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QUALITY QUANDARIES*

Checking Process Stability with the Variogram

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INTRODUCTION

It is a fundamental tenet of statistical quality control that all processes vary. But if stable and in a state of statistical control, we can have a high degree of confidence that the process will continue to produce output that only rarely vary outside given limits. Indeed, if the variability is sufficiently small relative to our customer's requirements and the process is in a state of statistical control, then we need not check every individual item. In other words, we can trust the process will continue to produce "good" parts and therefore leave it alone for shorter periods of time because it is *predictable*. All we need is to occasionally check to verify that the process remains in statistical control. It is this principle of predictability and the strategy of "trust but verify" that was Dr. Shewhart's primary economic rationale for introducing statistical process control based on sampling as opposed to 100% inspection.

So what is required for a process to be in a state of statistical control? According to the authoritative ANSI/ISO/ASQC Standard A3534-2-1993, a state of statistical control is defined as "[A] state in which the variations among the observed sampling results can be attributed to a system of chance causes that does not appear to change with time." There is general agreement that this definition implies that when in a state of statistical control, the mean and standard deviation of the process

remain constant over time. However, the definition is sometimes also interpreted to imply that consecutive observations must be statistically independent. However, this latter condition is unnecessarily restrictive.

In traditional applications of statistical process control (SPC) where the quality characteristic typically is a mechanical dimension and often a process output, we agree that autocorrelation frequently is a sign of more fundamental trouble and that it might be productive to hunt down the assignable cause. However, SPC is increasingly used to control process in- and out-put parameters such as temperature and pressure that are typically sampled at relatively high frequency. Under such circumstances, autocorrelation may simply be inherent to the process and not something that can be removed. In fact, trying to compensate for it may be counterproductive.

Fortunately, it is not necessary for the observations to be independent for a process to be stable and predictable. A stationary time series exhibits a stable probability distribution of its output. Both the mean and the standard deviation are constant and independent of time as required and the process is predictable.

Once we relax the condition of independence, it is difficult to establish that a given process is stationary. Stationary but positively autocorrelated processes may exhibit prolonged cycles. Thus given a finite set of data from a process, it may in practice be difficult to ascertain whether the process is stationary or not. The autocorrelation function used in the analysis of time series sometimes provides ambiguous answers. However, in this column we will demonstrate the use of an alternative tool called the variogram that can be helpful in determining whether a process is stationary or not.

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EXAMPLE: TEMPERATURE READINGS FROM A CERAMIC FURNACE

To provide an illustration of a stationary but autocorrelated process, consider the hourly temperature observations from the large ceramic furnace we used in a previous column (Bisgaard and Kulahci, 2004). A time series plot of the data is shown in Fig. 1. We see that although the process seems to vary around a fixed mean and show limited variability, it does exhibit periodicities, and it can be hard to distinguish from a process that is not in statistical control.

We previously showed that the furnace data can be modeled as a stationary second order autoregressive AR(2) time series process

$$\tilde{z}_t = \phi_1 \tilde{z}_{t-1} + \phi_2 \tilde{z}_{t-2} + a_t$$

where $\tilde{z}_t = z_t - \mu$ are deviations from the mean and a_t random shocks. We found that the parameter estimates were $\hat{\phi}_1 = 0.9824$ and $\hat{\phi}_2 = -0.3722$. We also showed that with these parameter estimates, the AR(2) model satisfied the stationarity conditions

$$\begin{aligned}\phi_2 + \phi_1 &< 1 \\ \phi_2 - \phi_1 &< 1 \\ -1 &< \phi_2 < 1\end{aligned}$$

indicating that the process is most likely stationary, and therefore in a state of statistical control (see Box et al., 1994). Modeling the process and checking that

the parameter estimates satisfy stationarity conditions is one way to test for stationarity. However, it would be desirable to have a simple exploratory tool to investigate whether a process is stationary or not without having to model it first. The variogram is such a tool.

PERIODICITIES IN STATIONARY PROCESSES

Before we introduce the variogram, let us first discuss why data may exhibit cycles and specifically the reason for the apparent cyclic pattern in the data shown in Fig. 1. We believe it is not as unusual as one might think. The second order autoregressive process was first investigated by the Cambridge statistician G. Udney Yule in 1927 in a paper entitled, "On a method of investigating periodicities in disturbed series, with special reference to Wölfer's sunspot numbers." In this paper, Yule wanted to explain how periodicities in times series data may occur. To this end, he provided a nice physical illustration that may also be instructive in our case. First he reminded the reader that the horizontal movement of a pendulum "when left to itself" in a room can be modeled in continuous time as a second order homogeneous differential equation. It is well-known that the solution to this second order differential equation is a damped sinusoidal curve. Yule then proceeded to explain that a second order autoregressive model is the discrete time equivalent of a second order linear differential equation with constant coefficients. But, as he

Figure 1. Time series plot of hourly temperature readings from a ceramic furnace.

Figure 2. The theoretical spectral density of an AR(2) model with parameters similar to the ceramic furnace.

explained, suppose “boys get into the room and start pelting the pendulum with peas, sometimes from one side and sometimes from the other.” The pendulum, he argued, will then exhibit horizontal movements that will follow a second order autoregressive model with random inputs or shocks, a_t . In other words, the system will continue to exhibit second order dynamic behavior. But, rather than vary as a regular sinusoidal curve, “the graph will remain surprisingly smooth, but amplitude and phase will vary continuously.”

It is often possible to approximate the dynamic behavior of a system with second order differential equations. Indeed, it does not seem far-fetched to imagine that our ceramic furnace with its very considerable inertia approximately resembles the dynamic behavior of a second order system. Thus, we can expect an oscillatory behavior analogous to a pendulum disturbed by naughty boys shooting peas at it. In other words, because of the inertia, the furnace temperature may exhibit damped random oscillations around a fix mean but essentially remain in a state of control. Indeed, attempts to compensate for such inherent fluctuations will likely increase rather than decrease the variability.

Let us further explore the issue of inherent periodicities of a stationary time series. The frequency spectrum is a graph that shows the amplitude of the sinusoidal components for a range of frequencies. For the present set of parameters of the AR(2) model fitted to the furnace data, it can be shown (see Box et al., 1994, p. 63) that the theoretical frequency spectrum is as shown in Fig. 2. In the present case, the spectrum shows

a peak at a frequency around $f_0 \approx 0.07$ corresponding to a period $p = 1/f$ of approximately 14 hours. Thus the prevalent cycle is about 14 hours. This matches well with the pattern seen in the time series plot in Fig. 1.

STATIONARY OR NOT STATIONARY?

In practice there is no clear demarcation line between a stationary and a non-stationary process. A process that is nearly non-stationary will wander randomly away from its mean and not return for considerable time lags. Based on a finite record it will therefore be difficult to distinguish such a process from one that is truly non-stationary.

The most basic assessment of stationarity is simply to plot a sufficiently long series of data to see if the process appears stationary. Another approach is to plot the autocorrelation. If the autocorrelation does not dampen out within, say 15 to 20 lags, then the process is likely not stationary. However, if the process is not stationary it will continue to wander off and the sample variance will continue to increase as the record gets longer. Thus the autocorrelation is, strictly speaking, not defined for non-stationary processes.

An alternative and more flexible tool is the variogram; for a detailed discussion, see Box et al. (1994) and Box and Luceno (1997). This tool is well defined and applicable to stationary as well as non-stationary processes. To understand how it works suppose $\{z_t\}$ is a time series. The variogram G_m measures the

Figure 3. The theoretical variogram for the AR(2) model fitted to the furnace data.

variance of differences m time units apart relative to the variance of the differences one time unit apart. Specifically, the variogram is defined as

$$G_m = \frac{V\{z_{t+m} - z_t\}}{V\{z_{t+1} - z_t\}}, \quad m = 1, 2, \dots \quad (1)$$

where G_m is plotted as a function of the lags, m .

For a stationary process, $G_m = (1 - \rho_m)/(1 - \rho_1)$. But for a stationary process, as m increases, $\rho_m \rightarrow 0$. Hence, G_m when plotted as a function of m will reach an asymptote $1/(1 - \rho_1)$. However if the process is non-stationary, G_m will instead monotonically increase. For a stationary process with positive auto-correlation and no seasonality, the intuitive interpretation of the variogram is as follows: because of the

Figure 4. Sample variogram for the ceramic furnace data.

positive autocorrelation, consecutive observations are expected to be similar. The variance of the first differences will therefore be less than the variance of the differences two lags apart, three lags apart, etc. However, as m gets large the differences m lag and $m + 1$ lag apart will eventually be very similar. Thus while the variogram for small m 's tends to get larger as m increases, it will eventually reach a steady state.

Figure 3 provides a plot of the theoretical variogram for the AR(2) model with parameter estimates $\hat{\phi}_1 = 0.9824$ and $\hat{\phi}_2 = -0.3722$. We see that the variogram after 8 or 9 lags seems to settle down implying that the process is stationary.

In practice, we need to estimate the variogram directly from the time series data. Thus we need an expression for the sample estimate of G_m . The literature is a bit ambiguous about how the sample variogram should be computed. However, Haslett (1997) has shown that a good estimate can be obtained by simply using the usual sample squared standard deviation applied to the differences with appropriate modifications for changing sample sizes that occur when we take differences. Specifically, he suggests using

$$\hat{V}\{z_{t+m} - z_t\} = s_m^2 = \frac{\sum_{t=1}^{n-m} (d_t^m - \bar{d}^m)^2}{n - m - 1} \quad (2)$$

where $d_t^m = z_{t+m} - z_t$ and $\bar{d}^m = (n - m)^{-1} \sum d_t^m$. Hence the sample variogram is given by

$$\hat{G}_m = \frac{s_m^2}{s_1^2}, \quad m = 1, 2, \dots \quad (3)$$

Figure 4 shows the sample variogram for the furnace data. As we should expect, the sample estimate differs somewhat from the theoretical variogram. However, aside from sample variations, the general appearance of the sample variogram does seem to indicate that it converges to a stable level confirming our previous assessment that the process most likely is stationary.

It should be noted that the sample variogram typically is not provided as a standard pull-down menu item by statistical software packages used by quality engineers. However, it is relatively simple to compute. All that is needed is to compute successive differences for a number of lags. To produce Fig. 4 in MINITAB, we produced difference columns for up to 15 lags and then computed the sample variances for each. The ratios of these sample variances to the sample variance

of the first differences produced the sample variogram given in Fig. 4.

CONCLUSION

Modern quality control methods are increasingly being used to monitor complex industrial processes. In that context, data are typically sampled automatically at a relatively high frequency. It should therefore be expected that the data is positively autocorrelated. When positively autocorrelated, a stationary process may wander off for considerable length of time before it returns to its mean. Thus it can be difficult for the quality engineer to assess whether the process is stationary or not. The most fundamental requirement will always be to get sufficiently long records. However, once such records have been obtained, the variogram is a simple and useful exploratory tool that can be used by quality professionals to investigate whether a process is stationary or not.

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