



**UNIVERSITÀ  
DEGLI STUDI  
DI BERGAMO**

Dipartimento  
di Ingegneria Gestionale,  
dell'Informazione e della Produzione

## **Lesson 16.**

# **Fault diagnosis IV**

## **Knowledge-based approaches**

**DATA SCIENCE AND  
AUTOMATION COURSE**

**MASTER DEGREE SMART  
TECHNOLOGY ENGINEERING**

TEACHER

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# Outline

1. Schematic of the approach
2. Review of PCA
3. Statistical process monitoring



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## 1. Schematic of the approach

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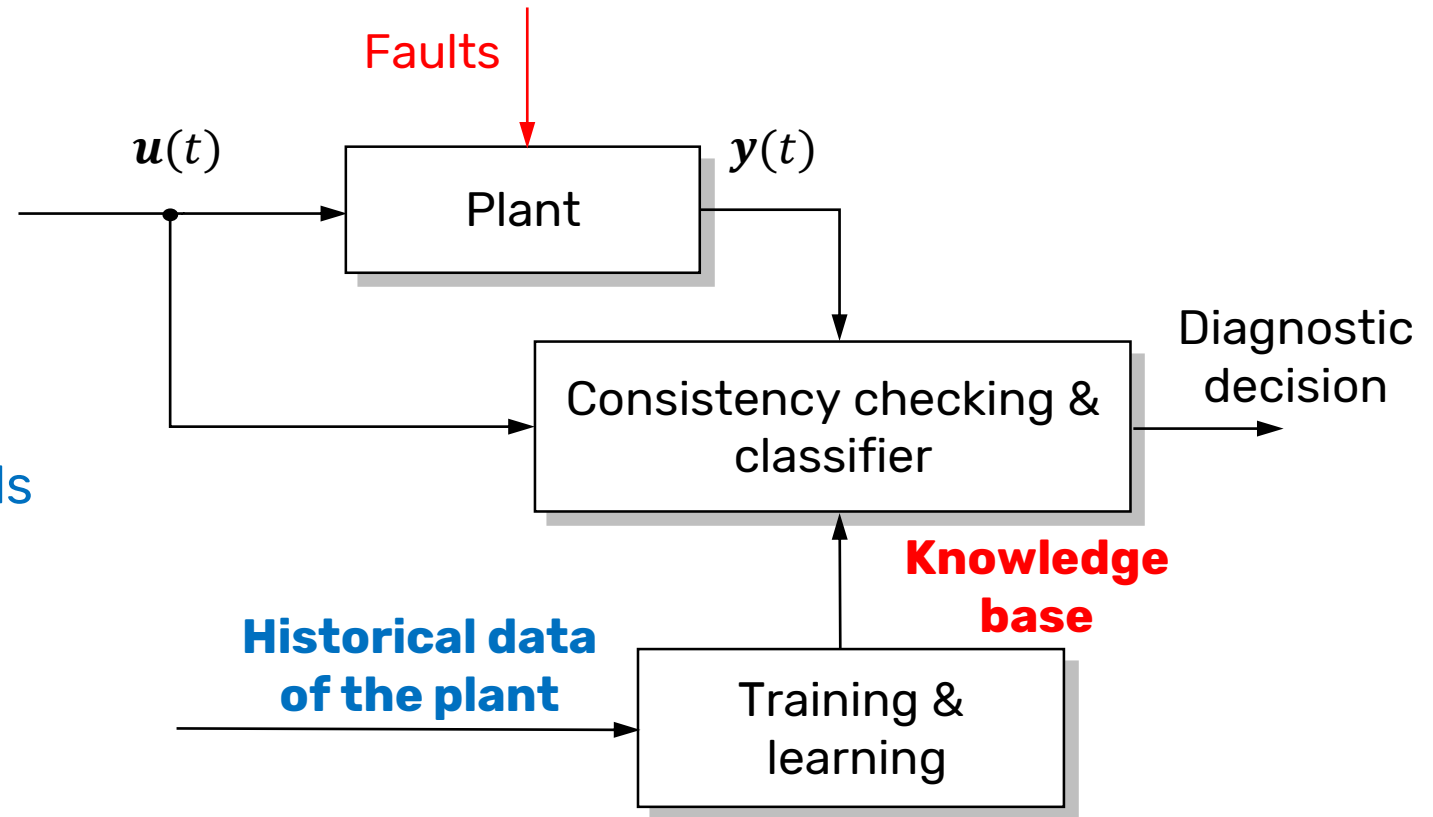
# Knowledge-based fault diagnosis

Great amount of historical data available:

- There is **not a prior knowledge** about the faults, and it has to be **extracted from data**
- **Training vs testing** phases

## Common approaches are:

- Machine learning classifiers
- Statistical Process monitoring methods  
(control charts, PCA indicators,...)



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# PCA algorithm

## Inputs

- $q$ : the number of dimensions to retain (can be  $q = d$ )
- The training set  $\mathcal{D} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ ,  $\mathbf{x} \in \mathbb{R}^d$  (do not consider dummy variables  $x_0 = 1$ )

## Data pre-processing

- Remove the feature (column) mean for each column of the data matrix  $X \in \mathbb{R}^{N \times d}$
- Standardize each feature element for the respective feature standard deviation
- Each feature now has mean 0 and standard deviation 1
- Define the normalized data matrix as  $\tilde{X} \in \mathbb{R}^{N \times d}$



# PCA algorithm

Perform a **Singular Value Decomposition** (SVD) of the matrix  $\tilde{X} \in \mathbb{R}^{N \times d}$

$$\tilde{X} = USV^T$$

$$U = \begin{bmatrix} \vdots & \dots & \vdots \\ & \ddots & \\ & & \dots \end{bmatrix}_{N \times N}$$

$$S = \begin{bmatrix} \vdots & \dots & \vdots \\ & \ddots & \\ & & \dots \end{bmatrix}_{N \times d}$$

$$V^T = \begin{bmatrix} \vdots & \dots & \vdots \\ & \ddots & \\ & & \dots \end{bmatrix}_{d \times d}$$

- The columns  $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_N$  of  $U$  form an orthonormal basis of  $\mathbb{R}^N$
- The columns  $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$  of  $V$  form an orthonormal basis of  $\mathbb{R}^d$
- The diagonal elements  $s_1, s_2, \dots, s_{\min\{N,d\}}$  in  $S$  are **nonnegative** and called **singular values** of  $\tilde{X}$

# PCA algorithm

From  $\tilde{X} = USV^T$  we get  $V = \begin{bmatrix} | & | & \dots & | \\ \mathbf{v}_1 & \mathbf{v}_2 & \dots & \mathbf{v}_N \\ | & | & \dots & | \end{bmatrix} \in \mathbb{R}^{d \times d}$

- The columns  $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$  of  $V$  are called **principal component loadings** and they are the **eigenvectors** of the covariance matrix  $\Sigma = \frac{1}{N} \tilde{X}^T \tilde{X}$
- Select the first  $q \leq d$  columns of  $V$ , obtaining the **reduced** matrix  $V_q \in \mathbb{R}^{d \times q}$
- Compute the projected data  $Z = \tilde{X} \cdot V_q \in \mathbb{R}^{N \times q}$  (**principal component scores**)
- It is possible to recover the original data, up to an **approximation**, by computing

$$\tilde{X}_r = Z \cdot V_q^T \in \mathbb{R}^{N \times d}$$



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# Introduction to SPM

In PCA, the **projected** data (scores) can be computed as  $Z = \tilde{X} \cdot V_q \in \mathbb{R}^{N \times q}$

It is possible to **reconstruct** the data, using only  $q$  components, as  $\tilde{X}_r = Z \cdot V_q^T \in \mathbb{R}^{N \times d}$

The reconstructed data matrix therefore reads as  $\tilde{X}_r = \tilde{X} \cdot V_q \cdot V_q^T \in \mathbb{R}^{N \times d}$

The data  $\tilde{X}$  can be decomposed as  $\tilde{X} = \tilde{X}_r + E$ . The matrix  $E \in \mathbb{R}^{N \times d}$  is called **residual matrix**

The subspace  $\mathcal{S}_v$ , spanned by the columns of  $V_q$  is called **the principal component subspace (PCS)**:  $\mathcal{S}_v = \text{span}(V_q)$ .

Its orthogonal complement  $\mathcal{S}_e$  is the **residual subspace (RS)**



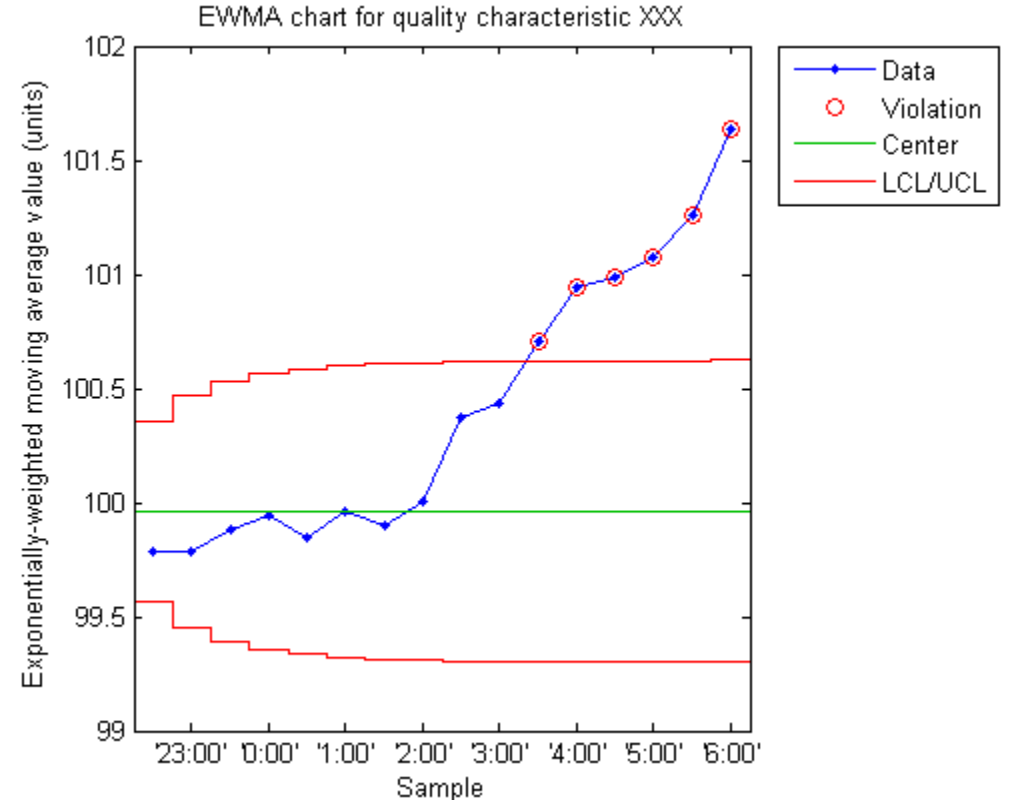
# Introduction to SPM

The simplest Statistical Process Monitoring (SPM) approaches consists of univariate statistical **control charts**:

- Shewart chart
- CUSUM (Cumulative Sum)
- EWMA (Exponentially Weighted Moving Average)

However, they do not take into account the **correlation** between variables

**Multivariate statistics** are needed. We discuss two indexes related to the PCA algorithm



# $T^2$ statistic

The Hotelling's  $T^2$  index measures variations in the **principal component subspace**

$$T^2(\mathbf{x}) = \underset{1 \times 1}{\tilde{\mathbf{x}}^T} \underset{1 \times d}{V_q} \underset{d \times q}{\cdot} \underset{q \times q}{S_q^{-2}} \underset{q \times 1}{\cdot} \underset{1 \times q}{V_q^T} \underset{1 \times d}{\tilde{\mathbf{x}}} = \underset{1 \times q}{\mathbf{z}^T} \underset{q \times q}{\cdot} \underset{q \times q}{S_q^{-2}} \underset{q \times 1}{\cdot} \underset{1 \times q}{\mathbf{z}}$$

where  $S_q$  consists in the first  $q$  rows and  $q$  columns of the matrix  $S$ .

The  $T^2$  statistic is a **scaled squared 2-norm** of an observation vector  $x$  from its mean.

The scaling on  $x$  is in the direction of the  $q$  **eigenvectors** and is inversely proportional to the **standard deviation** along the eigenvectors (each  $s_i^2$  equals the eigenvalue  $\lambda_i$  of the covariance matrix  $\tilde{X}^T X$ ).

This allows a scalar threshold to characterize the data variability in the entire  $\mathbb{R}^{q \times 1}$  space

# $T^2$ statistic

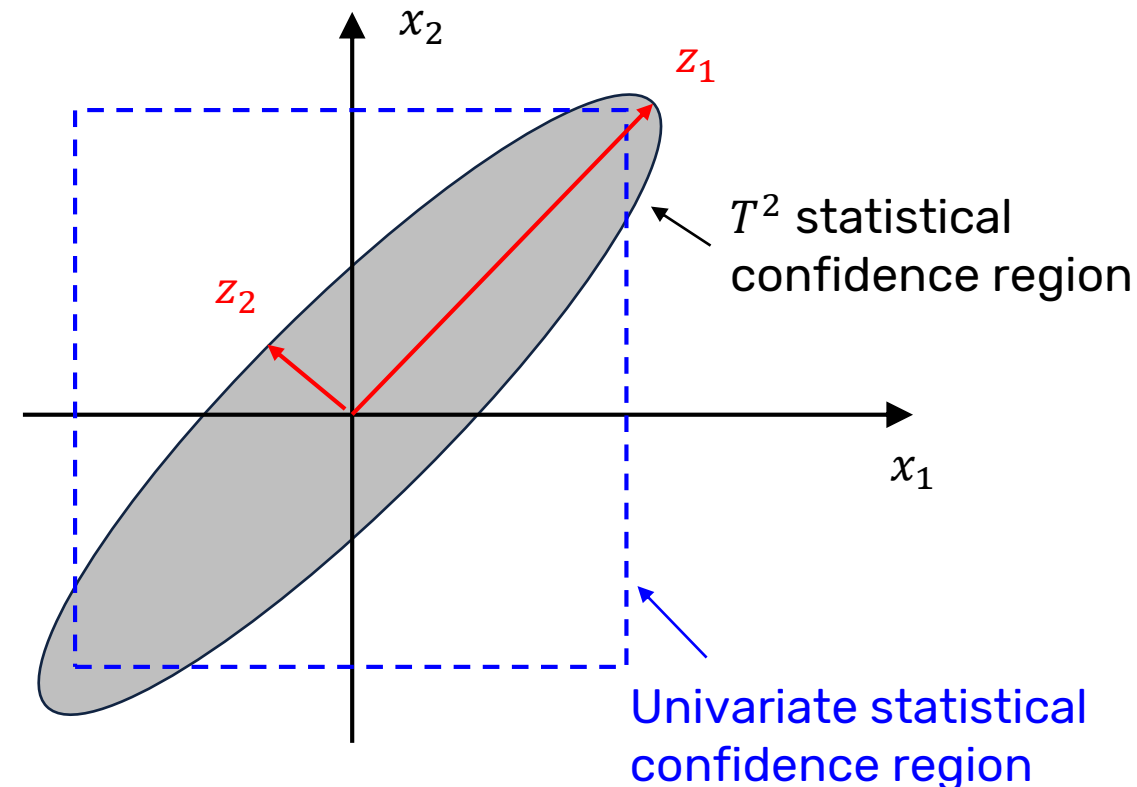
Given a level of significance  $\alpha$ , appropriate **thresholds**  $T_\alpha^2$  for the  $T^2$  statistic can be determined **automatically**

Given an observation vector  $\mathbf{x}$ , we have that:

1. The observation is **in-control** if  $T^2(\mathbf{x}) \leq T_\alpha^2$
2. The observation is **out-of-control** (there is a fault) if  $T^2(\mathbf{x}) > T_\alpha^2$

The confidence region is an **ellipsoid** that

«stretches» depending on the correlation between the variables



# $T^2$ statistic

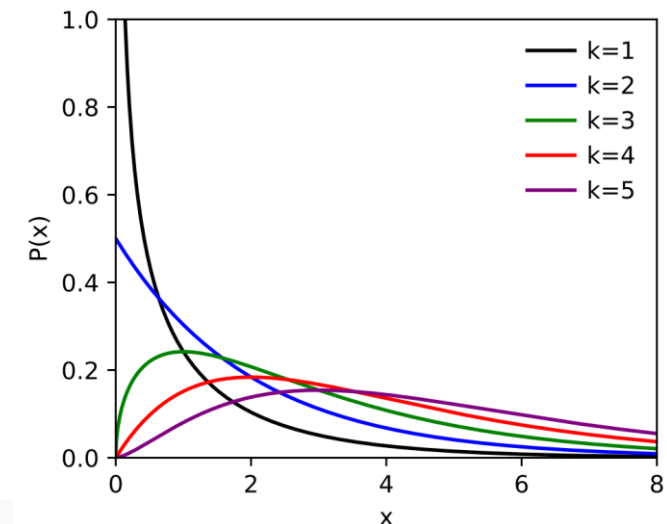
The  $T^2$  statistic can be interpreted as measuring the **systematic variations** of the process, and a violation of the threshold would indicate that the systematic variations are out-of-control

An usual **assumption** is that the observations  $x$  follow a multivariable Normal distribution

If the **mean** and the **covariance** matrix of the observations are **known** (or if not but  $N$  is high), the  $T^2$  statistic follows a Chi-quadro distribution, and a threshold can be set as

$$T_{\alpha}^2 = \chi_{\alpha}^2(q)$$

where  $\chi_{\alpha}^2(q)$  indicates the  $(1 - \alpha)$  percentile of a Chi-quadro distribution with  $q$  degrees of freedom



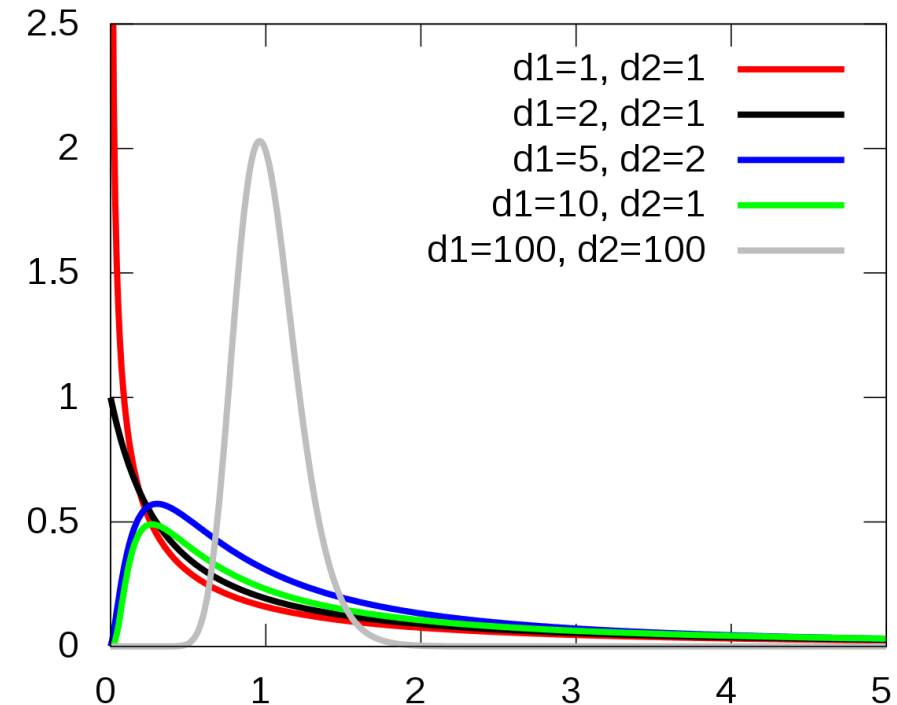
# $T^2$ statistic

If the mean and the covariance matrix are **not known but estimated**, the  $T^2$  statistic follows a Fisher distribution, and a threshold can be set as

$$T_{\alpha}^2 = \frac{q(N-1)(N+1)}{N(N-q)} F_{\alpha}(q, N-q)$$

where  $F_{\alpha}(q, N-q)$  indicates the  $(1-\alpha)$  percentile of the Fisher distribution with  $q$  and  $N-q$  degrees of freedom

**Fisher distribution**



# SPE ( $Q$ ) statistic

The  $Q$  statistic, also known as the **squared prediction error (SPE)**, is a squared 2-norm measuring the deviation of the observations projected **on the residual subspace**

$$Q(\mathbf{x}) = \mathbf{r}^T \mathbf{r} \quad \mathbf{r} = \tilde{\mathbf{x}} - \tilde{\mathbf{x}}_r = \left( I - V_q \cdot V_q^T \right) \tilde{\mathbf{x}}$$

$1 \times 1$        $d \times 1$        $d \times d$        $d \times q$        $q \times d$        $d \times 1$

The  $Q$  statistic measures the random **variations** of the process, for example, that are associated with **measurement noise**

Since the  $Q$  statistic does not directly measure the variations along each loading vector but measures the total sum of variations in the residual space, it does not suffer from an over-sensitivity to inaccuracies in the smaller singular values (contrary to the  $T^2$ )



# SPE ( $Q$ ) statistic

The threshold  $Q_\alpha$  for the  $Q$  statistic can be computed as

$$Q_\alpha = g^{\text{SPE}} \chi_\alpha^2(h^{\text{SPE}})$$

$$g^{\text{SPE}} = \frac{\theta_2}{\theta_1}$$

$$h^{\text{SPE}} = \frac{\theta_1^2}{\theta_2}$$

$$\theta_1 = \sum_{i=q+1}^d s_i^2$$

$$\theta_2 = \sum_{i=q+1}^d (s_i^2)^2$$

where  $\chi_\alpha^2(h^{\text{SPE}})$  indicates the  $(1 - \alpha)$  percentile of a Chi-quadro distribution with  $h^{\text{SPE}}$  degrees of freedom

# $T^2$ and SPE statistics

Since the **principal component subspace** typically contains **normal process variations** with large variance that represent signals, and the **residual subspace** contains mainly **noise**, the normal region defined by the control limit for  $T^2$  is usually much larger than that of SPE

Therefore it usually takes a much **larger fault magnitude** to exceed the  $T^2$  control limit

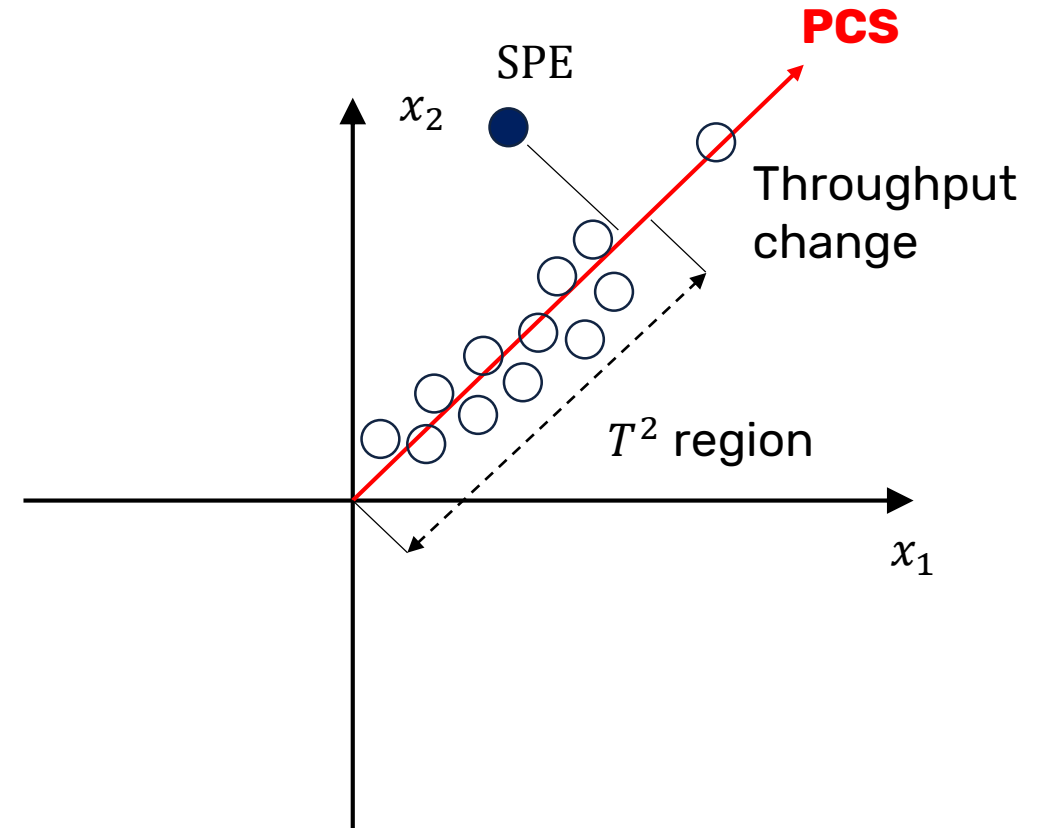
The normal region defined by the SPE control limit includes residual components that are mainly noise. Therefore faults with **small to moderate magnitudes** can easily exceed the SPE control limit



# $T^2$ and SPE statistics

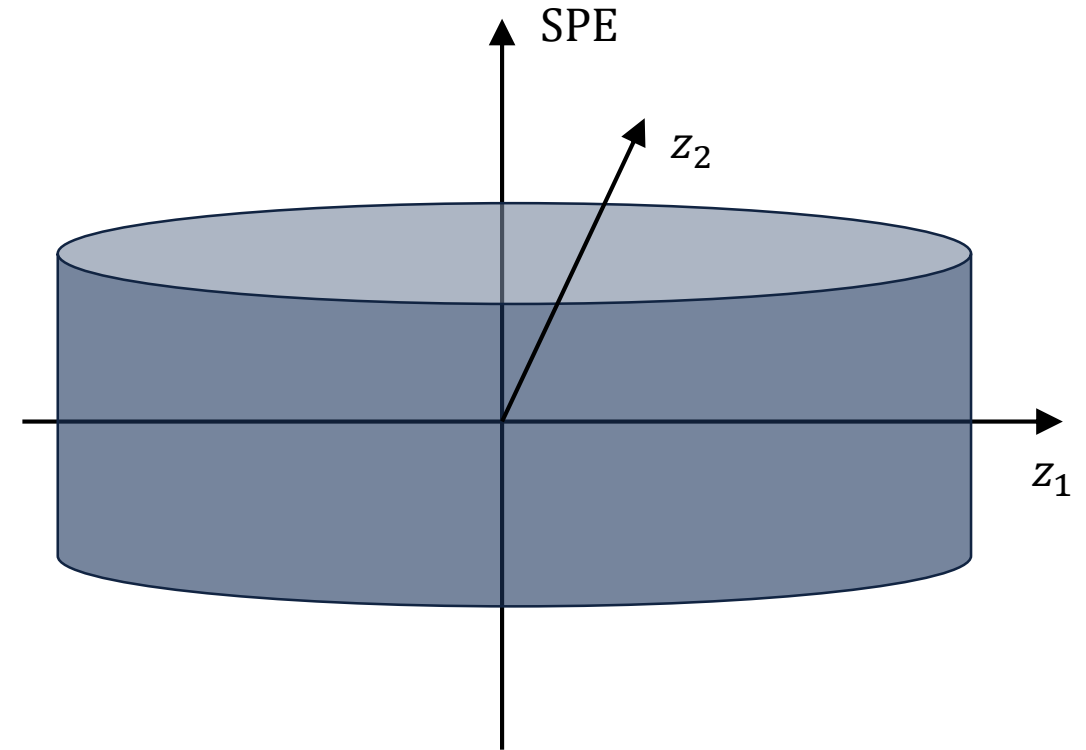
Furthermore, if a sample exceeds the  $T^2$  limit only, but does not violate the SPE limit, it does not break the correlation structure but simply shifts further away from the origin in the PCS.

This case could be a fault, but it **could also be a change in the operating region** which is not necessarily a fault



# $T^2$ and SPE statistics

The  $T^2$  and  $Q$  statistics along with their appropriate thresholds detect **different types of faults**, and the advantages of both statistics can be utilized by employing the two measures together. When these two statistics are utilized along with their respective thresholds, it produces a **cylindrical in-control region**



# $T^2$ and SPE statistics

The monitoring algorithm based on the  $T^2$  and  $Q$  statistics can be summarized as follows:

## Phase 1: training or set-up

1. Using  $X$ , compute the mean  $\hat{\mu}_j$  and the standard deviation  $\hat{\sigma}_j$  of each feature  $j$ .
2. Using  $\hat{\mu}_j, \hat{\sigma}_j$  normalize training data  $X$  to zero mean and standard deviation one,  $\tilde{X}$
3. Compute  $USV^T \leftarrow \text{svd}(\tilde{X})$ . Select  $q$  and compute  $V_q, S_q$
4. Select  $\alpha$  and compute the thresholds  $T_\alpha^2, Q_\alpha$

## Phase 2: usage

1. Normalize a new data  $\mathbf{x}^*$  using  $\hat{\mu}_j$  and  $\hat{\sigma}_j$
2. Compute the statistics  $T^2(\mathbf{x}^*)$  and  $Q(\mathbf{x}^*)$  using  $V_q$  and  $S_q$
3. Compare  $T^2(\mathbf{x}^*)$  with  $T_\alpha$  and  $Q(\mathbf{x}^*)$  with  $Q_\alpha$  to detect abnormalities in process data

# Extensions and further considerations

The presented rationales are used for fault detection. Fault isolation can be performed by **contribution plots**, which compute the contribution of each variable to the fault decision

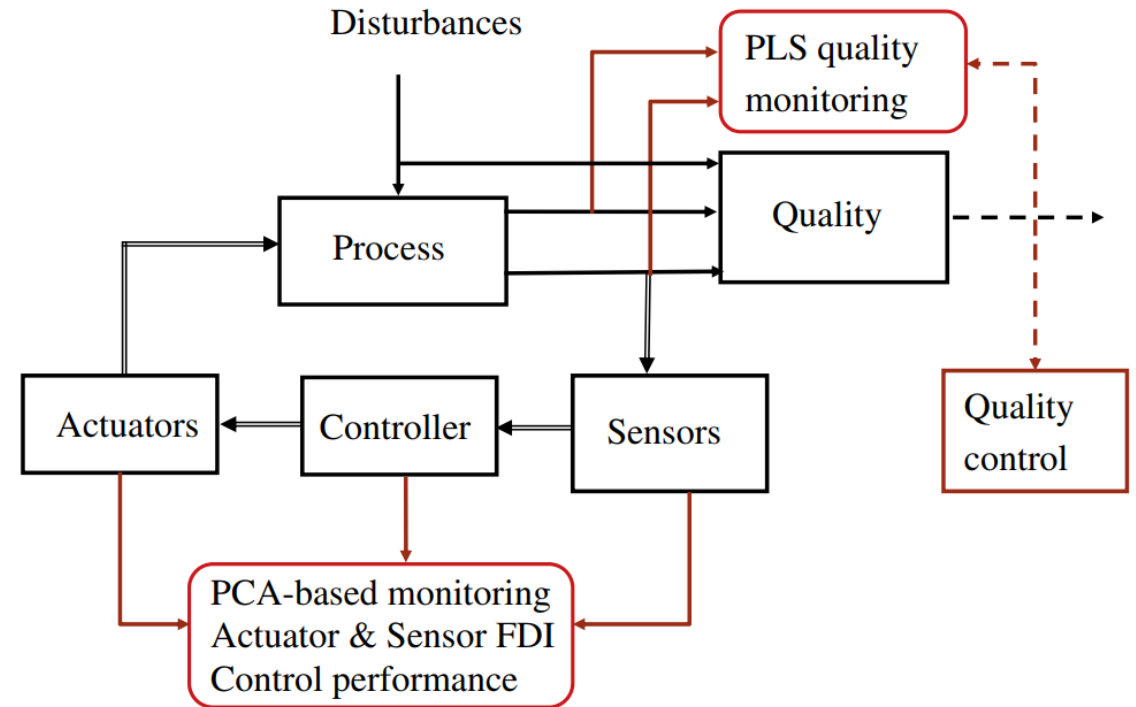
The PCA model can be extended to consider dynamical systems (**dynamic PCA**). If we suppose that  $\mathbf{x} = [y_t \ u_t]^T$ , we can define a matrix  $X(h)$ , where  $h$  defines the order of the system, as

$$X(h) = \begin{bmatrix} y_t & u_t & y_{t-1} & u_{t-1} & \cdots & y_{t-h} & u_{t-h} \\ y_{t-1} & u_{t-1} & y_{t-2} & u_{t-2} & & y_{t-h-1} & u_{t-h-1} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ y_{t+h-N} & u_{t+h-N} & y_{t+h-N-1} & u_{t+h-N-1} & \cdots & y_{t-n} & u_{t-n} \end{bmatrix}$$

# Extensions and further considerations

The method of **Partial Least Squares (PLS)** is a dimensionality reduction technique for **maximizing the covariance** between the predictor (independent) matrix  $X$  and the predicted (dependent) matrix  $Y$  for each component of the reduced space

A popular application of PLS is to select the matrix  $Y$  to contain only **product quality data** which can even include off-line measurement data, and the matrix  $X$  to contain all other **process variables**



# References

1. Russell, Evan L., Leo H. Chiang, and Richard D. Braatz. Data-driven methods for fault detection and diagnosis in chemical processes. Springer Science & Business Media, 2012.
2. Qin, S. Joe. "Survey on data-driven industrial process monitoring and diagnosis." Annual reviews in control 36.2 (2012): 220-234.
3. Mazzoleni, M., Previdi, F., Scandella, M., & Pispola, G. (2019). Experimental Development of a Health Monitoring Method for Electro-Mechanical Actuators of Flight Control Primary Surfaces in More Electric Aircrafts. IEEE Access, 7, 153618-153634.
4. Alcalá, C. F., & Qin, S. J. (2009). Reconstruction-based contribution for process monitoring. Automatica, 45(7), 1593-1600.
5. Joe Qin, S. (2003). Statistical process monitoring: basics and beyond. Journal of Chemometrics: A Journal of the Chemometrics Society, 17(8-9), 480-502.

