Outlier detection in autocorrelated manufacturing processes

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ABSTRACT

In this simulation study, different schemes for monitoring production processes with of autocorrelated data are compared. A time series forecast is applied to the autocorrelated process and the resultant residuals are monitored by a control chart and two common tracking signals. Performance comparisons of different monitoring schemes have been typically based on the Average Run Length (ARL) criterion but we offer the the Cumulative Distribution Function (CDF) as an alternative and more informative performance evaluation criterion. This study compares the performance of the Individuals Control Chart (ICC), the Smoothed Error Tracking Signal (ETS), and the Cumulative Sum (CTS) Tracking Signal (CTS) in terms of their ability to detect the presence of additive outliers. Based on the CDF, we found that the Individuals Control Chart offers the greatest probability of early detection of an additive outlier in an autocorrelated process.

Keywords: autocorrelation, control charts, tracking signals

Introduction

The occurrence of large unusual observations is not uncommon in time series data. These outliers may be due to recording errors or to one-time unique situations such as an unexpected change in demand for a product or a change in a production system. Fox (1972) defines two types of outliers that may occur in practice; *additive outliers,* corresponding to external disturbances that affect the value of a single observation; and, *innovational outliers*, or *step shifts*, refering to internal disturbances that change the value of an observation and all other successive observations. Typically in process control environments, the performance of monitoring schemes have been compared based on only in terms of their ability to detect step shifts or innovational outliers (Montgomery, 2013). However, which monitoring scheme detects the presence of an additive outlier most quickly is also of great interest in determining abnormal process behavior, a measurement error, a recording error or incorrect specifications based on distributional assumptions. (Walfish, 2006).

Autocorrelation implies the existence of a relationship between the outcomes produced in different time periods by the same process. With advances in measurement technology along with more frequent sampling, today's manufacturing processes often yield observations that are autocorrelated. The inertia effects present in most manufacturing processes coupled with the advent of automated gages that sample processes more frequently, often render most process data autocorrelated (Montgomery and Mastrangelo 1991, Woodall and Faltin 1993).

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This paper compares the performance of an Individuals Control Chart (ICC), the Smoothed Error Tracking Signal (ETS) and the Cumulative Tracking Signal (CTS) in monitoring residuals from exponential smoothing forecasts applied to autoregressive process data of order one, denoted by AR(1), in the presence of additive outliers. Montgomery and Mastrangelo (1991) show that a number of chemical and manufacturing processes conform to this model. The study shows that the Individuals Control Chart offers the highest probability of early detection of an additive outlier in AR(1) processes.

Literature review

The presence of autocorrelation creates unique problems to the performance of process monitoring schemes. Positive autocorrelation tends to increase the frequency of out-of-control signals that are detected by monitoring schemes. Positive autocorrelation occurs most often in production environments and chemical operations (Woodall and Faltin, 1993).

The performance of control charts in the presence of autocorrelation has been explored by a number of authors. Superville and Adams (1994) compare the performance of the Individuals chart, the Cumulative Sum (CUSUM) chart, and the Exponentially Weighted Moving Average (EWMA) chart in terms of their ability to detect *step shifts* in autocorrelated processes. Superville and Adams (1995) compare the performance of these charts to different tracking signals again in their ability for early detection of step shifts in autocorrelated process. Lu and Reynolds (1999) suggest the use of a combined Shewhart-EWMA chart for autocorrelated data. Lianjie, Daniel and Fugee (2002) suggest the use of a triggered CUSCORE chart on residuals. Lee et al. (2009) propose distribution-free charts for monitoring shifts in the mean of autocorrelated processes. Wu and Yu (2010) advocate a neural network approach for monitoring the mean and variance of an autocorrelated process. Chang and Wu (2011) present a Markov Chain approach to calculating the ARL for control charts on autocorrelated process data. Superville and Yorke (2012) compare the performance of Individuals, CUSUM and EWMA charts in detecting additive outliers in an autocorrelated process.

In the field of statistical process control, control charts have traditionally been used to monitor production processes. In the forecasting and time series fields, tracking signals perform a similar function, the monitoring of forecasting systems. The statistical tools are similar in both fields and have a common purpose, namely to provide timely information concerning changes in the systems.

Alwan and Roberts (1988) have proposed a method for monitoring autocorrelated data that involves the application of a time-series forecast to the process and monitoring the residuals. Unusual behavior in the process should result in a large error that is reflected as a signal on a control chart or tracking signal. Traditionally, monitoring tools have been compared on the basis of Average Run Lengths (ARLs).

The ARL is the expected number of observations in which a single period outlier is detected by the monitoring scheme as as an out-of-control situation. However, simple exponential smoothing forecasts recover quickly from step increases as well as additive outliers in the time series process that it monitors. This would suggest that the performance of forecast-based schemes should be based on the probability of "early detection" rather than on the ARL. As any average measure, the ARL is inflated by long run lengths, and thus it is an inadequate measure of quick recovery, especially with monitoring schemes characterized by short run lengths. Hence the cumulative distribution function (CDF) of the run lengths is offered as an alternative criterion to the average run length (ARL) for the selection of an appropriate monitoring scheme. The CDF provides the cumulative probability of a detecting a signal occurring by the ith time period after a disturbance.

A model of autocorrelated data

A time series model that is widely used in inventory and quality control applications is the autoregressive integrated moving average (ARIMA) model (Box and Jenkins 1976). The ARIMA(p,d,q) model is denoted by

$$\Phi_p(B)\,\nabla^d X_t = \Theta_q(B)\varepsilon_t \tag{1}$$

where $\Phi_p(B) = (1 - \phi_1 B - \phi_2 B^2 - ... - \phi_p B^p)$ is an autoregressive polynomial of order p, $\Theta_q(B) = (1 - \theta_1 B - \theta_2 B^2 - ... - \theta_q B^q)$ is a moving average polynomial of order q, B is the backshift operator, ∇ is the backward difference operator, and ε_t, the white noise, is a sequence of independent normal random errors with mean zero and variance σ^2, denoted by $\varepsilon_t \sim N(0, \sigma^2)$.

A special case of the ARIMA model that has been found to be useful in production and quality control environments is the ARIMA(1,0,0), referred to as the first-order autoregressive model and denoted by AR(1). It is represented by

$$X_t = \xi + \phi X_{t-1} + \varepsilon_t \tag{2}$$

where ϕ is the autocorrelation coefficient and ξ is the drift, or average increase per period, of the series. Without loss of generality, it is assumed in this article that $\varepsilon_t \sim N(0,1)$ and $\xi = 0$. Montgomery and Mastrangelo (1991) show that a number of chemical and manufacturing processes conform to this model.

The simple exponential smoothing forecast, also known as the exponentially weighted moving average (EWMA) forecast is given by

$$F_{t+1} = \alpha_F X_t + (1 - \alpha_F)F_t\ , \qquad 0 \leq \alpha_F \leq 1 \tag{3}$$

where X_t represents the process observation at time period t, and F_{t+1} represents the one-step-ahead forecast for observation X_{t+1} at time period t. The forecast error at time period t, denoted by e_t, is defined as

$$e_t = X_t - F_t.$$

Alwan and Roberts (1988) have observed that processes that do not drift too rapidly are well modeled by simple exponential smoothing. For the AR(1) model with no drift, Cox (1961) has shown that optimal simple exponential smoothing in terms of minimum mean square forecast error is given by

$$\alpha_F = 1 - ½[(1 - \phi)/\phi], \qquad 1/3 < \phi \leq 1 \tag{4}$$

where ϕ is the parameter of the AR(1) process. This result is used in the simulations discussed in the following sections.

Monitoring schemes for residuals

In this study, the Individuals Control Chart (ICC), and the Smoothed Error (ETS) and Cumulative Sum (CTS) tracking signals are applied to exponential smoothing residuals and their performances evaluated.

The Individuals Control Chart

The Individuals Control Chart applied to residuals requires an estimate of the variance of the residuals. Defining the *i*th moving range to be

$$MR_i = |e_i - e_{i-1}|, \qquad i = 2, 3, ..., m \tag{5}$$

and

$$\overline{MR} = \frac{1}{m-1}\sum_{i=2}^{m} MR_i, \tag{6}$$

the control limits are

$$\overline{X} \pm C_1 MR/d_2 \tag{7}$$

where the constant C_1 is typically set to 3.0 resulting in an ARL of 370 for independent observations. Montgomery (2013) has tabulated values for C_1 and d_2. For comparing monitoring scheme performance in this simulation study, control limits are set to achieve an in-control ARLs of 250 for each monitoring scheme. Values for these control limits are provided in the "Simulation results" section of this paper.

The Smoothed Error Tracking Signal

Trigg's (1964) Smoothed Error tracking signal (ETS) is given by

$$ETS_t = |E_t / MAD_t| \tag{8}$$

where

$$E_t = \alpha_1 e_t + (1 - \alpha_1)E_{t-1}, \qquad 0 \leq \alpha_1 \leq 1 \tag{9}$$

and

$$MAD_t = \alpha_2 |e_t| + (1 - \alpha_2)MAD_{t-1}, \qquad 0 \leq \alpha_2 \leq 1. \tag{10}$$

Typically, $E_0 = 0$ and MAD_0 is set equal to its expected value which is approximately equal to 0.8 σ_e (where σ_e is the standard deviation of the residuals). A signal occurs if ETS_t exceeds a critical value K_1. Gardner (1983) suggests that the value of K_1 should be set to achieve a desired in-control ARL. For comparing monitoring scheme performance in this simulation study, control limits are set to achieve an in-control ARLs of 250 for each monitoring scheme.

The Cumulative Sum Tracking Signal

Brown's (1959) Cumulative Sum tracking signal (CTS) is given by

$$CTS_t = \left| SUM_t / MAD_t \right| \tag{11}$$

where

$$SUM_t = e_t + SUM_{t-1} \,. \tag{12}$$

The value of MAD_0 is set equal to its expected value as with ETS_0. The value of SUM_0 is set equal to zero. A signal occurs if the value of CTS_t exceeds a critical value K_2. Gardner (1983) suggests that the value of K_2 should be set to achieve a desired in-control ARL. For comparing monitoring scheme performance in this simulation study, control limits are set to achieve an in-control ARLs of 250 for each monitoring scheme.

Concerning the choice of parameters for the forecast model α_F (equation 4) and tracking signals (α_1 and α_2), McKenzie (1978) and Gardner (1985) recommend that $\alpha_F \geq \alpha_1$, with $\alpha_1 = 0.1$ commonly used in practice. Small values of α_1 allow the ETS to respond more quickly to small disturbances in the demand process. Traditionally, the smoothing parameters in the numerator and denominator of the ETS have been set equal to each other, that is, $\alpha_1 = \alpha_2$. More recently, McClain (1988) has suggested that the smoothing parameter in the MAD model (equation 10), α_2, be smaller than the parameter in the error model (equation 9), α_1, so that the variance of the residuals may be stabilized.

Performance evaluation: ARL vs. CDF

The ARL is the standard criterion on which the relative performance of both tracking signals and control charts has been traditionally based. However, exponentially smoothed forecasts tend to recover quickly from disturbances in the time series that it monitors. The impact of forecast recovery on the ARLs of control charts applied to residuals has been discussed by Wardell, Moskowitz, and Plante (1994) and others. In general, the rate of forecast recovery depends on the type of shift, the underlying model of the series, and the forecasting equation used. Forecast recovery is shown to significantly impact the ARLs of all monitoring schemes.

Concerning forecast recovery in the presence of additive outliers, consider for example, an exponential smoothing forecast applied to an AR(1) process in which an additive outlier occurs in the process. Figure 1 shows a sequence of fifty observations from an AR(1) process with $\phi = 0.9$ and the optimal exponentially smoothed forecasts (with $\alpha_F = 0.9444$). Figure 2 displays the resulting residuals.

At time period 31, an additive outlier occurs. The forecast lags behind the observed data at time period 32 resulting in a large forecast error. By time period 33, the forecast has adjusted to the new level of the process. The residuals have returned to values close to zero as they were prior to the step increase. Notice that the '*window of opportunity*' available for detection of this time-series disturbance is quite small. This 'quick' adjustment is bound to happen at other instances, but sometimes an outlier will result in a much longer run; the average ARL of such a monitoring scheme will tend to be inflated by very large runs that seldom occur.

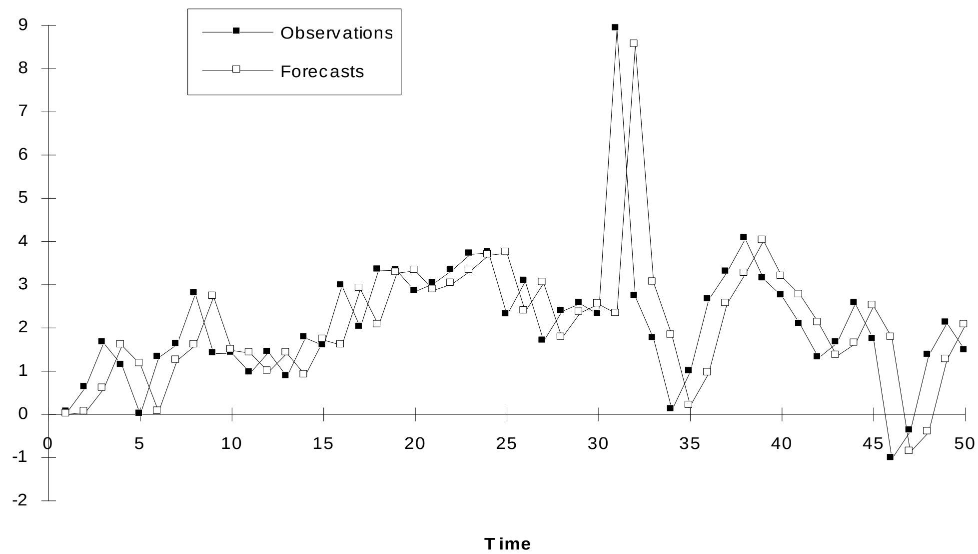

Figure 1. Observations from an AR(1) process with $\phi = 0.9$ and exponentially smoothed forecasts with $\lambda = 0.9444$. An additive outlier of size $3\sigma_p$ occurs at observation 31.

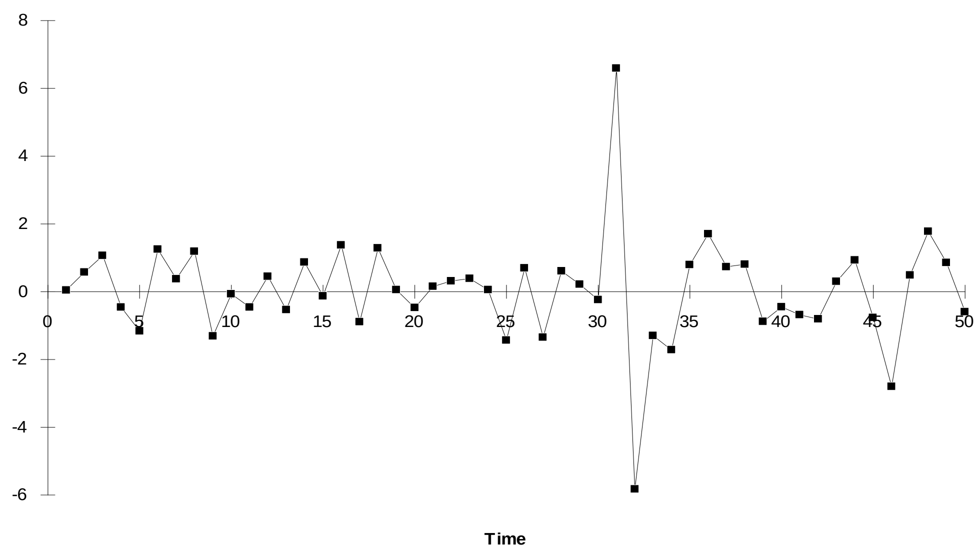

Figure 2. Residuals from an AR(1) process with $\phi = 0.9$ and exponentially smoothed forecasts with $\lambda = 0.9444$. An additive outlier of size $3\sigma_p$ occurs at observation 31.

The need to select monitoring schemes that provide quick detection of process disturbances, leads one to investigate the cumulative probability of a signal following a process disturbance as a meaningful criterion for the comparison of forecast-based monitoring schemes.

The use of the cumulative distribution functions (CDF) as an evaluation criterion is not new. Barnard (1959), Bissell (1968) and Gan (1991) recommend its use for control charts of independent observations. McClain (1988) advocates its use for forecast-based schemes which incorporate tracking signals. The CDF measures the cumulative percentage of disturbances in a time series that are detected early.

Design of the simulation study

In this simulation study, three monitoring schemes were compared. They are the traditional Shewhart control charts, or ICC, the ETS, and the CTS as defined earlier. ARLs and CDFs are provided for each monitoring scheme for outliers of size $3.0\sigma_p$, where $\sigma^2_p = \sigma^2 / (1-\phi^2)$, is the variance of an AR(1) process.

The initial values of the smoothed-error for the ETS (eq. 8) and the sum of errors for the CTS (eq. 11) were set to zero as suggested by Gardner (1985) and McClain (1988). The smoothing constants $\alpha_1$and α_2 were set to 0.10 as suggested by McKenzie (1978).

The simulation study was conducted as follows:

i) AR(1) series with autoregressive parameter values of ϕ =0.0, 0.5, 0.7, and 0.9 and N(0,1) were generated by the International Mathematical and Statistical (IMSL) (2010) subroutine RNARM / DRNARM. The subroutine generates a time series from a specified Autoregressive Moving Average (ARMA) model. The parameter ξ was set equal to zero, without loss of generality.
ii) The first fifty observations were used to allow for a burn-in period, for 1000 renderings of the series,
iii) The forecast is started at time period 2 with its initial value set equal to the first observed data point.
iv) After the burn-in period and before any disturbance in the process, fifty (50) preliminary sequences of residuals (each sequence consisting of 5000 observations) are used to estimate the mean and variance of the residuals. The residuals from theses preliminary samples are not monitored by a control chart or tracking signal but are only used to estimate the mean and variance of the forecast errors.
v) Ttracking signals and control charts are constructed based on the estimates obtained in step (iv). The initial MAD values were set to $0.8\sigma_e$ (σ_e is the standard deviation of the residuals) as suggested by Montgomery, Johnson and Gardiner (1990).
vi) At observation 51, an additive outlier of size $3.0\sigma_p$ (where $\sigma^2_p = \sigma^2 / (1-\phi^2)$), was introduced to each time series that was generated in step 1. The ICC, ETS and CTS are applied to the residuals. Each monitoring scheme is allowed to run until a single signal occurs. At this point, a single run length is recorded and the monitoring scheme reset for the next iteration.

vii) Steps (i)-(iii), (v) and (vi) were repeated 1000 times resulting in 1000 run lengths. These 1000 run lengths are used to estimate the ARLs and CDFs after an additive outlier of size $3.0\sigma_p$.

Simulation results

Table 1 displays parameters and control limits used in the simulation study.

TABLE 1
Parameters and Control Limits Used in the Simulation Study (in-control ARL =250)

Parameters used in the Simulation			**Control Limits**		
Φ	**λ_F**	**α_1=α_2**	**ICC**	**ETS**	**CTS**
0.0	0.0000	0.1	2.880	0.658	23.250
0.5	0.5000	0.1	1.577	0.466	5.500
0.7	0.7857	0.1	0.660	0.459	5.433
0.9	0.9444	0.1	0.166	0.546	8.900

For all monitoring schemes, control limits were obtained for an in-control ARL of 250. Table 2 shows simulated ARLs and CDFs for the Individuals control charts and the ETS and CTS tracking signals applied to the optimal exponential smoothing residuals from an AR(1) process with ϕ ranging from 0.0 to 0.9. Outliers are simulated as $3\sigma_p$. The results can be summarized as follows:

1. With the exception of the case where ϕ=0.9, the magnitude of the ARLs for the autocorrelated cases (ϕ>0) are significantly larger than for the independent case (ϕ=0). The difference in ARL magnitudes can be attributed to the quick recovery of the EWMA forecast. Recall that the ARL, as an average measure, is inflated by long run lengths. It is unable to adequately reflect short run lengths that are indicative of quick forecast recovery. For forecast-based schemes, ARLs are not informative.

2. Based on CDFs, the Individuals Control Chart provides a higher probability of early detection of an outlier for the autocorrelated cases where ϕ=0.5 and 0.7. This occurs although the Individuals Control Chart may have a longer ARL than any other monitoring scheme. As an example, consider the case where ϕ=0.5. The Individuals control chart provides the highest probability of early detection on the first observation after the outlier (60.5%) despite having a longer ARL (92.7) than the other monitoring schemes. The detection of an outlier early, that is, within the first few observations after the occurrence of an outlier is critical since the forecast recovers quickly. This suggests the use of the Individuals control chart for the autocorrelated cases.

TABLE 2

Average Run Lengths and Percentage of Signals detected by the *i*th observation after an outlier of size 3σ_p. Residuals are from AR(1) processes with autoregressive parameters ϕ.

ϕ	Monitoring Scheme	ARL	CDF – Cum. Prob. of number of periods where outlier is detected					
			1	2	3	4	5	6
0	**ICC**	1.8	54.2	79.0	90.5	96.1	98.2	98.9
	ETS	4.3	3.9	12.7	30.5	53.9	75.7	92.2
	CTS	21.9	0.0	0.0	0.0	0.0	0.0	0.0
0.5	**ICC**	92.7	60.5	64.0	64.3	64.8	64.9	65.2
	ETS	43.1	12.6	32.8	48.3	60.0	67.5	72.6
	CTS	4.5	5.4	21.6	40.3	58.7	73.0	83.2
	ICC	42.9	84.9	85.2	85.4	85.4	85.5	85.5
0.7	**ETS**	90.0	20.2	34.1	40.5	46.6	49.4	52.4
	CTS	6.4	9.9	22.6	34.5	45.9	54.2	61.7
	ICC	1.0	100	100	100	100	100	100
	ETS	61.9	30.2	35.6	38.0	39.5	39.8	40.3
0.9	**CTS**	52.6	0.9	2.0	3.1	5.0	7.6	10.3

Conclusion

This paper compared forecast-based quality control schemes for monitoring autocorrelated observations in the presence of additive outliers. The quick recovery property of forecasting tools suggests that comparisons of control charts and tracking signals applied to residuals be based on the CDF on the run lengths and not on the ARL. The Individuals control chart is recommended over the Smoothed Error and CUSUM tracking signals as it offers the highest probability of early detection of an additive outlier in an AR(1) process.

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