2.4 T^2 Statistic

Let the data in the training set, consisting of m observation variables and n observations for each variable, be stacked into a matrix $X \in \mathcal{R}^{n \times m}$, given by

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \cdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nm} \end{bmatrix}, \tag{2.5}$$

then the sample covariance matrix of the training set is equal to

$$S = \frac{1}{n-1} X^T X. \tag{2.6}$$

An eigenvalue decomposition of the matrix S,

$$S = V \Lambda V^T, \tag{2.7}$$

reveals the correlation structure for the covariance matrix, where Λ is diagonal and V is orthogonal ($V^T V = I$, where I is the identity matrix) [104]. The projection $\mathbf{y} = V^T \mathbf{x}$ of an observation vector $\mathbf{x} \in \mathcal{R}^m$ decouples the observation space into a set of uncorrelated variables corresponding to the elements of $\mathbf{y}$. The variance of the i^{th} element of $\mathbf{y}$ is equal to the i^{th} eigenvalue in the matrix Λ. Assuming S is invertible and with the definition

$$\mathbf{z} = \Lambda^{-1/2} V^T \mathbf{x}, \tag{2.8}$$

the Hotelling's T^2 statistic is given by [143]

$$T^2 = \mathbf{z}^T \mathbf{z}. \tag{2.9}$$

The matrix V rotates the major axes for the covariance matrix of $\mathbf{x}$ so that they directly correspond to the elements of $\mathbf{y}$, and Λ scales the elements of $\mathbf{y}$ to produce a set of variables with unit variance corresponding to the elements of $\mathbf{z}$. The conversion of the covariance matrix is demonstrated graphically in Figure 2.4 for a two-dimensional observation space ($m = 2$).

The T^2 statistic is a scaled squared 2-norm of an observation vector $\mathbf{x}$ from its mean. The scaling on $\mathbf{x}$ is in the direction of the eigenvectors and is inversely proportional to the standard deviation along the eigenvectors. This allows a scalar threshold to characterize the variability of the data in the entire m-dimensional observation space. Given a level of significance, appropriate threshold values for the T^2 statistic can be determined automatically by applying the probability distributions discussed in the next section.

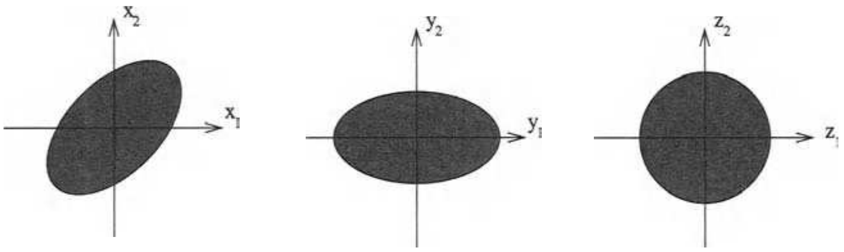

Fig. 2.4. A graphical illustration of the covariance conversion for the T^2 statistic

2.5 Thresholds for the T^2 Statistic

Appropriate thresholds for the T^2 statistic based on the level of significance, α, can be determined by assuming the observations are randomly sampled from a multivariate normal distribution. If it is assumed additionally that the sample mean vector and covariance matrix for normal operations are equal to the actual mean vector and covariance matrix, respectively, then the T^2 statistic follows a χ^2 distribution with m degrees of freedom [209],

$$T_\alpha^2 = \chi_\alpha^2(m). \tag{2.10}$$

The set $T^2 \leq T_\alpha^2$ is an elliptical confidence region in the observation space, as illustrated in Figure 2.5 for two process variables $m = 2$. Applying (2.10) to process data produces a confidence region defining the in-control status whereas an observation vector projected outside this region indicates that a fault has occurred. Given a level of significance α, Figure 2.5 illustrates the conservatism eliminated by employing the T^2 statistic versus the univariate statistical approach outlined in Section 2.3. As the degree of correlation between the process variables increases, the elliptical confidence region becomes more elongated and the amount of conservatism eliminated by using the T^2 statistic increases.

When the actual covariance matrix for the in-control status is not known but instead estimated from the sample covariance matrix (2.6), faults can be detected for observations taken outside the training set using the threshold given by

$$T_\alpha^2 = \frac{m(n-1)(n+1)}{n(n-m)} F_\alpha(m, n-m) \tag{2.11}$$

where $F_\alpha(m, n-m)$ is the upper $100\alpha\%$ critical point of the F-distribution with m and $n-m$ degrees of freedom [209]. For a given level of significance, the upper in-control limit in (2.11) is larger (more conservative) than the

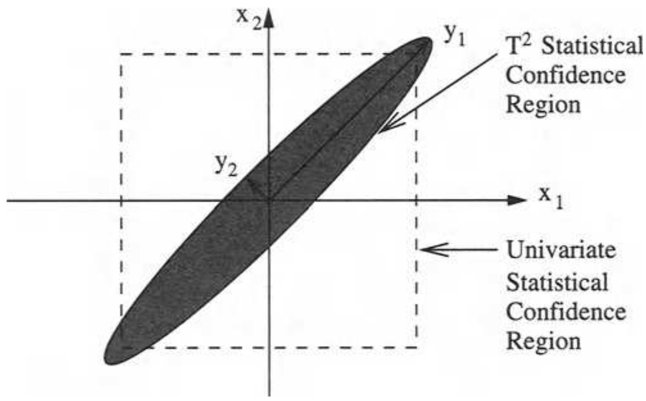

Fig. 2.5. A comparison of the in-control status regions using the T^2 statistic (2.9) and the univariate statistics (2.2) and (2.3) for two process variables [272, 307]

limit in (2.10), and the two limits approach each other as the amount of data increases ($n \to \infty$) [308].

When the sample covariance matrix (2.6) is used, the outliers in the training set can be detected using the threshold given by

$$T_\alpha^2 = \frac{(n-1)^2(m/(n-m-1))F_\alpha(m, n-m-1)}{n(1+(m/(n-m-1))F_\alpha(m, n-m-1)}. \tag{2.12}$$

For a given level of significance, the upper in-control limit in (2.12) is smaller (less conservative) than the limit in (2.10), and the two limits approach each other as the amount of data increases ($n \to \infty$) [308]. Equation (2.12) is also appropriate for detecting faults during process startup, when the covariance matrix is determined recursively on-line because no data are available *a priori* to determine the in-control limit.

The upper control limits in (2.10), (2.11), and (2.12) assume that the observation at one time instant is statistically independent to the observations at other time instances. This can be a bad assumption for short sampling intervals. However, if there are enough data in the training set to capture the normal process variations, the T^2 statistic can be an effective tool for process monitoring even if there are mild deviations from the normality or statistical independence assumptions [30, 171].

There are several extensions that are usually not studied in the process control literature, but for which there are rigorous statistical formulations. In particular, lower control limits can be derived for T^2 [308] which can detect shifts in the covariance matrix (although the upper control limit is usually used to detect shifts in mean, it can also detect changes in the covariance matrix) [114].

The above T^2 tests are multivariable generalizations of the Shewhart chart used in the scalar case. The single variable CUSUM and EWMA charts can be generalized to the multivariable case in a similar manner [171, 203, 292, 338]. As in the scalar case, the multivariable CUSUM and EWMA charts can detect small persistent changes more readily than the multivariable Shewhart chart, but with increased detection delay.

2.6 Data Requirements

The quality and quantity of the data in the training set have a large influence on the effectiveness of the T^2 statistic as a process monitoring tool. An important question concerning the training set is, "How much data is needed to statistically populate the covariance matrix for m observation variables?" This question is answered here by determining the amount of data needed to produce a threshold value sufficiently close to the threshold obtained by assuming infinite data in the training set.

For a given level of significance α, a threshold based on infinite observations in the training set, or equivalently an exactly known covariance matrix, can be computed using (2.10), and the threshold for n observations in the training set is calculated using (2.11). The relative error produced by these two threshold values,

$$\epsilon = \frac{\dfrac{m(n-1)(n+1)}{n(n-m)}F_\alpha(m, n-m) - \chi^2_\alpha(m)}{\chi^2_\alpha(m)}, \tag{2.13}$$

indicates the sufficiency of the data amount n, where a large ϵ implies that more data should be collected. Table 2.2 shows the data requirements using (2.13) for various numbers of observation variables, where $\epsilon = 0.10$ and $\alpha = 0.5$; this implies that the medians of the T^2 statistic using (2.10) and (2.11) differ by less than 10%. The table indicates that the required number of observations is approximately 10 times the dimensionality of the observation space. The data requirements given in Table 2.2 do not take into account sensitivities that occur when some diagonal elements of Λ in (2.8) are small. In such cases the accuracy of the estimated values of the corresponding diagonal elements of the inverse of Λ will be poor, which will give erratic values for T^2 in (2.9). This motivates the use of the dimensionality reduction techniques described in Part III of this book.