Mean Shifts

A type of effect that one would like to be able to detect when it occurs within a time series is *mean shift*. This is when the mean of a time series process changes by a fixed quantity for several consecutive observations. The following example illustrates how orthogonal residuals and marginal residuals can be used together to identify a mean shift.

A data set of 125 observations was simulated using the formula

$$y_i = 2 - 5x_i + 7x_i^2 + e_i$$

where e_i was an AR(1) process with a coefficient of $\phi = 0.85$ and with $\sigma^2 = (2.5)^2$. The variable x_i was randomly generated from the continuous uniform distribution $\mathrm{U}[1, 4]$. To simulate a mean shift, the value for e_i of observations 70 through 85 was increased by 10 units. Figure 6 illustrates the relationship between y_i and x_i. The process y_i and the mean-shifted values can be easily seen in Figure 7.

Table 2 shows the result of fitting a quadratic relationship between y_i and x_i.

As evident from the studentized orthogonal residuals in Figure 8, observations 69, 70 and 85 have orthogonal residuals remarkably different from the other values. From this, it could be concluded that the only noticeable feature of the data is the presence of a few outliers. In fact, the mean shift is responsible for these large residual values.

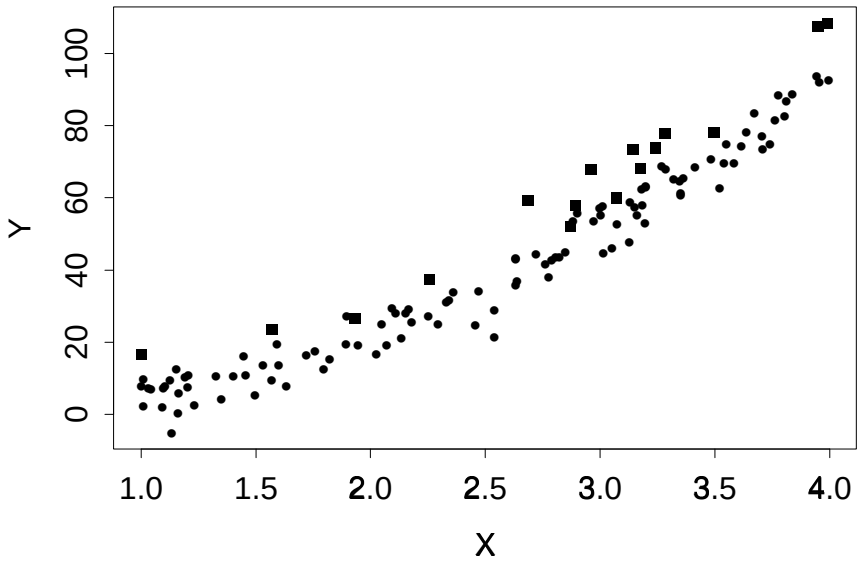

Figure 6: *Plot of y_i vs x_i for the mean shift simulation data. The mean-shifted observations are indicated with squares.*

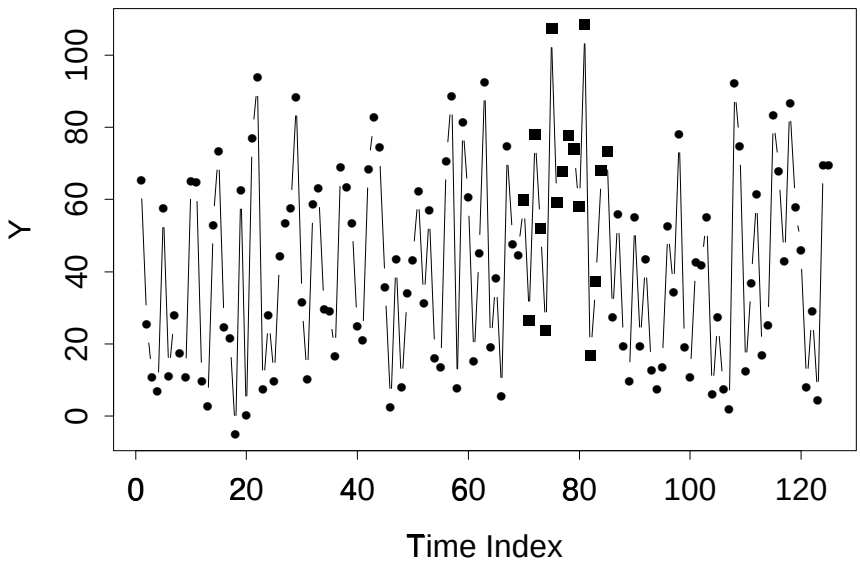

Figure 7: *Plot of y_i in time order for the mean shift simulation data. The mean-shifted observations are indicated with squares.*

Parameter	**Estimate**	**Std.Err**
Intercept	6.30	2.49
X	-7.23	1.37
X^2	7.49	0.28
AR(1) Model		
Lag 1 Coefficient	0.875	
σ	2.921	

Table 2: Summary of parameter estimation for the mean shift simulation data.

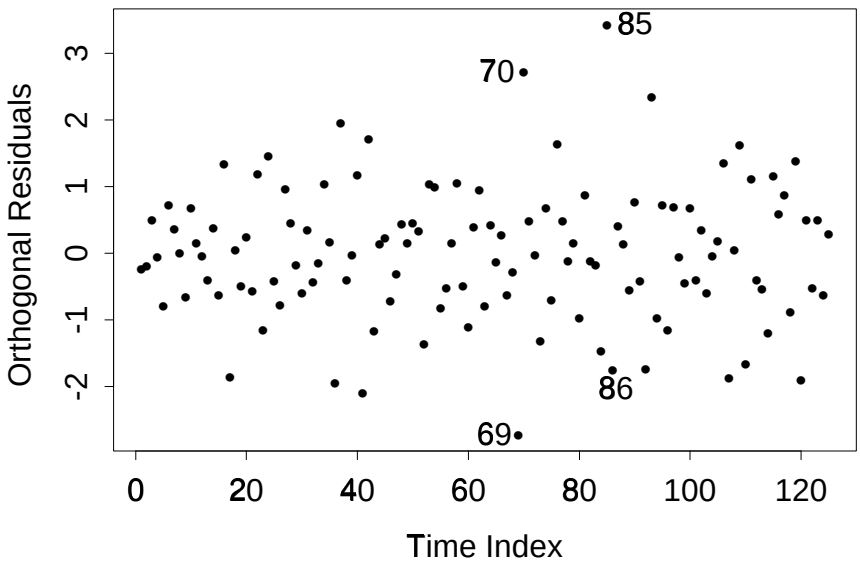

Figure 8: *Plot of studentized orthogonal residuals for the mean shift simulation data.*

Consider the low-order autocorrelation of orthogonal residuals as discussed in Section 3.1, and the covariance properties as discussed regarding (5). The residual for observation i will depend on the $(i-1)^{th}$ and $(i+1)^{th}$ observations. Observation 85 has the same time series process mean as observation 84, but not observation 86. Consequently, observation 85 has a large orthogonal residual value. Similarly observations 69 and 70 have large residual values. Observation 86 would also be expected to have a large residual value but the orthogonal residual plot reveals that it does not have a remarkable residual value.

Observations 71 through 84 all have the same time series process mean as their neighbours, and therefore do not have large orthogonal residual values.

As part of model checking, one would examine the marginal residuals next. When there may be mean shifts, it can be useful to view the plot of marginal residuals. Due to their autocorrelated nature, marginal residuals can provide insight into the underlying time series process. Figure 9 suggests that observations 70 through 85 do not follow the trend for marginal residuals established by the other observations. The conclusion to be reached here is that the mean shift apparent in Figure 9 is responsible for the indication of outliers in the plot of orthogonal residuals, and not the presence of three outlying observations. This example highlights how it can be useful to consider the orthogonal residual plot and marginal residual plot together.

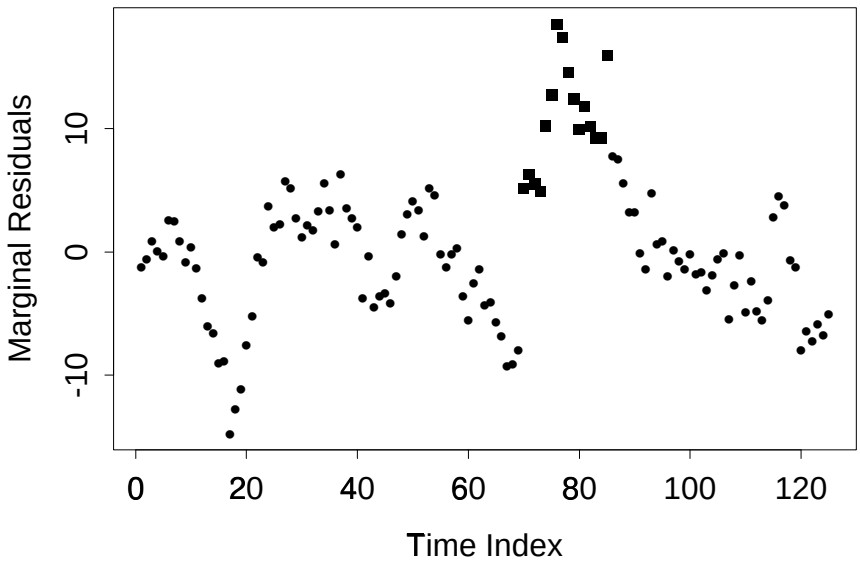

Figure 9: *Plot of marginal residuals for the mean shift simulation data. The mean-shifted observations are indicated with squares.*

4.3 Mis-specification

To demonstrate how orthogonal residuals can be used to identify model mis-specification, consider the mean shift simulation data presented above. A quadratic relationship was used to model the relationship between y_i and x_i, based on the pattern suggested in Figure 6. Suppose a straight line relationship were fitted instead. Table 3 details the resulting parameter estimates, and reveals that a higher order time series error model was fitted.

Parameter	**Estimate**	**Std.Err**
Intercept	-32.03	2.04
X	29.37	0.61
AR(2) Model		
Lag 1 Coefficient	0.354	
Lag 2 Coefficient	0.193	
σ	6.761	

Table 3: Summary of parameter estimation for the mean shift simulation data when the quadratic term has been omitted from the model.

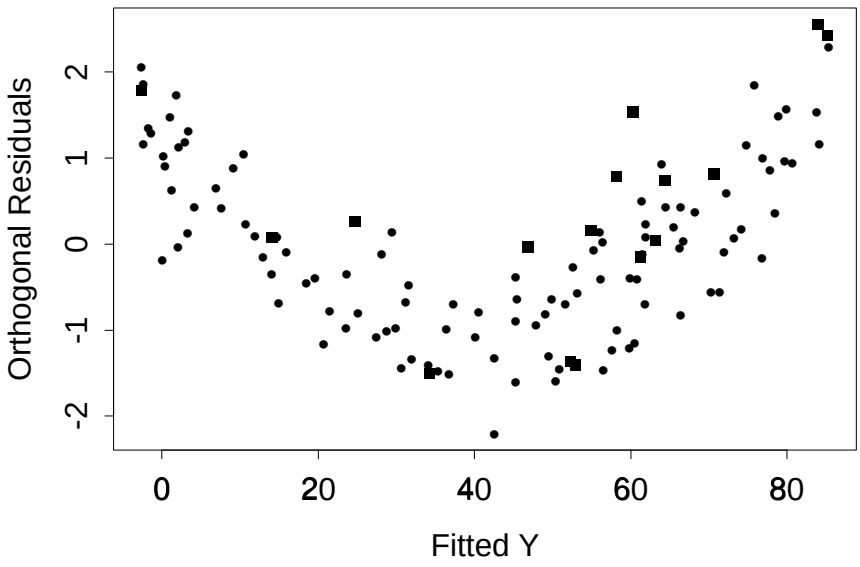

Figure 10: *Plot of studentized orthogonal residuals for fitting a mis-specified model to the mean shift simulation data. The mean-shifted observations are indicated with squares.*

The studentized orthogonal residuals, shown in Figure 10, display a quadratic pattern, suggesting that the fitted regression model has been mis-specified. Note that the pattern induced by mis-specification overwhelms any other features in the plot, such as the presence

of possible outliers indicated in the orthogonal residual plot for the correctly specified model, Figure 8. When the marginal residuals are plotted against the fitted values (not shown), a quadratic pattern, similar to that displayed in Figure 10, is evident.

5 Conditional Residuals

For the time series regression model, it is possible to calculate the expectation of Y_t conditional on previous values of the observations. Let $\mathbf{Y}_t^{(p)}$ denote the partitioned vector $[Y_{t-p}\ Y_{t-p+1}\ \cdots\ Y_{t-1}\ |\ Y_t]'$. Then $\boldsymbol{Y}_t^{(p)}$ has a multivariate normal distribution with mean

$$[f(\boldsymbol{X}_{t-p})\ f(\boldsymbol{X}_{t-p+1})\ \cdots\ f(\boldsymbol{X}_{t-1})\ |\ f(\boldsymbol{X}_t)]'$$

and covariance matrix

$$\begin{bmatrix} \boldsymbol{\Sigma}_p & \boldsymbol{\gamma}_p \\ \boldsymbol{\gamma}_p' & \gamma(0) \end{bmatrix}$$

where $\boldsymbol{\Sigma}_p$ has $(i,j)^{th}$ element $\gamma(|i-j|)$ $(1 \le i,j \le p)$, and $\boldsymbol{\gamma}_p$ has ith element $\gamma(p-i)$. Then, applying equation (8a.2.11) of Rao (1973), we obtain

$$\begin{aligned} \mathrm{E}[Y_t \,|\, Y_{t-1},\ldots,Y_{t-p},\boldsymbol{X}] &= f(\boldsymbol{X}_t) + \boldsymbol{\gamma}_p\boldsymbol{\Sigma}_p^{-1}\left(\begin{bmatrix} Y_{t-p} \\ Y_{t-p+1} \\ \vdots \\ Y_{t-1} \end{bmatrix} - \begin{bmatrix} f(\boldsymbol{X}_{t-p}) \\ f(\boldsymbol{X}_{t-p+1}) \\ \vdots \\ f(\boldsymbol{X}_{t-1}) \end{bmatrix}\right) \\ &= \phi_1 Y_{t-1} + \phi_2 Y_{t-2} + \cdots + \phi_p Y_{t-p} \\ &\quad + f(\boldsymbol{X}_t) - \phi_1 f(\boldsymbol{X}_{t-1}) - \cdots - \phi_p f(\boldsymbol{X}_{t-p}) \end{aligned}$$

because $\boldsymbol{\gamma}_p\boldsymbol{\Sigma}_p^{-1} = [\phi_p\ \phi_{p-1}\ \cdots\ \phi_1]$ by the Yule-Walker equations (see, for example, Brockwell and Davis, 1991, p.239).

The difference between Y_t and this expectation will be referred to as the *conditional residual* (for $t > p$)

$$\begin{aligned} \hat{z}_t &= Y_t - \hat{\phi}_1 Y_{t-1} - \hat{\phi}_2 Y_{t-2} - \cdots - \hat{\phi}_p Y_{t-p} - \hat{f}(\boldsymbol{X}_t) + \hat{\phi}_1 \hat{f}(\boldsymbol{X}_{t-1}) + \cdots + \hat{\phi}_p \hat{f}(\boldsymbol{X}_{t-p}) \\ &= \hat{\Phi}_p(B)\hat{e}_t. \end{aligned}$$

Assuming that the regression model has not been mis-specified, the conditional residuals will be estimates for the unobservable z_t. A plot of conditional residuals can then be used to assess whether $\hat{z}_t$ satisfies model assumptions.

An alternative approach for deriving the conditional residuals is to transform the terms

in model (2) so that the transformed errors are uncorrelated. Let $\boldsymbol{P}$ be a lower triangular matrix such that $\boldsymbol{\Sigma}^{-1} = \boldsymbol{P}'\boldsymbol{P}$. Then multiplying (2) by $\boldsymbol{P}$ we obtain $\boldsymbol{PY} = \boldsymbol{PX\beta} + \boldsymbol{Pe}$. The covariance matrix for this transformed model is $\text{Var}(\boldsymbol{Pe}) = \boldsymbol{P}'\text{Var}(\boldsymbol{e})\boldsymbol{P} = \boldsymbol{I}$, so the error terms are independent with unit variance.

The effect of the transformation is easy to understand, for example, in the AR(1) case where

$$\boldsymbol{P} = \frac{1}{\sigma}\begin{bmatrix} \sqrt{1-\phi^2} & 0 & 0 & \cdots & 0 & 0 \\ -\phi & 1 & 0 & \cdots & 0 & 0 \\ 0 & -\phi & 1 & \ddots & & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & & \ddots & \ddots & 1 & 0 \\ 0 & 0 & \cdots & 0 & -\phi & 1 \end{bmatrix}.$$

Then, for $t > p$, the tth term of $\boldsymbol{Pe}$ is $\frac{1}{\sigma}(e_t - \phi e_{t-1}) = z_t/\sigma$. However, this transformed model also allows the calculation of conditional errors for $1 \leq t \leq p-1$.

Generally, for $t > p$, the $(t,i)^{th}$ element of $\boldsymbol{P}$ is

$$P_{t,i} = \begin{cases} 1/\sigma & i = t \\ -\phi_k/\sigma & i = t-k, \quad k = 1,\ldots,p \\ 0 & \text{otherwise;} \end{cases}$$

(see Knottnerus, 1991, p.15). Consequently, $\boldsymbol{P}Y_t = \Phi_p(B)Y_t/\sigma$, $\boldsymbol{PX}_t = \Phi_p(B)\boldsymbol{X}_t/\sigma$ and $\boldsymbol{P}e_t = \Phi_p(B)e_t/\sigma = z_t/\sigma$, for $t > p$. Therefore, the conditional residuals are $\hat{z}_t = \hat{\sigma}\hat{\boldsymbol{P}}\hat{e}_t$, where $\hat{\sigma}$ and $\hat{\boldsymbol{P}}$ are estimates of σ and $\boldsymbol{P}$. The quantities $\hat{\boldsymbol{P}}\hat{e}_t = \hat{z}_t/\hat{\sigma}$ will be referred to as *standardised* conditional residuals.

A relationship exists between conditional residuals and orthogonal residuals. This is demonstrated by premultiplying the standardised conditional residual by $\hat{\boldsymbol{P}}'$, yielding

$$\begin{aligned} \hat{\boldsymbol{P}}'\hat{\boldsymbol{z}}/\hat{\sigma} &= \hat{\boldsymbol{P}}'\hat{\boldsymbol{P}}\hat{\boldsymbol{e}} \\ &= \hat{\boldsymbol{\Sigma}}^{-1}\hat{\boldsymbol{e}} \\ &= \hat{\boldsymbol{v}}. \end{aligned}$$

For an AR(1) error model, $\hat{\sigma}\hat{v}_t = \hat{z}_t - \hat{\phi}\hat{z}_{t+1}$ for $t \geq 2$, which is a non-invertible MA(1) process. This result is as expected from the results in Section 3.1. In general, $\hat{\sigma}\hat{v}_t = \hat{\Phi}_p(B^{-1})\hat{z}_t$ (for $t > p$) is a non-invertible MA(p) process, where B^{-1} denotes the forward shift operator.

A different method of transformation is presented by Seber (1977, p.172), which results in

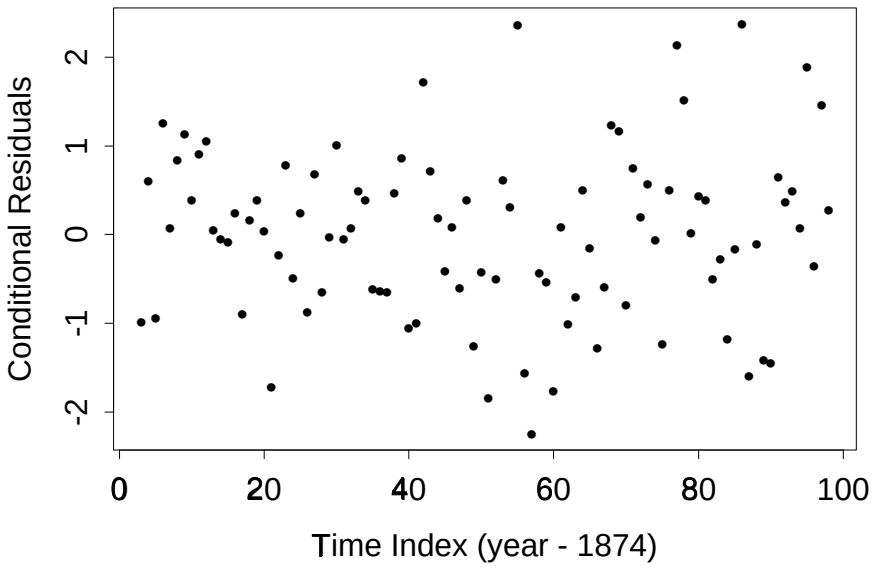

Figure 11: *Plot of standardised conditional residuals for the Lake Huron data.*

Best Linear Unbiased Scaled (BLUS) residuals. This produces a set of $(n-p)$ transformed residuals, as opposed to the n residuals produced from the methods described above.

5.1 Lake Huron Example

Figure 11 is a plot of standardised conditional residuals for the Lake Huron data set examined above. The conditional residuals are uncorrelated and appear to indicate that model assumptions regarding z_t are satisfied.

5.2 Interpreting Conditional Residuals

As stated above, the conditional residual $\hat{z}_t$ is an estimate of the unobservable z_t when the model has not been mis-specified. However, mis-specification of the time series error model can greatly affect the conditional residuals. Consider an example where the following AR(3) time series error model is appropriate

$$e_t = \phi_1 e_{t-1} + \phi_2 e_{t-2} + \phi_3 e_{t-3} + z_t$$

but where an AR(1) error model is used in the time series regression model. The resulting conditional residuals are no longer a function of z_t alone. This error model mis-specification may result in conditional residual plots with patterns induced by autocorrelation.

Therefore, the procedure used to fit a time series regression model to data affects the way the conditional residuals should be interpreted. A procedure that allows the error model to be optimally chosen through an iterative procedure (such as in iterative GLS) will usually result in conditional residuals demonstrating a white noise pattern. If instead, a procedure is used where the analyst specifies the error model, patterns in the conditional residuals may be attributable to mis-specification of the error model rather than, say, mean shifts or outliers.

Further complications can arise when the regression model is mis-specified. If the error model is fixed by the analyst, unexplained variation that exists because of the regression model mis-specification will not be accounted for in the time series error model. This unexplained variation will thus be present in the conditional residuals, resulting in patterns in residual plots.

The situations outlined above indicate the sensitivity of the conditional residual to model mis-specification. Due to this sensitivity, it is suggested that conditional residuals be only examined once the orthogonal and marginal residuals have been analysed and any apparent model mis-specification has been corrected.

6 Unified Use Of Residuals

The presentation of marginal, orthogonal and conditional residuals provides a regime for model checking and analysis. The following example illustrates how these three types of residuals can be used in a unified manner.

In a metal production facility a response y_i depends on another variable x_i and measurements of both are recorded over time. Thirty-six pairs of observations are shown in Figure 12, where a linear relationship between y_i and x_i appears appropriate. (The data presented are a linear transformation of observations recorded directly from the production plant. For reasons of confidentiality, the names of the variables and their origin cannot be disclosed.) Observations 23 and 24 are numbered as they are prominent in the plots to follow. Note also the points depicted as squares in the top-hand right corner of the plot; these correspond to observations 12 through 14.

Figure 13 is a plot of y_i in time order and shows evidence of autocorrelation. Note that observations 12 through 14 appear to be inconsistent with the trend set by the other observations. These observations are not necessarily outliers, as they also have large x_i values as shown in Figure 12.

A straight line relationship between the two variables was fitted, and the result is sum-

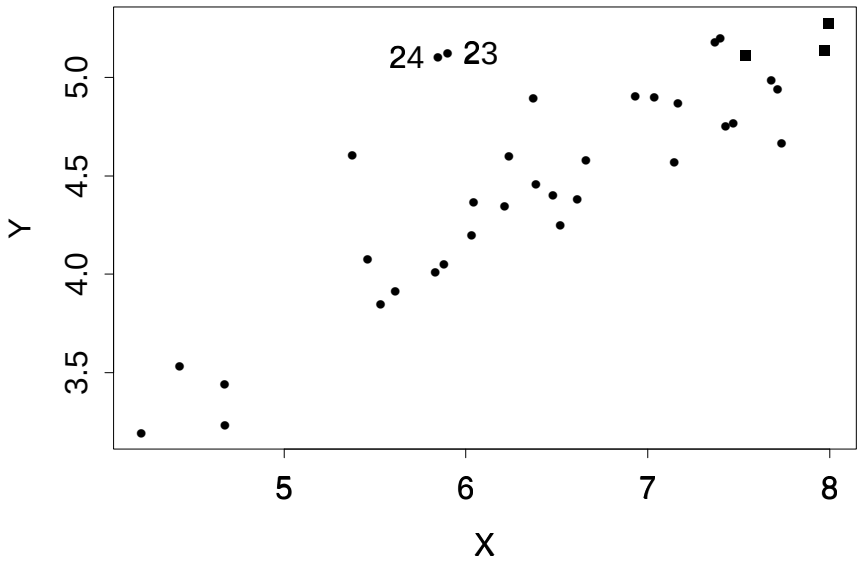

Figure 12: *Plot of y_i vs x_i for the metal production data. Observations 12 through 14 are denoted with a square. Observations 23 and 24 are numbered.*

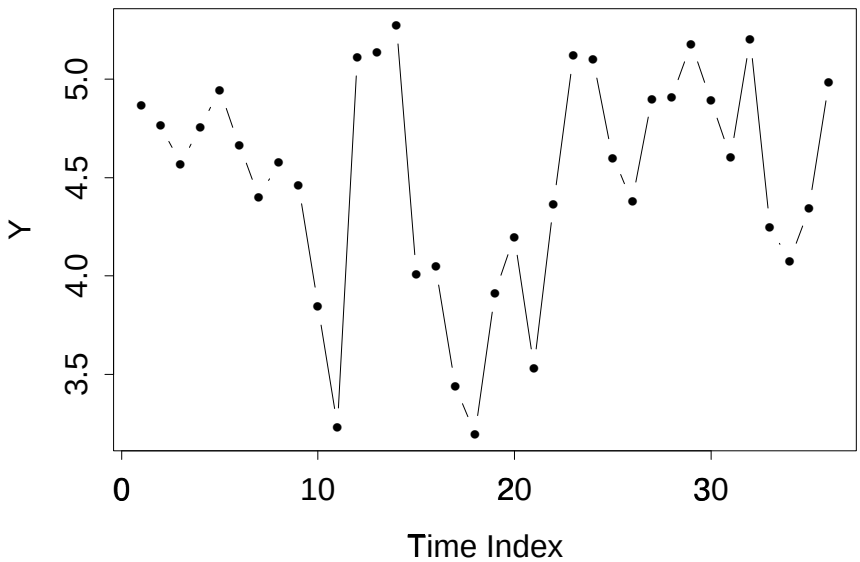

Figure 13: *Plot of y_i in time order for the metal production data.*

Parameter	Estimate	Std.Err
Intercept	1.415	0.3259
X	0.479	0.0478
AR(1) Model		
Lag 1 Coefficient	0.583	
σ	0.255	

Table 4: Summary of parameter estimation for the metal production data.

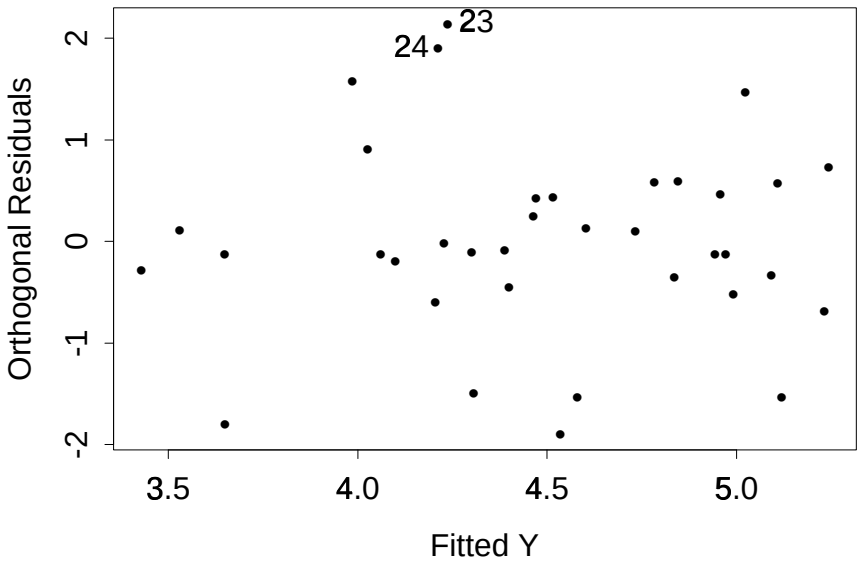

Figure 14: *Studentized orthogonal residual plot for the metal production data. Observations 23 and 24 are numbered.*

marised in Table 4.

To assess the fit of the model in Table 4, the orthogonal residuals presented in Figure 14 are examined. This plot does not reveal any mis-specification or any other problems in the fitted regression model. Observations 23 and 24 are again labelled.

Examining the marginal residuals, Figure 15, reveals the underlying time series error process. In this plot, observation numbers 23 and 24 have residual values that are inconsistent with the trend established by the other values. These two observations do not follow the time series error model assumed to be responsible for autocorrelation in the observations.

Finally, the conditional residuals are presented in Figure 16. This plot confirms observation 23 to be discordant. Since observations 23 and 24 are both large and have similar y_i values,

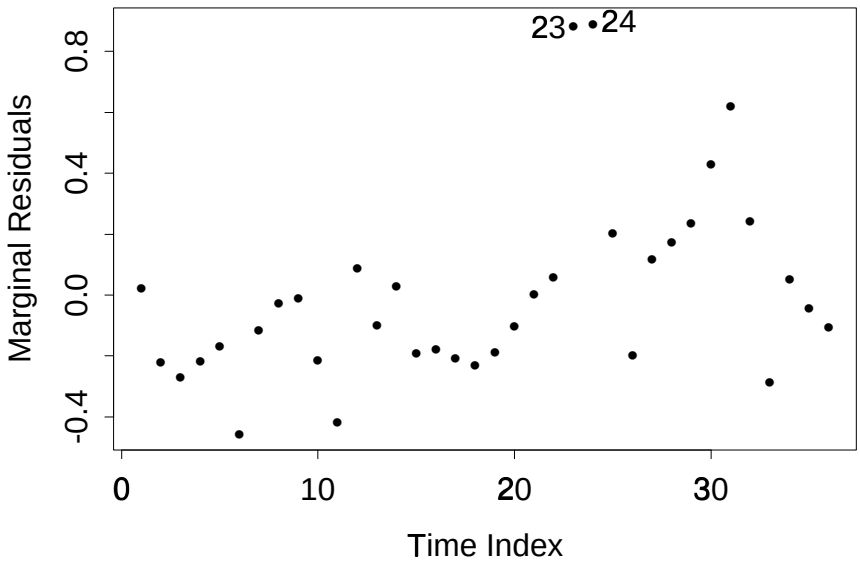

Figure 15: *Marginal residual plot for the metal production data. Observations 23 and 24 are numbered.*

the resulting conditional residual for observation 24 is not discordant.

The apparently inconsistent conclusions between the three residual plots illustrates the point that these plots should be interpreted differently. In the metal production data above, observations 23 and 24 have been highlighted as unusual observations. As far as the regression model is concerned, these observations are not outliers. The y_i and x_i values for these observations are consistent with other observations. However, the marginal residual values suggest these observations to be discordant. Reconciling these two conclusions suggests that the process was producing y_i values (with associated x_i values) consistent with other observations, but that these values were not expected at time points 23 and 24 – these observations were produced contrary to the underlying autocorrelation. One could surmise that some special cause was in effect over these two times.

7 Conclusion

We have considered the need for suitable residual diagnostic plots for time series regression. Although the marginal residual may be intuitively appealing, it has been shown that it is not suitable for identifying mis-specification in the regression model. However, it is useful in checking the unobserved time series error process assuming the regression model is correctly specified. For identifying model mis-specification, we have proposed the orthogonal residual which is orthogonal to both the fitted values and covariates, and which

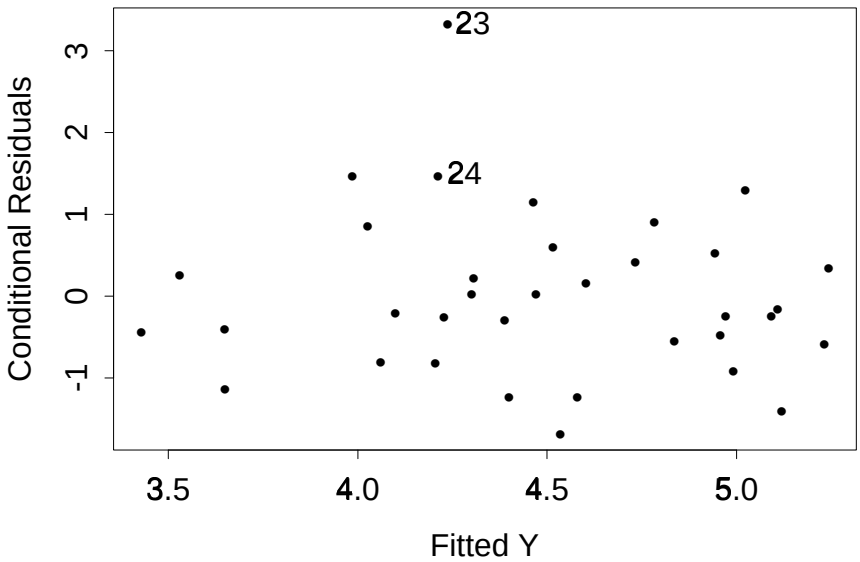

Figure 16: *Conditional residual plot for the metal production data. Observations 23 and 24 are numbered.*

possesses low-order autocorrelation. When used in conjunction with marginal residual plots, the orthogonal residual plots can help identify mean shifts and other patterns. Finally, conditional residuals have been shown to be useful in checking the white noise error component. These residuals are sensitive to the regression and error model fitted, and it is suggested that they be analysed only after orthogonal and marginal residuals are examined.

Together, these three residuals provide the means for examining various aspects of the fitted model and for identifying problems such as model mis-specification, mean shifts and outliers.

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