Statistical Approaches to Fault Analysis in Multivariate Process Control

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Abstract

After a brief review of some statistical approaches to multivariate process control, we present a technique for determining root causes when information is available on likely out of control scenarios or fault types. We utilize linear dimension reduction techniques such as principal component analysis or partial least squares to limit the number of latent variables to study. While using historical in control data is important in establishing control means and limits, these data often have less structure for dimension reduction than do data which come from known fault types. If these latter data are available, the expanded data set can be analyzed for dimension reduction, using the in control data to set limits in the reduced set. When a sequence of points is then seen to be beyond the control limits, the distance to the nearest known fault type is measured. If the dimensions can be reduced to two, these can be plotted as well. The new problem is classified into one of the existing fault types when its distance to it becomes smaller than a pre-specified criterion. If it remains out of control, but fails to approach an existing fault type, a new fault paradigm is created. Our approach is demonstrated on a simulated chemical process.

KEYWORDS: multivariate process control; principal components; partial least squares; quality control

1. Introduction

In multivariate quality control one desires to monitor a large number of process (or predictor) variables in order to keep a number of quality (or response) variables in control. Should a change in the quality variables occur, whether manifested as a change of level, trend, outlying data point or other significant pattern, rapid detection is desired. Because of the large number of variables involved, it is not practical to monitor each variable, via the traditional univariate charting techniques such as Shewhart charts, cumulative sum (CUSUM) charts, or exponentially weighted moving average (EWMA) charts. Often, however, there is some level of analytical redundancy in the process in the sense that a significant correlation may exist either among the variables within each set and/or between the predictor and response variables. This redundancy can be exploited to reduce the dimensionality of the monitoring problem. In such a case, dimension reduction techniques such as principal component analysis (PCA) or partial least squares (PLS) can be employed to significantly simplify the problem. See, for example, MacGregor et al. [1], Piovoso et al.[2], or Mejdell and Skogestad [3]. While this facilitates detection of an out of control process, it complicates the root cause analysis, because it is often unclear on which original variable(s) the new point is out of control, and hence what action needs to be taken to correct the problem.

In order to choose the appropriate target values for the center line of the control chart and sensible control limits for detection, historical data from the process must be available, unless one is willing to set arbitrary goals not based on the current performance of the process. Unfortunately, it is precisely when the process is in control that the least amount of dimension reduction is possible. Therefore it is important to have data available when the process is not in control, preferably in specific known fault types.

While many dimension reduction techniques are available, we shall restrict our discussion to the two widely used methods of Principle Component Analysis (PCA) and Partial Least Squares (PLS). These two methods both attempt to reduce the dimension of the original variable space by finding a reduced set of new variables that capture the structure or essential features of the original variables. These new variables or directions are just linear combinations of the original variables. Ideally, the number of new variables will be one or two. In this case, one can monitor the variables directly by plotting new data on a one or two dimensional graph. We review these dimension reduction techniques first, and compare their behavior with ordinary least squares. In section 3 we discuss how fault information can be used to identify and classify the fault type of the new points. Finally we summarize our findings.

2. Dimension reduction

Before briefly explaining how PCA and PLS reduce the number of variables, we will review what ordinary least squares (OLS) regression does. Let us put the process variables in a matrix $\mathbf{X}$ and the quality variables in a matrix $\mathbf{Y}$, and refer to these as the X and Y variables respectively. For ease of comparison we will assume that all the variables have been centered and scaled so that each X and each Y variable has mean 0 and standard deviation 1. (This does not imply any loss of generality. The variables can be centered and scaled simply by subtracting their average and dividing by their standard deviation).

If we consider the following (univariate) model:

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \epsilon,$$

OLS find the estimates of the coefficients $\boldsymbol{\beta}$ via:

$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}.$$

One way of interpreting this is to view the resulting predicted values of $\mathbf{y}$,

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{b}$$

as a direction in X variable space, $b_1x_1 + \ldots + b_px_p$. This direction is chosen by the virtue that it is the single linear combination of the X's most correlated with the output $\mathbf{y}$.

In other words,

$$\mathbf{b} = \underset{||\mathbf{b}||=1}{argmax} \quad corr^2 \quad (\mathbf{y}, \mathbf{X}\mathbf{b})$$

2.1. PCA

By contrast, PCA finds its directions in $\mathbf{X}$ space not by choosing those having high correlations with $\mathbf{Y}$, but only by choosing. directions in X that have high variance. The first PCA direction is the linear combination of the X's that has maximum variance:

$$\mathbf{b_{pc}} = \underset{||\mathbf{b}||=1}{argmax} \quad var \quad (\mathbf{X}\mathbf{b}).$$

(See [4] for an excellent introduction to PCA.) Subsequent directions are found by finding the next linear combination orthogonal to the first direction that has the highest variance. The process can be continued until all p directions (linear combinations) are found, where p is the number of X variables. Typically, however, the idea is to find k directions, where $k < p$ that explain most of the variance of the X variables. That is, the sum of the variances of the k new variables is nearly the sum of the variance of the original p variables. Often, this value k is found by cross-validation, a method by which a part of the data set is used to estimate k and another part used to test the procedure (see *e.g.* [5]). However, most of the emphasis of cross-validation is concerned with prediction. For our purposes, we are simply looking to find a reasonably small k that will contain most of the variance of X.

The problem with PCA for the purposes of multivariate process control is that although it can capture the structure of the process variables, the quality variables Y play no role in the direction choosing. This maybe a serious limitation in the process control setting, if it is the quality variables that one is interested in monitoring. For this reason we discuss partial least squares as an alternative dimension reduction technique.

2.2. PLS

Partial Least Squares (or projection to latent structures) was originally developed by H. Wold ([6]) for applications to the social sciences. It has since been used extensively by chemometricians, and much of the development has taken place in the chemometric literature. There are a number of different algorithms to calculate the direction of PLS. Recently, Höskuldsson [7] has shown that PLS forms a compromise between the direction searches of OLS and PCA. (See also [8].)

PLS finds its directions by choosing the linear combinations of both the X's and Y's that have the maximal covariance of any such linear combinations. Subsequent directions are found first by "deflating" the $\mathbf{X}$ and $\mathbf{Y}$ matrices by these directions, and then repeating the search for maximal covariance directions. (De Jong [8] has developed an efficient algorithm to do this based on singular value decompositions.)

For univariate $\mathbf{y}$, maximizing the covariance is equivalent to maximizing the product of the squared correlation and variance:

$$\mathbf{b_{PLS}} = \underset{||\mathbf{b}||=1}{argmax} \quad corr^2 \quad (\mathbf{y}, \mathbf{X}\mathbf{b}) * \mathbf{var}(\mathbf{X}\mathbf{b})$$

Thus, PLS can be viewed as a "compromise" between PCA and OLS regression methods. (See also [9] for a general discussion of biased regression methods.)

Recently, Stone and Brooks [10] have placed these three techniques together(for univariate $\mathbf{y}$) in one framework known as continuum regression. They have shown that all three satisfy a criterion of the form:

$$(\mathbf{b}'\mathbf{X}'\mathbf{y})^{\mathbf{2}}(\mathbf{b}'\mathbf{X}'\mathbf{X}\mathbf{b})^{\alpha/(\mathbf{1}-\alpha)-\mathbf{1}}$$

where $0 \leq \alpha \leq 1$

The three special cases we have discussed are:

$\alpha = 0 \Rightarrow \mathrm{O}LS$
$\alpha = 1/2 \Rightarrow \mathrm{P}LS$
$\alpha = 1 \Rightarrow \mathrm{P}CR$

They recommend that the parameter α be chosen by cross-validation.

Assuming that k has been chosen, we can express the reduced set of process variables Z as:

$$\mathbf{Z} = \mathbf{T}\mathbf{X} \tag{1}$$

where $\mathbf{T}$ is a k x n matrix of weights. This expression is valid whether $\mathbf{T}$ is the outcome of any linear dimension reduction technique including PLS and PCA. We will refer to the variables Z as the latent variables.

3. Fault information

In standard methods for determining when a process is in control, it is imperative that the process be in control in order to obtain historical mean and control limits for detection. This insures that a base has been established against which to test future readings. The alternative of setting arbitrary limits based on goals, can be useful to track performance, but is not usually recommended for quality control monitoring.

Unfortunately, when the process in is control, there may be very little structure in either the X or Y variable space. Chemical plants are often subjected to disturbances in the compositions or flowrates of the feedstreams, as well as changes in ambient or cooling water temperatures. Such disturbances are typically small, and may be largely compensated for by the process controllers, giving relatively little correlation structure to sensor data to exploit using dimensionality reduction techniques. For example, a disturbance to the cooling water temperature is often rapidly compensated for by increased flowrate of cooling water under automatic control. If, as is often the case, cooling water temperature is not measured, no correlation need be measurable from plant data. Other disturbances cause correlated shifts in many measured variables, which can be characterized by projection onto a small number of principle components.

Less frequently, chemical plant are also subjected to disturbances and faults large enough that they cannot be fully compensated for by the process controllers. These disturbances may be large fluctuations in process inputs, or may be sensor, controller, or equipment failures. Some of these disturbances, such as miscalibration of devices providing online composition measurements or changes in the composition of a feedstream (particularly if natural products such as crude oil or wood are used) occur sufficiently often that data are available. In other cases, dynamic models are available on which different faults can be simulated to produce data sets showing the effect of significant disturbances.

Expanding the data set to include the data from these known faults, one can then apply the dimension reduction technique of one's choosing to the entire set. Control limits for the latent variables Z can be chosen by examining their behavior while the process is in control. If the dimension can be reduced to two, a bivariate plot of Z_2 vs. Z_1 can be drawn with, for example, 95% control ellipses to bound "in control" data. The ellipse can be found simply by examining the past history. An example is shown in figure 1. If the data do not reduce to two dimensions, the sum of the coefficients of the latent variables can be plotted instead.

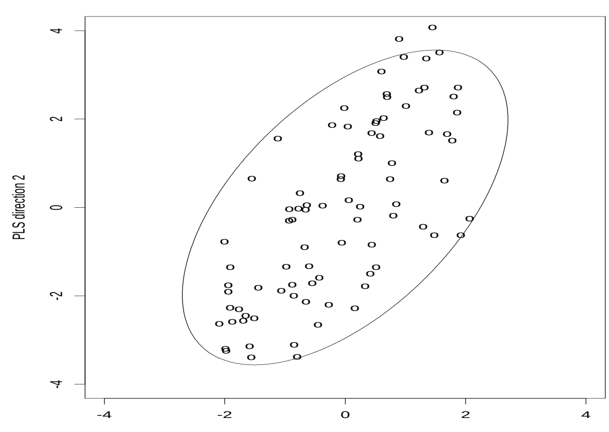


Figure 1

That is, for each observation, the sum of the squared coefficients of $\mathbf{T}$, normalized by their variances are plotted and used to detect out of control points. Specifically, if t_i denotes the i^{th} column of the matrix **T** in equation 1,

$$T^2 = \sum_{d=1}^{D} t_{id}^2/\sigma_d^2$$

The values of T^2 are plotted in time as shown in figure 2.

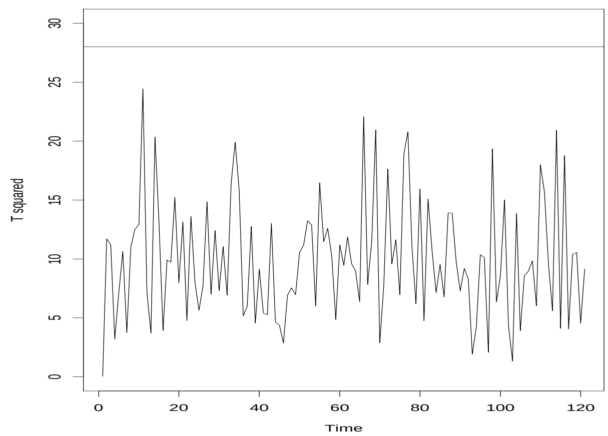
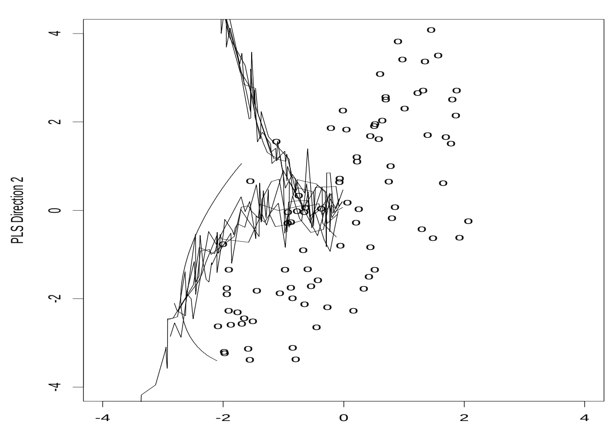


Figure 2

Control limits on T^2 are set from the historical in control data. For a point out of control, plots showing the contribution of the various process variables can be derived. See Miller *et al.* [11] for further details.

If information on various fault types is available, however, one can classify the new problem based on the distance to the fault. In two dimensions, an example is shown in figure 3. Here, the data are again plotted in the first two PLS directions over time. Notice



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