

- Quality variances during what are considered to be *normal* periods of operation can be quite large.
- Process and quality variables show significant *time* correlations (due to the process dynamics as well as the temporal correlations in these disturbances).
- There is significant incentive to reduce the variance even during *in-control* periods through adjustment of process condition (*e.g.*, temperature, pressure).

These considerations point to the following potential shortcomings of the traditional approaches:

- *Testing For a Wrong Hypothesis?*

The previously-discussed traditional methods can be considered as a kind of hypothesis testing. The hypothesis tested is:

During *in-control* epochs (i.e., periods of normal operations), the measured variable is serially independent with the mean and variance corresponding to the chosen target and the bound.

While the above hypothesis is reasonable in many industries like the automotive industries and parts industries where SQC has proven invaluable, *its validity is highly questionable for chemical and other process industries*. As mentioned above, in these industries, measured variables exhibit significant time correlation even in normal (*in-control*) situations.

- *Lack of Control Need During In-Control Period?*

SPC is based on the assumption that control adjustments should be made only when an abnormal (*out-of-control*) situation arises. This is

sensible for many industries (e.g, automotive industries) where there are assignable causes to be removed. In reality, quality variables in many chemical processes show significant variances even during *in-control* periods. The deviations are usually time-correlated giving opportunities for control through process input adjustments (which can lower the quality variance, leading to economic savings, more consistent products and less environmental problems, etc.). In most cases, little costs are associated with adjustments.

For the remainder, we will highlight the above limitations through simple examples and propose remedies / alternatives.

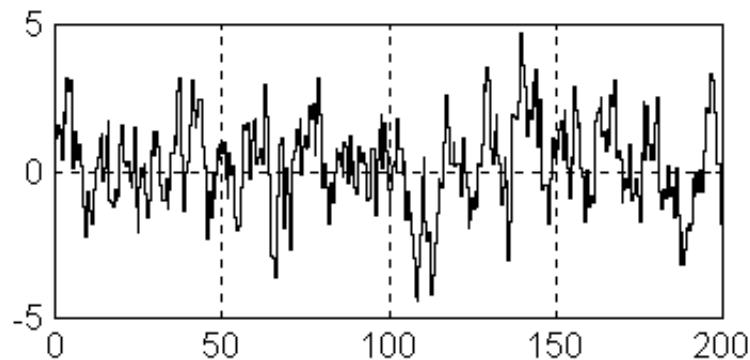
1.4.2 MOTIVATING EXAMPLE

The Simple First-Order Case.

To understand the limitation arising from ignoring the time correlation, consider the situation where the output follows the pattern

$$(y(k) - \bar{y}) = \alpha(y(k-1) - \bar{y}) + \varepsilon(k) \quad (1.18)$$

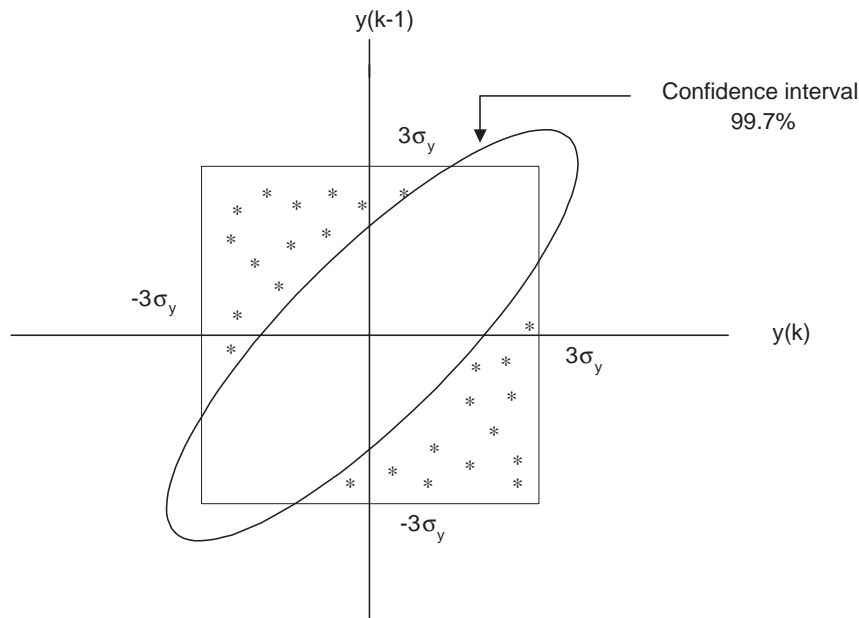
where $\varepsilon(k)$ is an independent (white) sequence with zero mean and variance σ_ε^2 . A plot of an example sequence is shown below.



Note that

$$\begin{aligned}
 & E \left\{ \begin{bmatrix} y'(k) \\ y'(k-1) \end{bmatrix} \begin{bmatrix} y'(k) & y'(k-1) \end{bmatrix} \right\} \\
 &= E \left\{ \begin{bmatrix} \alpha y'(k-1) + \varepsilon(k) \\ y'(k-1) \end{bmatrix} \begin{bmatrix} \alpha y'(k-1) + \varepsilon(k) & y'(k-1) \end{bmatrix} \right\} \\
 &= \begin{bmatrix} \alpha^2 \sigma_y^2 + \sigma_\varepsilon^2 & \alpha \sigma_y^2 \\ \alpha \sigma_y^2 & \sigma_y^2 \end{bmatrix} \tag{1.19}
 \end{aligned}$$

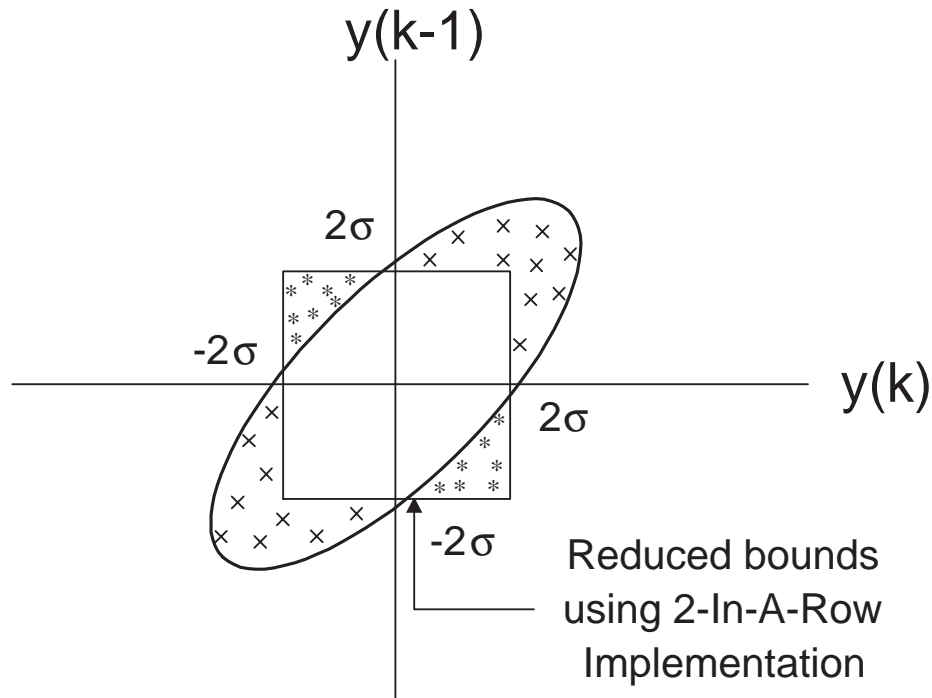
The plot of a confidence interval may look as below:



What's The Problem?

Note that, if $y'(k)$ is monitored through the Shewart chart, one would not be able to catch points marked with * that are outside the 99.7% confidence interval (missed faults).

In order to catch these points, one may choose to tighten the bounds. However, doing this may cause false alarms.



In short, by ignoring the time correlation, one gets bounds that are inefficient.

A Solution?

One solution is to model the sequence using a time series and decorrelate the sequence. For instance, one may fit to the data a time-series model of form

$$y'(k) = a_1 y'(k-1) + \varepsilon(k) \quad (1.20)$$

where $\varepsilon(k)$ is a white (time-independent) sequence. The one-step-ahead prediction based on the above model is

$$\hat{y}'(k|k-1) = a_1 y'(k-1) \quad (1.21)$$

The prediction error is

$$y'(k) - \hat{y}'(k|k-1) = (\alpha - a_1) y'(k-1) + \varepsilon(k) \quad (1.22)$$

Note that, assuming the model parameter matched the true value ($a = \alpha$), the prediction error is $\varepsilon(k)$ which is an independent sequence. Hence, the idea goes as follows:

Apply the statistical monitoring methods to the prediction error sequence $\varepsilon(k)$, since it satisfies the basic assumption of independence underlying these methods.

1.4.3 TIME-SERIES MODELS

Assuming the underlying distribution is stationary (during *in-control* periods), one can use a time series to model the temporal correlation.

Various Model Types

Different forms of time series models exist for modeling correlation of a time sequence. We will drop the notation $'$ and use y to represent y' for simplicity. The following is an Auto-Regressive (AR) model of order n :

$$y(k) = a_1y(k-1) + a_2y(k-2) + \cdots + a_ny(k-n) + \varepsilon(k) \quad (1.23)$$

The parameters can be obtained using the linear least squares method. A more complex model form is the following Auto-Regressive Moving Average (ARMA) model:

$$\begin{aligned} y(k) = & a_1y(k-1) + a_2y(k-2) + \cdots + a_ny(k-n) \\ & + \varepsilon(k) + c_1\varepsilon(k-1) + c_n\varepsilon(k-n) \end{aligned} \quad (1.24)$$

The above model structure is more general than the AR model, and hence much fewer terms (i.e., lower n) can be used to represent the same random sequence. However, the parameter estimation problem this time is nonlinear. Often, pseudo-linear regression is used for it.

General Model Form

The general form of a model for a stationary sequence is

$$y(k) = H(q^{-1})\varepsilon(k) \quad (1.25)$$

where $H(q^{-1})$ can be interpreted as a filter with $H(0) = 1$. For instance, for AR model,

$$H(q^{-1}) = \frac{1}{1 - a_1q^{-1} - \dots - a_nq^{-n}} \quad (1.26)$$

For ARMA model,

$$H(q^{-1}) = \frac{1 + c_1q^{-1} + \dots + c_nq^{-n}}{1 - a_1q^{-1} - \dots - a_nq^{-n}} \quad (1.27)$$

1.4.4 COMPUTATION OF PREDICTION ERROR

Key Idea

The one-step-ahead prediction based on model (1.25) is

$$\hat{y}(k|k-1) = E\{y(k)|y(k-1), \dots\} = (1 - H^{-1}(q^{-1}))y(k) \quad (1.28)$$

Note that, since the constant term cancels out in $(1 - H^{-1}(q^{-1}))$ (because $H(0) = 1$), it contains at least one delay and the RHS does not require $y(k)$.

The optimal prediction error is

$$y(k) - \hat{y}(k|k-1) = H^{-1}(q^{-1})y(k) = \varepsilon(k) \quad (1.29)$$

Hence, assuming the model correctly represents the underlying system, the prediction error should be white. In conclusion,

Compute $\varepsilon(k) = H(q^{-1})y(k)$ and monitor $\varepsilon(k)$ using the Shewart's method, etc.

by filtering the output sequence with filter $H^{-1}(q^{-1})$, one can decorrelate

the sequence, which results in an independent variable suitable for traditional SPC methods. $H^{-1}(q^{-1})$ can be thought of as *whitening filter*.

1.4.5 INCLUDING THE DETERMINISTIC INPUTS INTO THE MODEL

What's the Issue?

In many cases, variation of the output variable may not be entirely stochastic. That is, there may be deterministic inputs that contribute to the observed output behavior. Included in the deterministic inputs are

- measured disturbances
- manipulated inputs (e.g., setpoints to the existing loops)

In this case,

rather than viewing the output behavior as being entirely stochastic, we can add the effect of the deterministic input explicitly into the model for a better prediction.

Another option is to include them in the output vector. However, the former option is more convenient for designing a supervisory control system.

Model Form : Same As Before But With Extra Inputs

In the linear systems context, one may use a model of the form

$$y(k) = G(q^{-1})u(k) + H(q^{-1})\varepsilon(k) \quad (1.30)$$

For instance, the following is the ARX (Auto-Regressive with eXtra input) model.

$$\begin{aligned} y(k) = & a_1y(k-1) + a_2y(k-2) + \cdots + a_ny(k-n) \\ & + b_1u(k-1) + \cdots + b_mu(k-m) + \varepsilon(k) \end{aligned} \quad (1.31)$$

Another popular choice is the ARMAX (Auto-Regressive Moving Average with eXtra input) model, which looks like

$$\begin{aligned} y(k) &= a_1y(k-1) + a_2y(k-2) + \cdots + a_ny(k-n) \\ &\quad + b_1u(k-1) + \cdots + b_mu(k-m) \\ &\quad + \varepsilon(k) + c_1\varepsilon(k-1) + \cdots + c_n\varepsilon(k-n) \end{aligned} \quad (1.32)$$

Monitoring: No More Difficult!

The one-step-ahead prediction is given as

$$y(k|k-1) = G(q^{-1})u(k) + (I - H^{-1}(q^{-1}))(y(k) - G(q^{-1})u(k)) \quad (1.33)$$

and the prediction is once again

$$y(k) - y(k|k-1) = H^{-1}(q^{-1})(y(k) - G(q^{-1})u(k)) = \varepsilon(k) \quad (1.34)$$

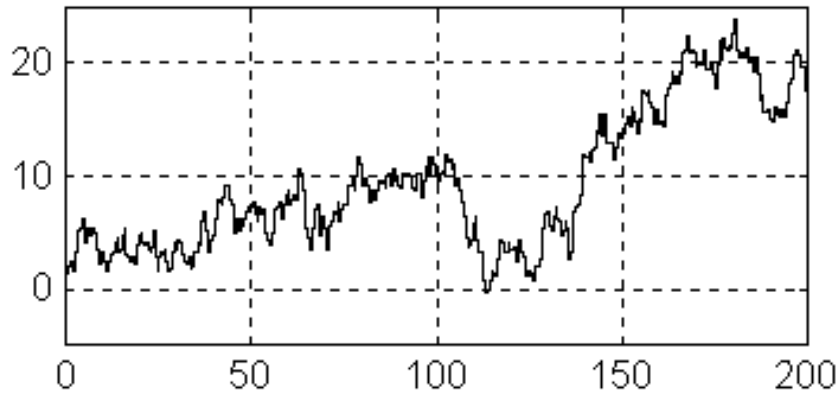
Control Opportunity: Additional Benefit

Having the deterministic inputs in the model also give opportunities to control the process (in addition to the monitoring). That is, one can manipulate the deterministic input sequence $u(k)$ to shape the output behavior in a desirable manner (e.g., no bias, minimum-variance).

1.4.6 MODELING DRIFTING BEHAVIOR USING A NONSTATIONARY SEQUENCE

Basic Problem

For many processes, even during what is considered to be *in-control* periods, variables do not have a fixed mean or level, but rather are drifting / *mean-shifting* (*nonstationary*). Shown below is an example of such a process:



Model Form

the following ARIMA model is the popular choice:

$$\begin{aligned}
 (1 - a_1q^{-1} - \dots - a_nq^{-n})y(k) &= (b_1q^{-1} + \dots + b_mq^{-m})u(k) \\
 &+ \underbrace{(1 + c_1q^{-1} + \dots + c_nq^{-n})}_{\text{integrator}} \frac{1}{1 - q^{-1}} \varepsilon(k)
 \end{aligned}
 \tag{1.35}$$

The above can be re-expressed as:

$$\begin{aligned}
 \Delta y(k) &= a_1\Delta y(k-1) + a_2\Delta y(k-2) + \dots + a_n\Delta y(k-n) \\
 &+ b_1\Delta u(k-1) + \dots + b_m\Delta u(k-m) \\
 &+ \varepsilon(k) + c_1\varepsilon(k-1) + c_n\varepsilon(k-n)
 \end{aligned}
 \tag{1.36}$$

Hence, simple differencing of input and output data gets rid of the stationarity.

More generally, a model for a nonstationary sequence takes the form of

$$\Delta y(k) = G(q^{-1})\Delta u(k) + H(q^{-1})\varepsilon(k)
 \tag{1.37}$$

Decorrelation: Just Needs Differencing!

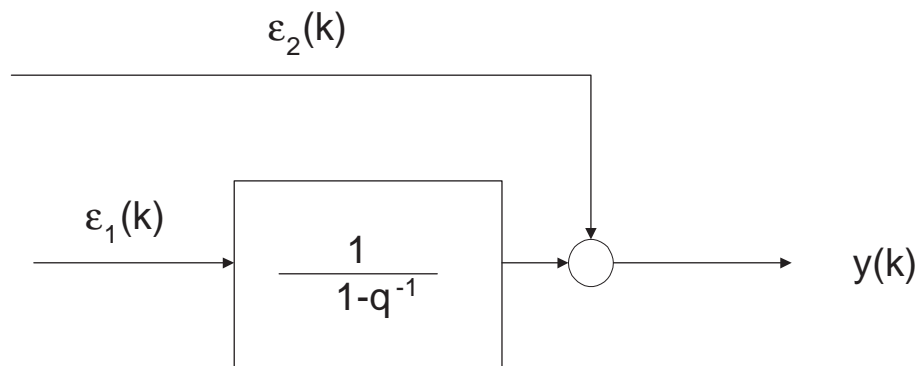
Once again, de-correlation can be done through

$$\varepsilon(k) = H^{-1}(q^{-1})(\Delta y(k) - G(q^{-1})\Delta u(k)) \quad (1.38)$$

Hence, the only extra thing required is differencing of the data, both in prior to the model construction and decorrelation through filtering with the model inverse.

Example

Consider the case where the output is sum of the following two random effects:



Then, the overall behavior of y can be expressed as

$$y(k) = \frac{1 - \alpha q^{-1}}{1 - q^{-1}} \varepsilon(k) \quad (1.39)$$

There also is a result that all nonstationary disturbances must tend toward the above model (integrated moving average process) as sampling interval gets larger.

For the above model,

$$\begin{aligned}
 y(k|k-1) &= \left(1 - \frac{1-q^{-1}}{1-\alpha q^{-1}}\right) y(k) \\
 &= \frac{(1-\alpha)q^{-1}}{1-\alpha q^{-1}} y(k) \\
 &= (1-\alpha)[y(k-1) + \alpha y(k-2) + \alpha^2 y(k-3) \cdots \cdots]
 \end{aligned}$$

This is the EWMA. Hence, EWMA is thought to provide more efficient monitoring under the postulated model due to its extrapolation capability.

In addition, the prediction error (or whitened output) becomes

$$\varepsilon(k) = \frac{\Delta y(k)}{1 - \alpha q^{-1}} \tag{1.40}$$

which can be written as

$$\varepsilon(k) = \alpha \varepsilon(k-1) + \Delta y(k) \tag{1.41}$$

This is EWMA for the differenced output.

1.4.7 MULTIVARIABLE TIME-SERIES MODEL

Getting Rid of Both the Spatial and Temporal Correlations

A natural next step is to consider the time correlation in the multivariate statistical monitoring context.

MIMO Time Series Model?

One option is to fit a multivariable time series model to the data. For instance, MIMO ARMA model looks like

$$y(k) = A_1 y(k-1) + \cdots + A_n y(k-n) + \varepsilon(k) + C_1 \varepsilon(k-1) + \cdots + C_n \varepsilon(k-n) \tag{1.42}$$

Once a model of the above form becomes available, one can then compute the prediction error as before (which is a white sequence) and apply the

chi-square monitoring.

The trouble is that multivariable time-series models are notoriously difficult to construct from data. It requires a special parametrization of the coefficient matrices and the resulting regression problem is nonconvex with many local minima.

State-Space Model?

A much better option is to fit the following state-space model instead:

$$\begin{aligned}x(k+1) &= Ax(k) + K\varepsilon(k) \\y(k) &= Cx(k) + \varepsilon(k)\end{aligned}\tag{1.43}$$

Such models may be developed from y data using one of the following options:

- computation of the autocorrelation function followed by factorization and model reduction.
- state-space realization using (modified) *subspace identification* techniques. The obtained model can be further refined using the prediction error minimization.

Once a model of the above form becomes available, $x(k)$ in the model can be updated recursively. The prediction error $\varepsilon(k) = y(k) - Cx(k)$ is a time-wise independent sequence and can be monitored using the chi-square statistics as before. The two-tier approach based on the principal component analysis should be utilized in this context as well.

Incorporating Deterministic Inputs

If there are deterministic inputs, one can include them in the model as before.

$$\begin{aligned}x(k+1) &= Ax(k) + Bu(k) + K\varepsilon(k) \\y(k) &= Cx(k) + \varepsilon(k)\end{aligned}\tag{1.44}$$

Model for Nonstationary Sequences

Finally, in the case that the outputs exhibit nonstationary, drifting-type behaviors, the data can be differenced before the model fitting and this results in a model of the form

$$\begin{aligned}x(k+1) &= Ax(k) + B\Delta u(k) + K\varepsilon(k) \\ \Delta y(k) &= Cx(k) + \varepsilon(k)\end{aligned}\tag{1.45}$$

1.5 REGRESSION

1.5.1 PROBLEM DEFINITION

We have two vector variables $x \in \mathcal{R}^n$ and $y \in \mathcal{R}^p$ that are *correlated*. We have a data set consisting of N data points, $\{(x(i), y(i)), i = 1, \dots, N\}$. We assume that x and y are both mean-centered (x and y represent the deviation variables from the respective means). Now, using the data, we wish to construct a prediction model

$$\hat{y} = f(x)\tag{1.46}$$

which can be used to predict y given a fresh data point for x .

Example

- In a distillation column, relate the tray temperatures to the end-point compositions. In this case $x = [T(1), T(2), \dots, T(n)]^T$ and $y = [x_D, x_B]^T$.
- In a polymer reactor, relate the temperature and concentration (trends) to the average molecular weight, polydispersity, melt index, etc. of the product.