Generalized Least Squares

- When Cov[$\boldsymbol{\varepsilon}$]=$\sigma^2\mathbf{G}$, where $\mathbf{G}$ is a known (symmetric) positive definite matrix and σ^2 is an unknown parameter, the generalized least squares estimation of $\boldsymbol{\beta}$ is given by

$$\hat{\boldsymbol{\beta}} = (\mathbf{Z}^T\mathbf{G}^{-1}\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{G}^{-1}\mathbf{Y}$$

$$Cov[\hat{\boldsymbol{\beta}}] = \sigma^2(\mathbf{Z}^T\mathbf{G}^{-1}\mathbf{Z})^{-1}$$

- When Cov[$\boldsymbol{\varepsilon}$]=$\boldsymbol{\Sigma}$, where $\boldsymbol{\Sigma}$ is a known (symmetric) positive definite matrix, the generalized least squares estimation of $\boldsymbol{\beta}$ is given by

$$\hat{\boldsymbol{\beta}} = (\mathbf{Z}^T\boldsymbol{\Sigma}^{-1}\mathbf{Z})^{-1}\mathbf{Z}^T\boldsymbol{\Sigma}^{-1}\mathbf{Y}$$

$$Cov[\hat{\boldsymbol{\beta}}] = (\mathbf{Z}^T\boldsymbol{\Sigma}^{-1}\mathbf{Z})^{-1}$$

U^2 Multivariate Control Chart Based on Generalized Least Squares

George C. Runger "Projections and the U^2 Multivariate Control Chart", Journal of Quality Technology, **28**(3), 1996

Test with Restricted Alternatives

- The optimality of T^2 test is under the implicit assumption that the mean shifts may occur in any direction with equal probability
- A common situation is that the likely shifts have some known structure – e.g., they may be expected to affect only a minority of the variables. Under these situations, it is possible to find more powerful and interpretable test statistics

Sensitivity of χ^2 Chart

- If the mean vector of **X** (p×1) shifts to $\boldsymbol{\mu}$ from $\boldsymbol{\mu}_0$, the average run length of a chi-square chart only depends on the following **noncentrality parameter**

$$\lambda \equiv n(\boldsymbol{\mu}-\boldsymbol{\mu}_0)^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}-\boldsymbol{\mu}_0)$$

- The detection sensitivity increases with λ.
- With the same λ, reduce the dimension of the data can increase detection sensitivity.

Mean Shifts in a Subspace

- One approach to reduce dimension is to sensitize a control chart to detect shifts in an arbitrary subspace of the variables.
- In some applications, knowledge of assignable causes suggests that shifts in the mean can only occur in a subspace (e.g., a subset of the variables).
- Denote **U** a k-dimensional subspace of the p-dimensional (full) space (p is the dimension of **X**).
- Let the $p \times k$ matrix **U** denote a matrix whose columns are a set of k orthonormal basis vectors for the subspace **U**.

Detection of Mean Shifts in Subspace U

- Assume $\mu_0 = \mathbf{0}$ and detect a mean shift of **X** from **0** along an arbitrary vector in the k-dimensional subspace **U**. (If $\mu_0 \neq \mathbf{0}$, replace **X** with $\mathbf{X}-\mu_0$)
- Define U^2 statistic as (n=1, each sample consists of an individual observation)

$$U^2 = \mathbf{X}^T \mathbf{\Sigma}^{-1} \mathbf{U} (\mathbf{U}^T \mathbf{\Sigma}^{-1} \mathbf{U})^{-1} \mathbf{U}^T \mathbf{\Sigma}^{-1} \mathbf{X}$$

- Plot U^2 over time to detect a shift in subspace **U**. U^2 has a chi-square distribution when the process is in-control with degrees of freedom equal to k, the rank of **U**. A control limit for U^2 chart can be selected as $\chi_k^2(\alpha)$.

Advantage of U^2 Chart

- If **X** has a mean shift to $\boldsymbol{\mu} \neq \mathbf{0}$ (out-of-control), then U^2 has a noncentral chi-square distribution with k degrees of freedom and noncentrality parameter $\lambda = \boldsymbol{\mu}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}$, which is the same as the noncentrality parameter for χ^2 chart for **X**.
- The advantage of U^2 chart is that the dimensionality has been reduced from p to k.

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Average Run Length Comparisons

TABLE 1. Average Run Length Comparisons for χ^2 and U^2 Control Charts

Chart	UCL	No. of Variables	Dimension of Shift Subspace	λ 1	λ 2	λ 3	λ 4
χ^2	40.00	20		117	74	49	34
U^2	25.19		10	93	51	31	21
U^2	18.55		6	74	37	22	14
U^2	12.84		3	52	24	14	9
χ^2	25.19	10		93	51	31	21
U^2	16.75		5	68	33	19	12
U^2	12.84		3	52	24	14	9
U^2	10.60		2	42	18	11	7

On-Target Average Run Length = 200.

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Releasing the Orthonormal Basis Assumption

- The requirements that the columns in **U** are orthonormal are not necessary in construction of U^2 chart.
- Let the $p \times k$ matrix $\boldsymbol{\Gamma}$ denote a matrix whose columns are a set of k linearly independent basis vectors for the subspace **U**.
- The U^2 statistic calculated based on $\boldsymbol{\Gamma}$ as follows

$$U^2=\mathbf{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\Gamma}(\boldsymbol{\Gamma}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\Gamma})^{-1}\boldsymbol{\Gamma}^T\boldsymbol{\Sigma}^{-1}\mathbf{X}$$

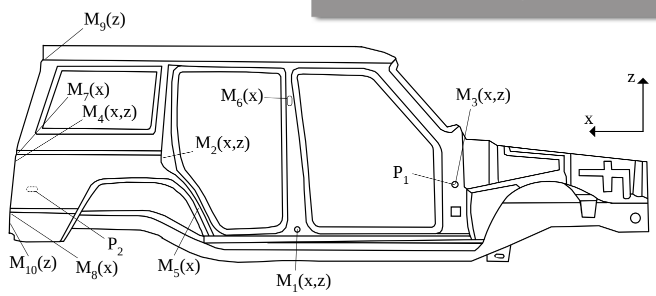
is equivalent to U^2 calculated from matrix **U**.

Example: Subset Assignable Causes

- A special case of subspace is the subset assignable cause, in which an assignable cause can only shift the mean of a subset of k variables.
- Let the variables in the mean-shift-possible subset be denoted as $k \times 1$ vector $\mathbf{X}_1$ and let the remaining p-k variables be denoted as $\mathbf{X}_2$.
- In this case, the U^2 statistic can be written as

$$U^2 = \mathbf{X}^T\boldsymbol{\Sigma}^{-1}\mathbf{X} - \mathbf{X}_2^T\boldsymbol{\Sigma}_{22}^{-1}\mathbf{X}_2$$

Auto-Body Assembly Example



- 10 measurement points on 2-D plane – p=20 measurements (two directions for each point) for each product
- Mean shifts on the 20 measurements are caused by two faults on locating pin P_1 and one fault on locating pin P_2. So the mean shifts are constrained in a subspace of dimension k=3.

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Gamma Matrix for Mean Shift Subspace of the Assembly Example

$$\Gamma = \begin{pmatrix} 0.9972 & -0.1157 & 0.1157 \\ -0.0093 & 0.6196 & 0.3804 \\ 1.0013 & 0.0519 & -0.0519 \\ -0.0179 & 0.2669 & 0.7331 \\ 1.0000 & 0 & 0 \\ 0 & 1.0000 & 0 \\ 1.0002 & 0.0086 & -0.0086 \\ -0.0265 & -0.0856 & 1.0856 \\ 0.9977 & -0.0931 & 0.0931 \\ -0.0150 & 0.3846 & 0.6154 \\ 1.0043 & 0.1766 & -0.1766 \\ -0.0106 & 0.5676 & 0.4324 \\ 1.0012 & 0.0476 & -0.0476 \\ -0.0265 & -0.0855 & 1.0855 \\ 0.9979 & -0.0865 & 0.0865 \\ -0.0265 & -0.0857 & 1.0857 \\ 1.0072 & 0.2961 & -0.2961 \\ -0.0246 & -0.0049 & 1.0049 \\ 0.9973 & -0.1099 & 0.1099 \\ -0.0266 & -0.0871 & 1.0871 \end{pmatrix}_{20\times 3}$$

$\mu_0=0,\ n=1,\ \alpha=0.01$

$$\mathbf{\Sigma} = \mathbf{\Gamma} \times \left(\frac{0.25}{6}\right)^2 \mathbf{I}_{(3\times 3)} \times \mathbf{\Gamma}^T + \left(\frac{0.25}{6}\right)^2 \mathbf{I}_{(20\times 20)}$$

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