Statistical process control (SPC)

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Goals

- Establishing an intelligent **information** system to describe the **process evolution,** able to**:**
  - ✓ **Detect abnormal** behaviour as fast as possible.
  - ✓ **Identify** the **source** of the **abnormal** behaviour.
  - ✓ **Correct** the **abnormal** behaviour and **avoid** it in the future.

Process control. The main idea

- Visualize the process evolution from a series of mesurements acquired during the process.
- Visualization tools should:
  - ✓ Be statistically sound,
  - ✓ Allow easy and fast detection of presence and source of abnormal behaviour.

Natural variability vs. special variability

Natural variability

Inherent to the process.

- Permanent.
- Produces a stable and predictable behaviour.
- In the presence of natural variability, the process is **UNDER CONTROL**.

Special variability

Fluctuations strange to the process.

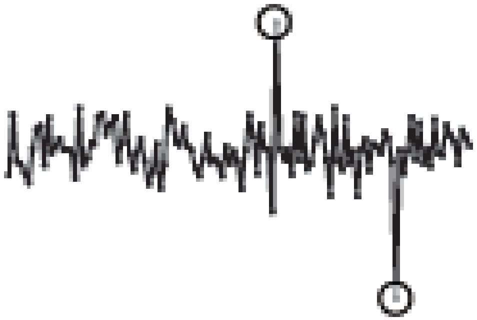
- Happens in unusual or specific circumstances.
- Causes an erratic and unpredictable process behaviour.
- In the presence of anomalous variability, the process is **OUT OF CONTROL.**

Natural variability vs. special variability

Natural variability

- Process under statistical control.
- Process working in **normal operating conditions** (**NOC**).

Special variability



- Process out of statistical control.
- Does not work in NOC conditions.

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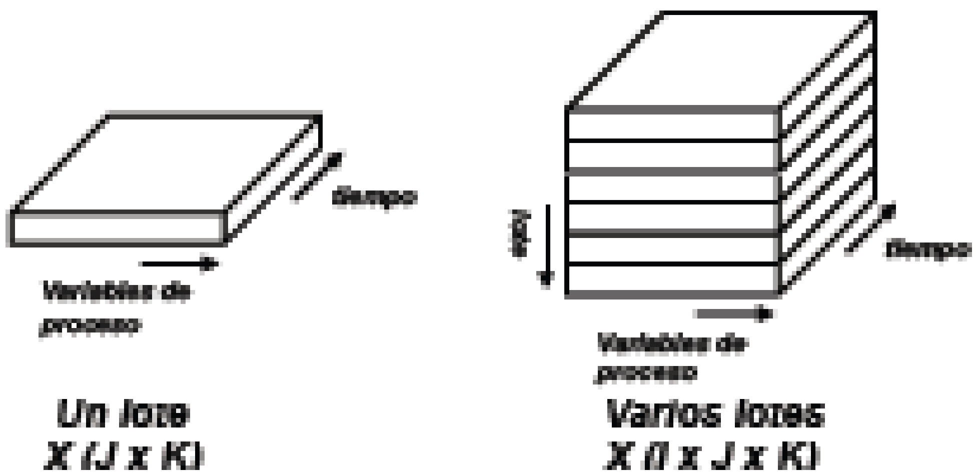
Process typology

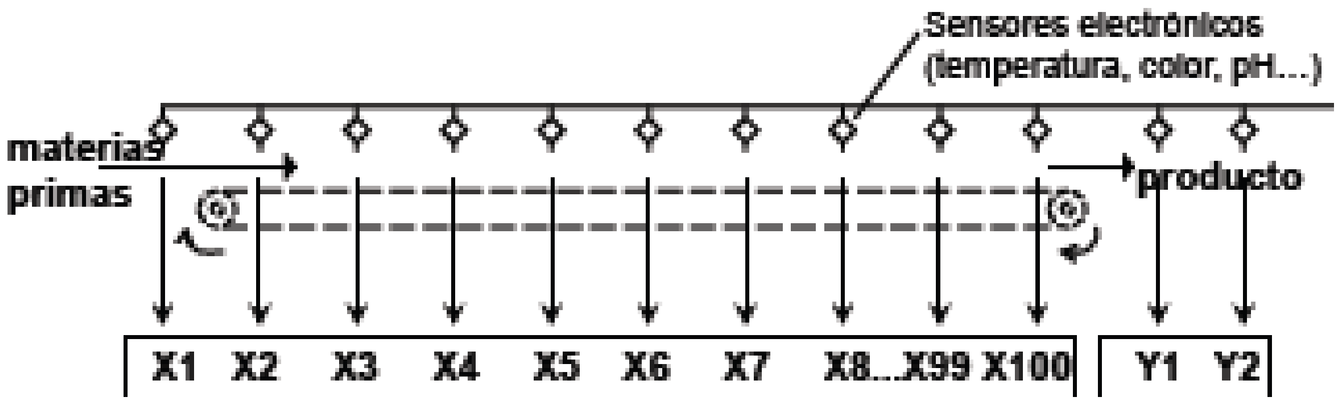
- **Batch processes.**
  - ✓ Done in a discontinuous way. Limited duration.
  - ✓ Several (or many) variables are controlled ‘on/in-line’ (*process vari*ables).
  - ✓ Few variables related to quality attributes are measured ‘off-line’ in the final product (*quality variables*).



*(Adapted from A. Ferrer)

Process typology

- **Continuous processes.**
  - ✓ Take place in a non-stop way.
  - ✓ Many process variables are controlled on or in-line.
  - ✓ Control of end product is done in real time by prediction of quality attributes based on previously established statistical models among process variables and quality variables.



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*(Adapted from A. Ferrer)

Tools for process control

- **Univariate SPC tools.**
  - ✓ Control charts based on a process or a quality variable.
    - Shewhart charts, CUSUM charts or EWMA charts.
- **Multivariate SPC tools (MSPC).**
  - ✓ Based on quality (**Y**) or on process variables (**X**).
    - Principal Component Analysis (PCA).
  - ✓ Based on models relating process (**X**) and quality variables (**Y**).
    - Partial Least Squares regression (PLS).

Tools for process control

- **Setting the model of Normal Operating Conditions.**
  - ✓ Establishing process control limits (univariate tools). Establishing boundaries of operational space (multivariate tools).
  - ✓ Limits or boundaries are set using historical data known to be under control.
- **Exploiting the model of Normal Operating Conditions.**
  - ✓ The model helps to predict whether observations from new processes are under or out of control.
  - ✓ Observations out of control are out of the control limits (univariate tools) or out of the space boundaries (multivariate tools).

Univariate SPC tools

- **Control charts.** Check the variability of a single quality attribute.
  - ✓ We need as many charts as quality attributes to control.
  - ✓ All of them work setting upper and lower control limits (UCL, LCL) that define normal variability.
  - ✓ Observations higher than UCL or lower than LCL are out of control.
  - ✓ The relationship among the different quality atrributes monitored is ignored.

Univariate SPC tools

Types of control charts

- **Shewhart chart**. Looks at the values recorded during the process independently from each other.
  - ✓ Detects observations IN or OUT of control.
  - ✓ Detects clear non-random behaviour trends that can be sign of process malfunction.
- **CUSUM, EWMA charts.** Relate current and past observations recorded during the process.
  - ✓ Detects observations IN or OUT of control.
  - ✓ Detects slight non-random behaviour trends that can lead to OUT OF CONTROL situations.

Univariate SPC tools

Shewhart chart (1920)

- Plots observations of a process and compares them with a target value (often, a mean value). UCL and LCL are usually set as ±3s with respect to the target value.

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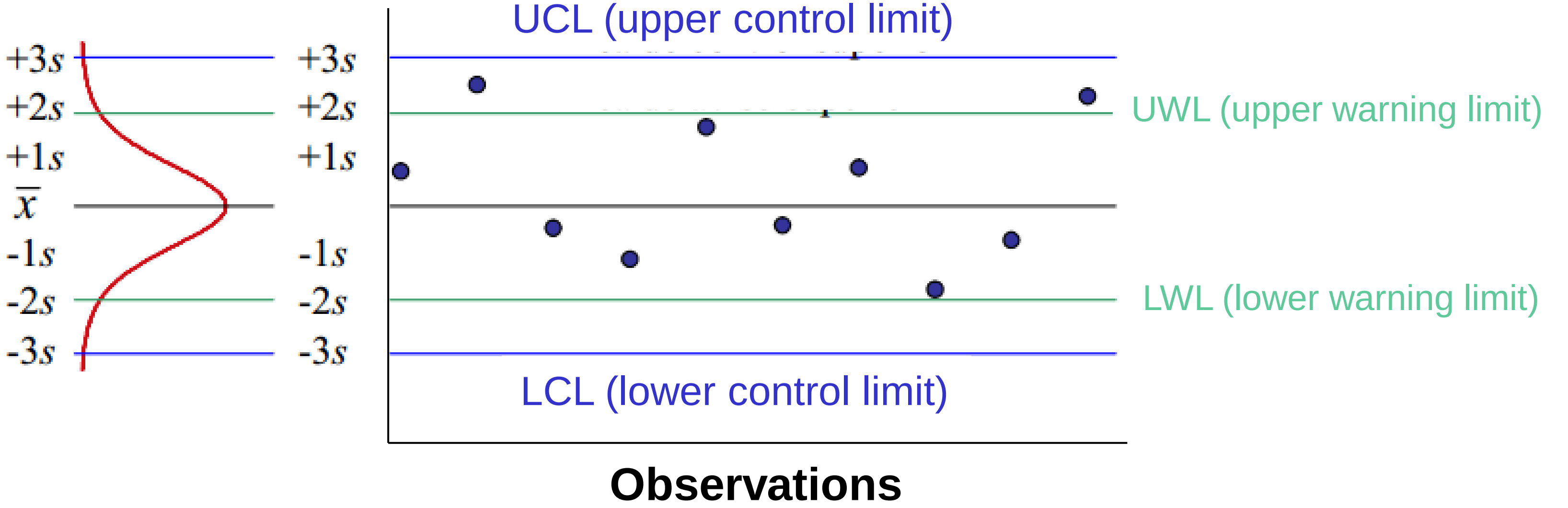

Observations above UCL or below LCL are out of control.

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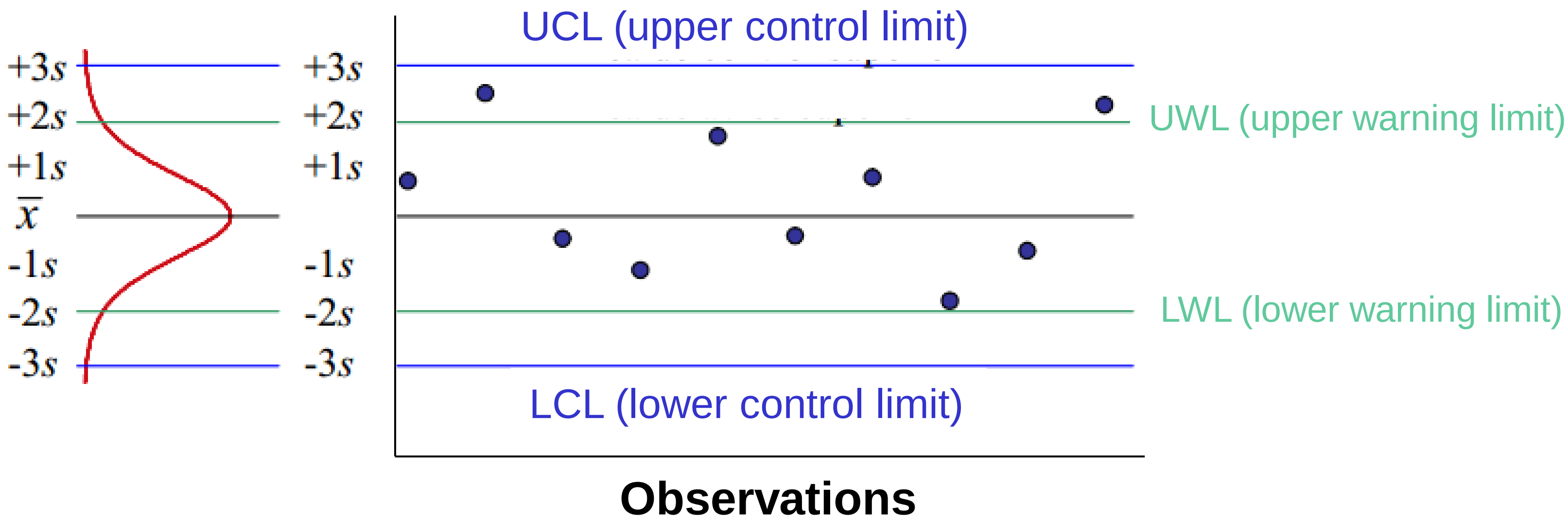
(*) Figure adapted from J. Riu. Gráficos de control de Shewhart.

Univariate SPC tools

Shewhart chart

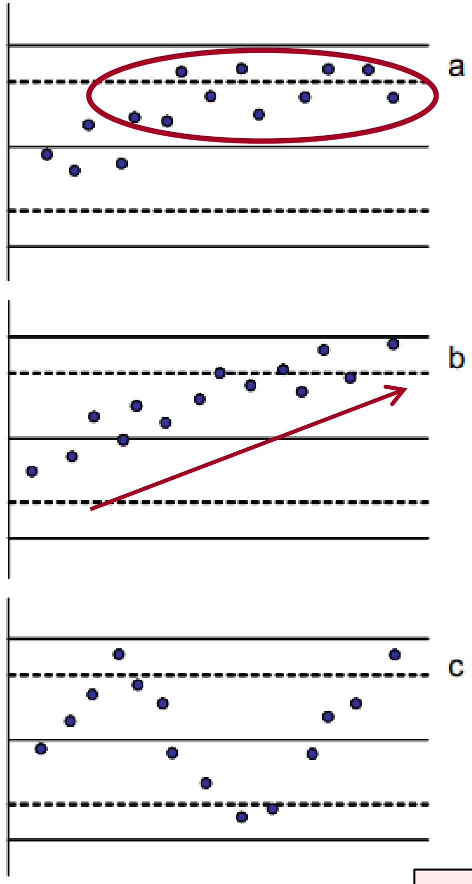


- **Supplementary rules for control (*Western Electric, 1956*)**
  - ✓ 2 out of 3 consecutive points between UCL and UWL or LCL and LWL.
  - ✓ 6 consecutive points systematically increasing or decreasing.
  - ✓ 9 consecutive points above (or below) target point.
  - ✓ Series of equal number of points alternating above or below target.

Univariate SPC tools

Shewhart chart

(*)



- ✓ **Presence of bias**: many consecutive observations above (or below) target value.
- ✓ **Monotonic (increasing or decreasing) trends.**
- ✓ **Periodic trends.**

Detects **non-random trends** in observations.
Can be a sign of **process malfunction**.

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(*) Figure adapted from J. Riu. Gráficos de control de Shewhart.

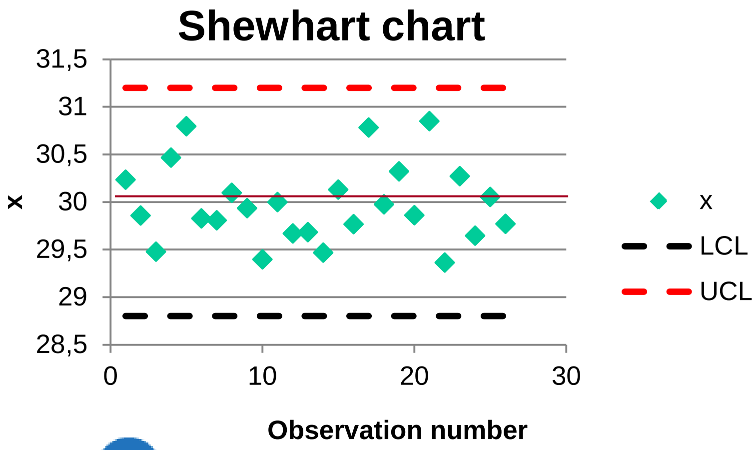
Univariate SPC tools

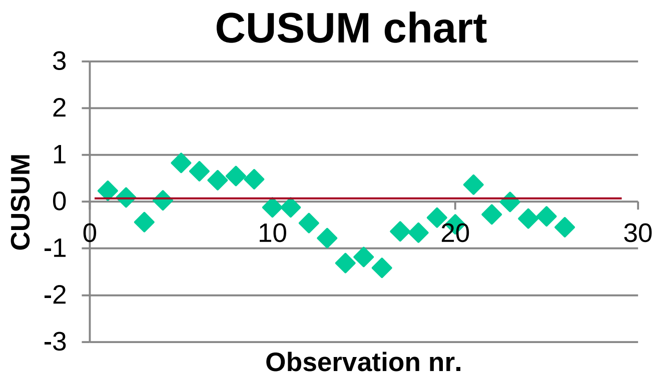
CUSUM chart (Page, 1954) (CUmulative SUM control chart)

- Takes into account the present observation and all the previous ones into the parameter $CUSUM_t$.

$$\mathbf{CUSUM_t} = \sum_{i=1}^{t}\left(x_i - \bar{x}\right)$$

- Allows detecting slight shifts from the ideal behaviour in a process.





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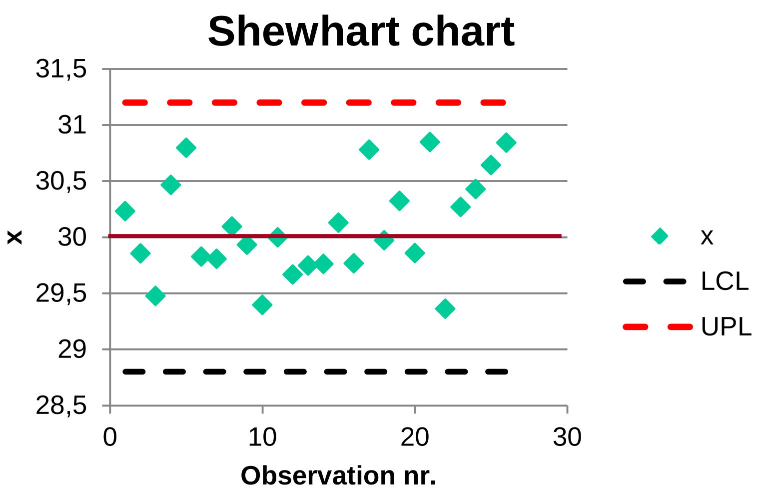
In a normal process, CUSUM charts move around zero.

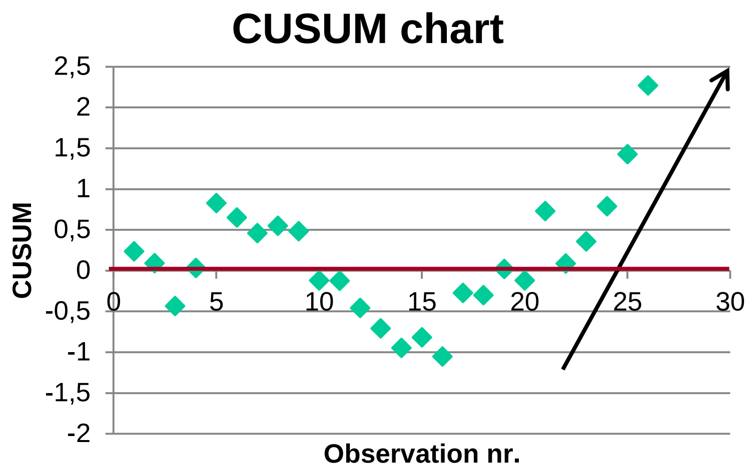
Univariate SPC tools

CUSUM chart (Page, 1954)

- Takes into account the present observation and all the previous ones into the parameter $CUSUM_t$.

$$\mathbf{CUSUM_t} = \sum_{i=1}^{t}\left(x_i - \bar{x}\right)$$





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CUSUM charts detect more easily slight abnormal trends in process behaviour.

Univariate SPC tools

CUSUM chart (Page, 1954)

- Takes into account the present observation and all the previous ones into the parameter $CUSUM_t$.

$$\mathbf{CUSUM_t} = \sum_{i=1}^{t} \left(\mathbf{x_i} - \overline{\mathbf{x}} \right)$$

Parameters for CUSUM chart

- ✓ **Sensibility of the system** (k). Shift from the mean value to be noticed. E.g. shift to notice, δ=1 $\Rightarrow$ 1σ, k = (δ/2)σ, k= 0,5σ.
- ✓ **Control limit (h)**. h = 5σ (or 4σ are the most used).

Univariate SPC tools

CUSUM chart (current visualization)

- Plot of C^+_i (positive deviations from the mean) and C^-_i (negative deviations from the mean) vs. Observation number.

- **Control limits**: set by h.

$$\mathbf{C}_\mathbf{i}^+ = \max\left\{0, \mathbf{C}_{\mathbf{i}-1}^+ + \underbrace{(\mathbf{x}_\mathbf{i} - \overline{\mathbf{x}}) - \mathbf{k}}_{\text{Positive deviations > k}}\right\}$$

$$\mathbf{C}_\mathbf{i}^- = \max\left\{0, \mathbf{C}_{\mathbf{i}-1}^- - \underbrace{(\mathbf{x}_\mathbf{i} - \overline{\mathbf{x}}) - \mathbf{k}}_{\text{Negative deviations > k}}\right\}$$

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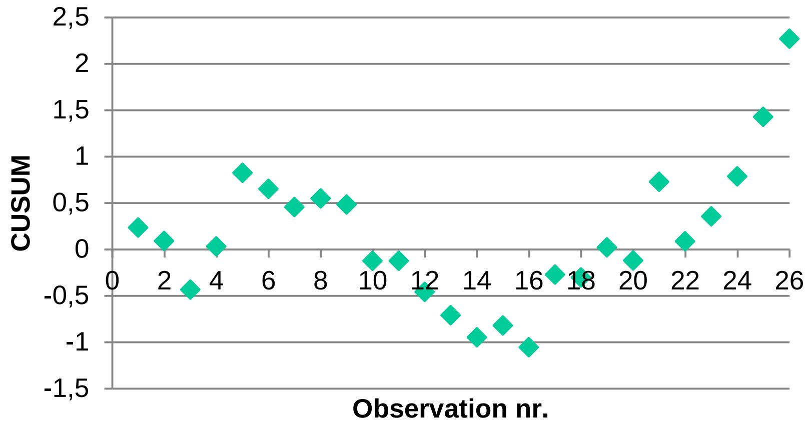
$$\mathbf{C}_0^- = 0, \quad \mathbf{C}_0^+ = 0$$

Univariate SPC tools

CUSUM chart (current visualization)

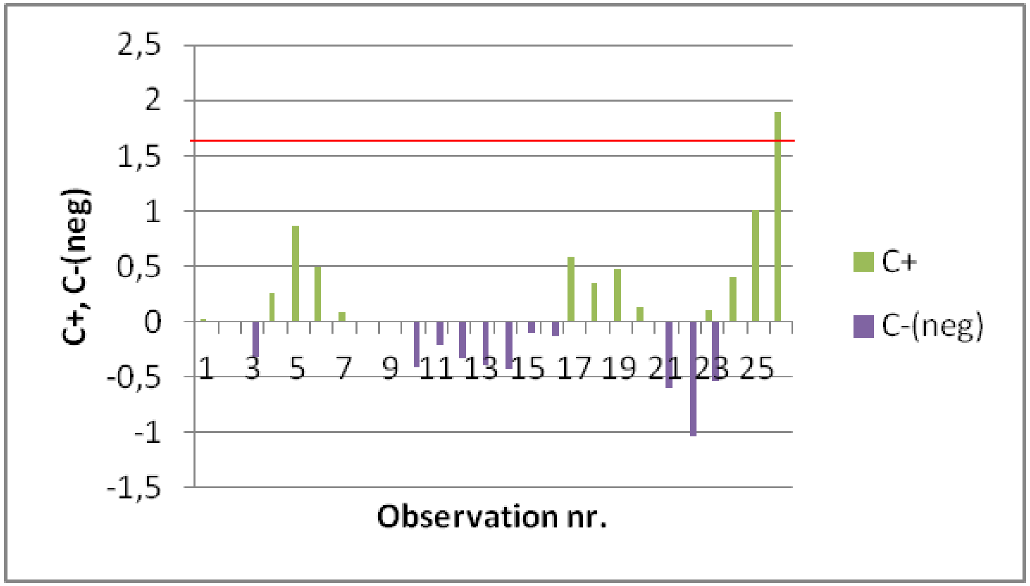
Classical CUSUM chart



Current CUSUM chart

k = 0,2

h = 1,6



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Univariate SPC tools

EWMA chart (Roberts, 1959)

(Exponentially Weighted Moving Average control chart)

- Takes into account the present observation and the past ones. The weight of past observations (λ) decreases exponentially as they are further from the current observation.
- The plotted statistic (y_i) is defined as follows:

$$\mathbf{y_i} = \underbrace{\lambda \mathbf{x_i}}_{\text{Weight of current observation}} + \underbrace{(1-\lambda)\mathbf{y_{i-1}}}_{\text{Weight of past observations}}$$

$$y_0 = \bar{x}$$

x_i current observation

λ weighting factor

$1 < \lambda < 0$

$\lambda \uparrow$ more importance to recent events

$\lambda \downarrow$ longer history of the process considered

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Univariate SPC tools

EWMA chart (Roberts, 1959)

(Exponentially Weighted Moving Average control chart)

- The plotted statistic (y_i) is defined as follows:

$$\mathbf{y_i} = \lambda \mathbf{x_i} + (1-\lambda)\mathbf{y_{i-1}}$$

- This is equivalent to:

$$\mathbf{y_i} = \lambda \mathbf{x_i} + \lambda(1-\lambda)\mathbf{x_{i-1}} + \lambda(1-\lambda)^2 \mathbf{x_{i-2}} + \lambda(1-\lambda)^3 \mathbf{x_{i-3}} + \cdots$$

Weights of further observations decrease exponentially!!

Usual λ values

$0,25 > \lambda > 0,05$

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Univariate SPC tools

EWMA chart (Roberts, 1959)

(Exponentially Weighted Moving Average control chart)

- Plots y_i vs. current observation number.

$$\mathbf{y_i} = \lambda \mathbf{x_i} + (1 - \lambda)\mathbf{y_{i-1}}$$

- **Limits of EWMA chart.**
  - ✓ Change with the number of observations considered.

$$\mathbf{UCL_i} = \bar{\mathbf{x}} + \mathbf{L}\sqrt{\mathbf{var(y_i)}} = \bar{\mathbf{x}} + \mathbf{L\sigma}\sqrt{\frac{\boldsymbol{\lambda}(1-(1-\boldsymbol{\lambda})^{2i})}{2-\boldsymbol{\lambda}}}$$

L = 3

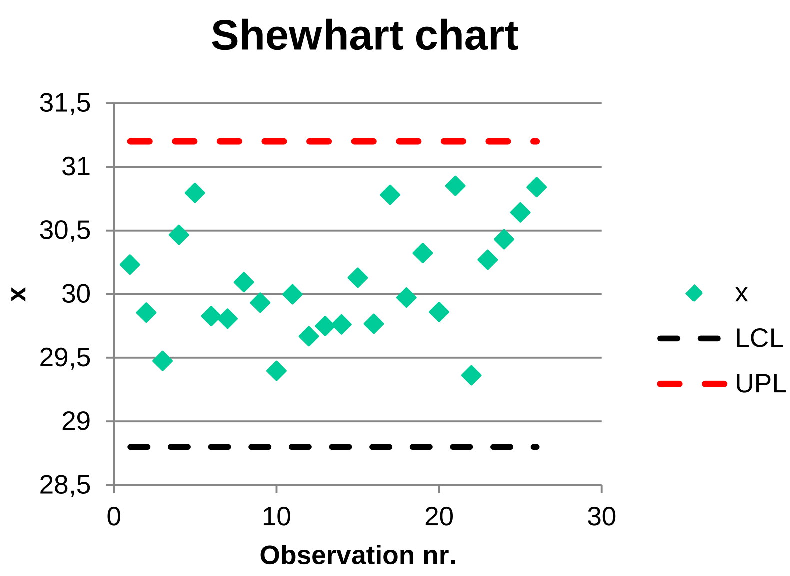
$$\mathbf{LCL_i} = \bar{\mathbf{x}} - \mathbf{L}\sqrt{\mathbf{var(y_i)}} = \bar{\mathbf{x}} - \mathbf{L\sigma}\sqrt{\frac{\boldsymbol{\lambda}(1-(1-\boldsymbol{\lambda})^{2i})}{2-\boldsymbol{\lambda}}}$$

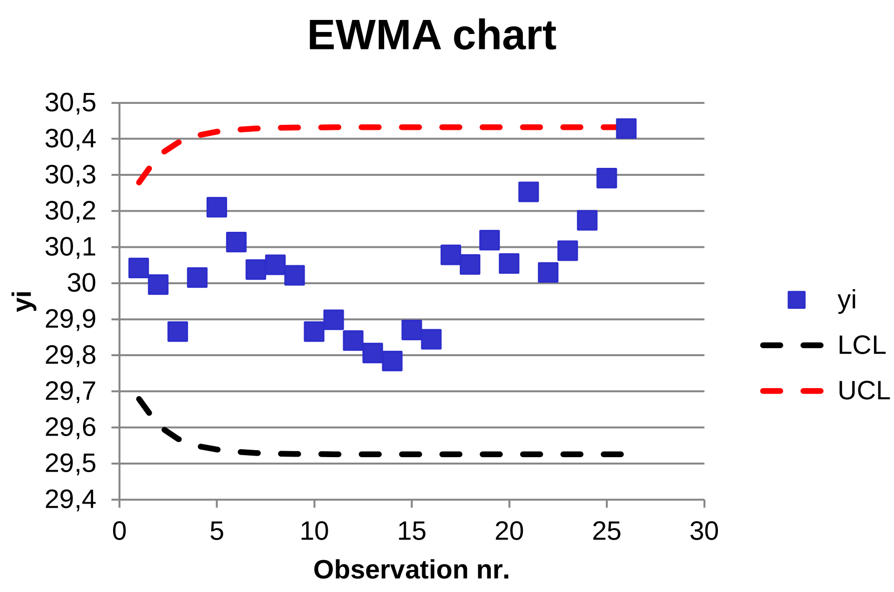
Univariate SPC tools

EWMA chart (Roberts, 1959)

(Exponentially Weighted Moving Average control chart)

$$\mathbf{y_i} = \lambda \mathbf{x_i} + (1-\lambda)\mathbf{y_{i-1}}$$





$\lambda = 0,25$

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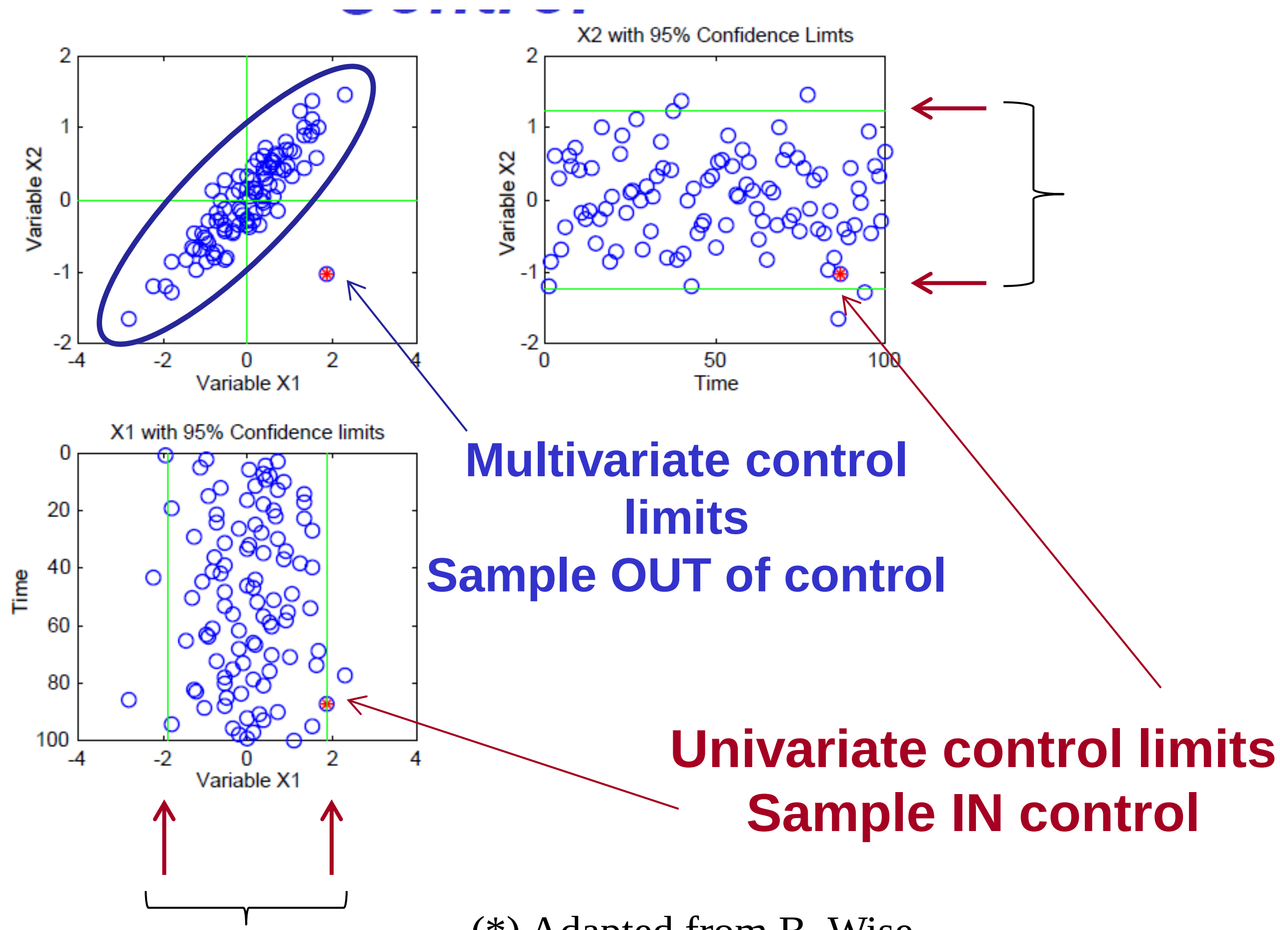
Limitations of univariate SPC charts

- One SPC chart is not sufficient to control a process.
- Univariate SPC charts ignore the relationship among variables to be controlled.

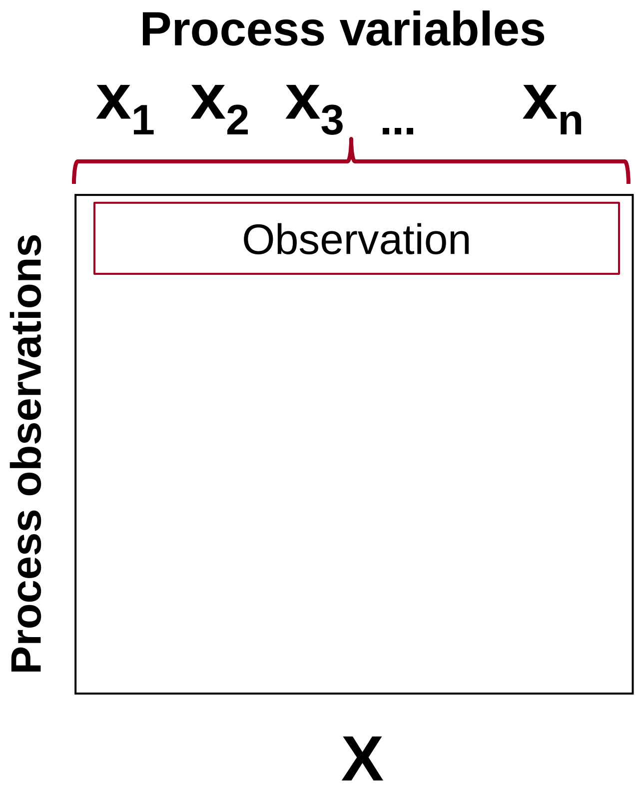


(*) Adapted from B. Wise.

Multivariate Statistical Process Control (MSPC)

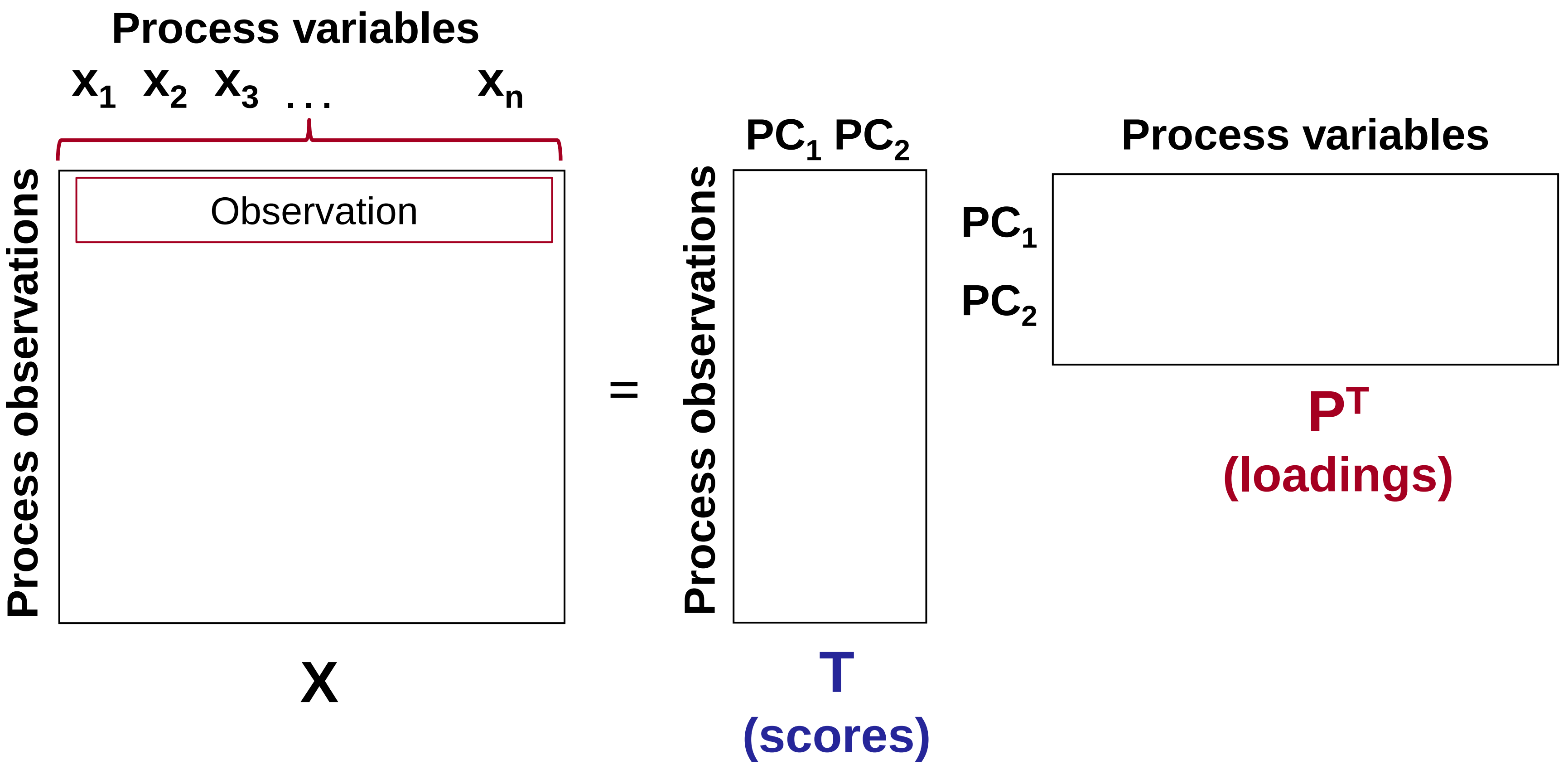
- Takes into account several variables at the same time.
- Considers correlation among variables.
- Can be carried out analysing one data table of process or quality variables.
  - ✓ **PCA-based process control.**
- Can be carried out relating a data table of process variables to another of quality variables.
  - ✓ **PLS-based process control.**

MSPC based on PCA



- Several variables characterize each process observation.
- All of them are analyzed simultaneously.
- For visualization, a low dimensional space (PC space) should be used.

MSPC based on PCA



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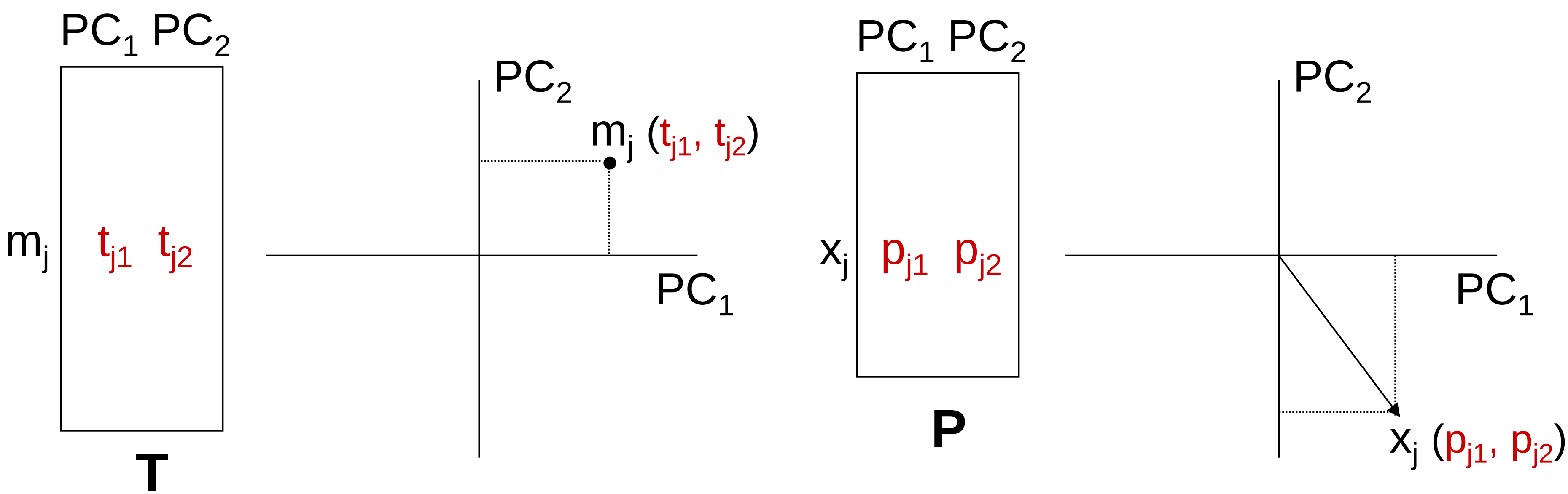
- PCs do not repeat information among them.
- PCs preserve the information in original variables.
- PCs are linear combinations of original variables.

MSPC based on PCA

$$X = T \, P^T$$

Scores plot (observation map in PC space)

Loadings plot (variable map in PC space)



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- PCA allows easier visualization of process observations (score plot) and process variables (loading plot).

MSPC based on PCA

Steps

- Building a PCA model from process data in NOC conditions.

$$\mathbf{X}_{\mathbf{NOC}} = \mathbf{T}_{\mathbf{NOC}} \boxed{\mathbf{P}^{\mathbf{T}}_{\mathbf{NOC}}} \text{ Model}$$

- Project new process data using the model developed in NOC conditions.

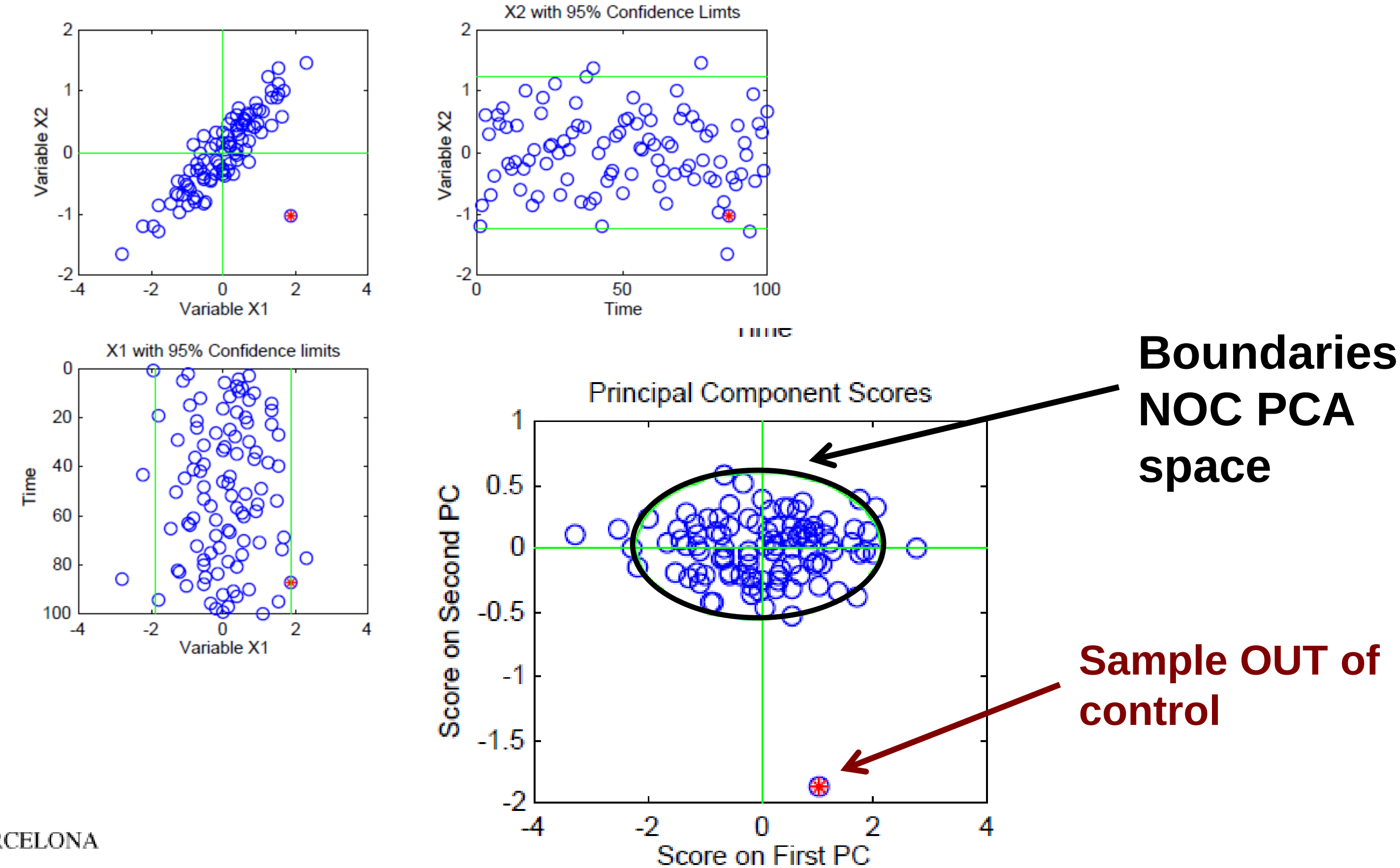
$$\mathbf{T}_{\mathbf{new}} = \mathbf{X}_{\mathbf{new}} \mathbf{P}_{\mathbf{NOC}}$$

- See whether the $\mathbf{T}_{\mathbf{new}}$ value is within the statistical boundaries of the score plot of NOC data.

MSPC based on PCA

Diagnostic tools based on PCA

- **Score plot.** Observations out of boundaries are OUT of control.



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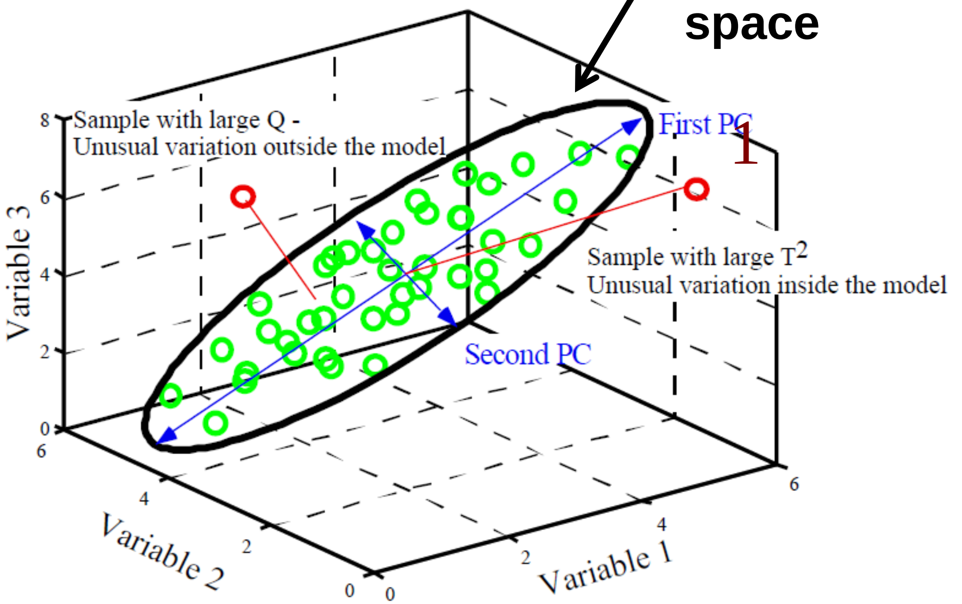
MSPC based on PCA

Diagnostic tools based on PCA

- **Score plot.** Observations out of boundaries are OUT of control.
  - ✓ **Type 1**. Observations are OUT of boundaries but follow the tendency of the NOC model (**T^2 chart**).
  - ✓ **Type 2.** Observations are OUT of boundaries and do not behave according to the model (**Q** or **SPE chart**).

Boundaries NOC PCA space



(*) Adapted from B. Wise.

MSPC based on PCA

Diagnostic tools based on PCA

- **T^2 charts.** Based on the Hotelling's T^2 statistic. Compare the magnitude of the scores of a new observation with those from NOC observations.

$$T^2_{obs} = \sum_{i=1}^{PC} \frac{t^2_{i,obs}}{s^2_{t_i}} = \sum_{i=1}^{PC} \frac{t^2_{i,obs}}{\lambda_i}$$

t_i Score value

s_{t_i} Variance of PC_i

λ_i Eigenvalue of PC_i

- **Q charts.** Show how big is the residual of the observation with respect to the projection in the PCA space.

$$T_{new} = X_{new} P_{NOC} \qquad \hat{X}_{new} = T_{new} P^T_{NOC}$$

$$Q = \sum_{i=1}^{nv} \left(\hat{x}_{new,i} - x_{new,i}\right)^2$$

MSPC based on PCA

Diagnostic tools based on PCA

- **T^2 chart.**

$$T^2_{obs} = \sum_{i=1}^{PC} \frac{t^2_{i,obs}}{s^2_{t_i}} = \sum_{i=1}^{PC} \frac{t^2_{i,obs}}{\lambda_{i_i}}$$

Upper control limit $$UCL(T^2) = \frac{A(m^2-1)}{m(m-A)} F(A, m-A), \alpha$$

A nr. of PCs in the model
m nr. of samples
α confidence limit

- **Q chart.**

$$Q = \sum_{i=1}^{nv} \left(\hat{x}_{new,i} - x_{new,i}\right)^2$$

Upper control limit

$$UCL(Q) = \theta_1 \left[\frac{h_0 p(\alpha)\sqrt{2\theta_2}}{\theta_1} + 1 + \frac{\theta_2 h_0 (h_0 - 1)}{\theta_1^2} \right]$$

$$\theta_k = \sum_{j=A+1}^{PC} (\lambda_j)^k$$

$$h_o = 1 - \frac{2\theta_1\theta_3}{3\theta_2^2}$$

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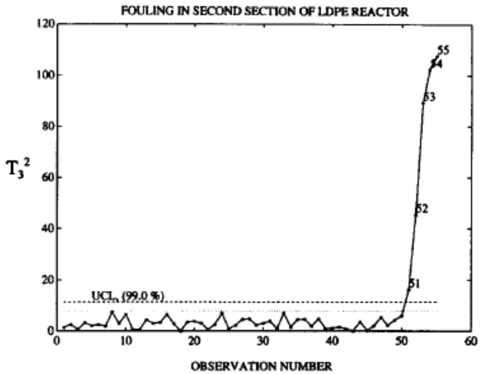
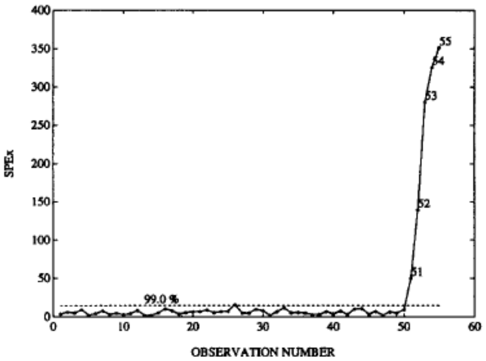
MSPC based on PCA

Diagnostic tools based on PCA

T^2 chart



Q chart



- **Abnormal observations in T^2:** they follow a normal process behaviour but are out of the domain identified as NOC. Maybe NOC conditions should be redefined.
- **Abnormal observations in Q or in Q and T^2 :** they show behaviour different from the process. The source(s) of abnormality should be identified.

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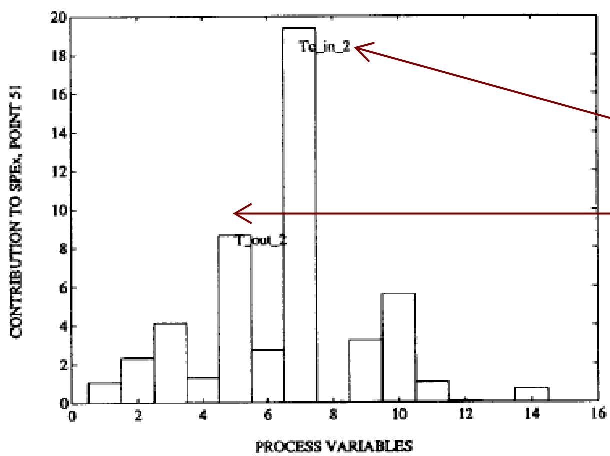
MSPC based on PCA

Sources of abnormal process behaviour
(contribution plots based on Q charts).

1. Identify abnormal observation (x_i)
2. Plot the residuals of observation x_i for each variable.

$$\mathbf{e_i = x_i - \hat{x}_i}$$

Contribution plot



High values in the contribution plot

variables responsible for abnormal behaviour.

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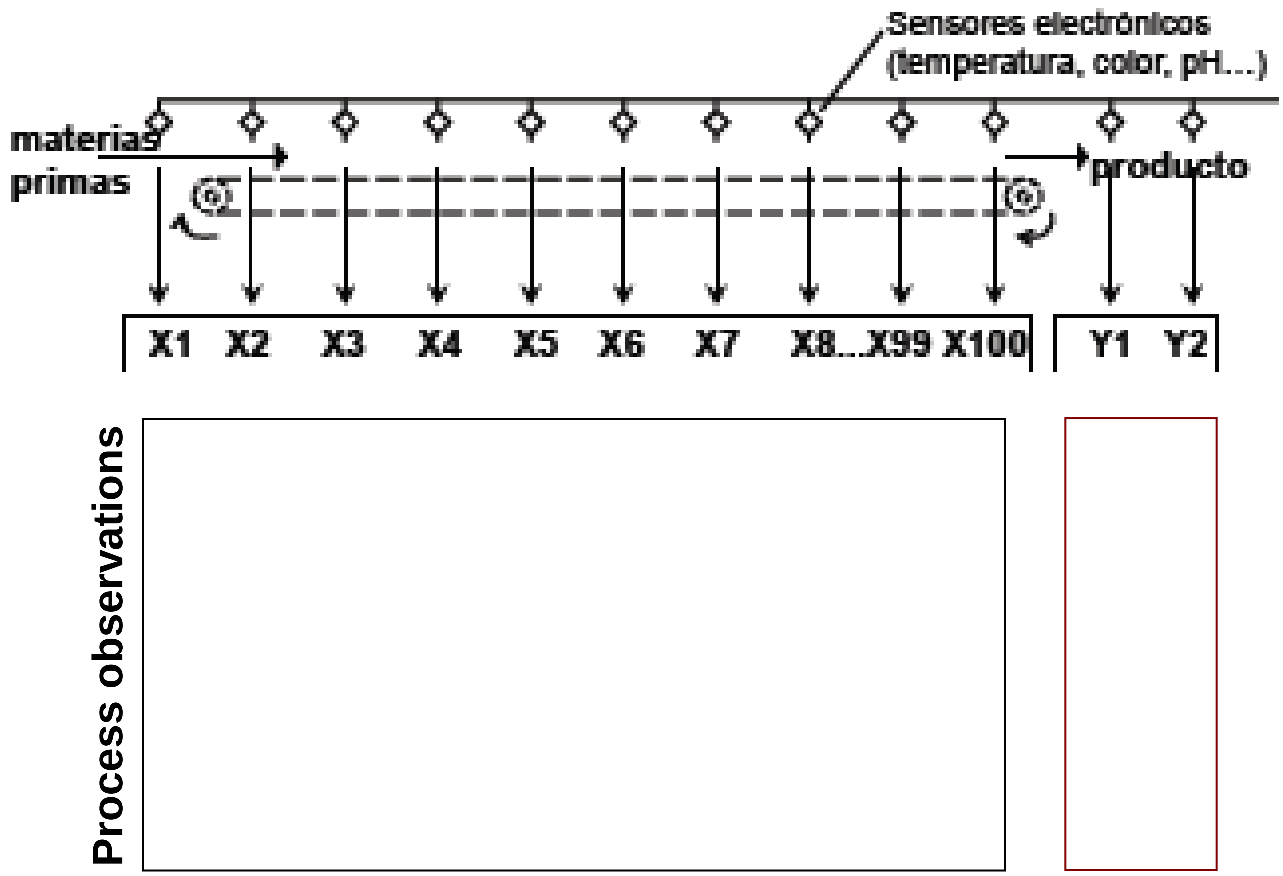
MSPC based on PLS

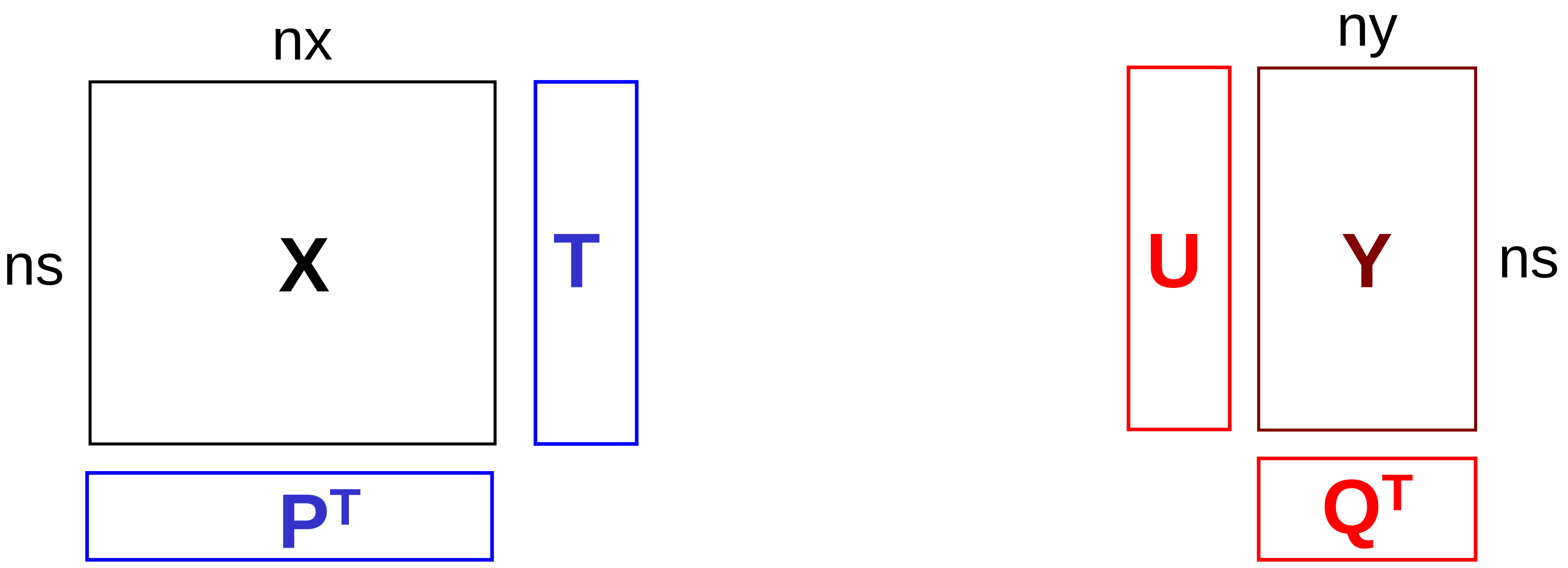


X
(process variables)

Y
(quality variables)

Relates **X** and **Y**

MSPC based on PLS. The concept.



$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E}$ ⇒ $\mathbf{U} = \mathbf{T}\mathbf{B}_{PLS}$ ⇐ $\mathbf{Y} = \mathbf{U}\mathbf{Q}^T + \mathbf{E'}$

- **X** and **Y** are decomposed in PLS components.
- PLS components describe the covariance between **X** and **Y**.

MSPC based on PLS

Steps

- Building a PLS model from process data in NOC conditions.

$X = T\boxed{P_{NOC}^T}$ **Model** $Y = U\boxed{Q_{NOC}^T}$ **Model** $U = T\boxed{B_{PLS}}$ **Model**

- Project new process data using the model developed in NOC conditions.

$T_{new} = X_{new}P_{NOC}$ $U_{new} = T_{new}B_{PLS}$ $Y_{new} = U_{new}Q_{NOC}^T$

- See whether the Y_{new} and T_{new} values are within the statistical boundaries of the plots of NOC data.

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Allows prediction of **Y** values in real time

MSPC based on PLS

- **T^2 chart** (on PLS scores of **X**)
- **Q chart** (on PLS scores of **X**)
- **Y predicted chart** (prediction of quality attributes).
  - ✓ Shewhart chart.

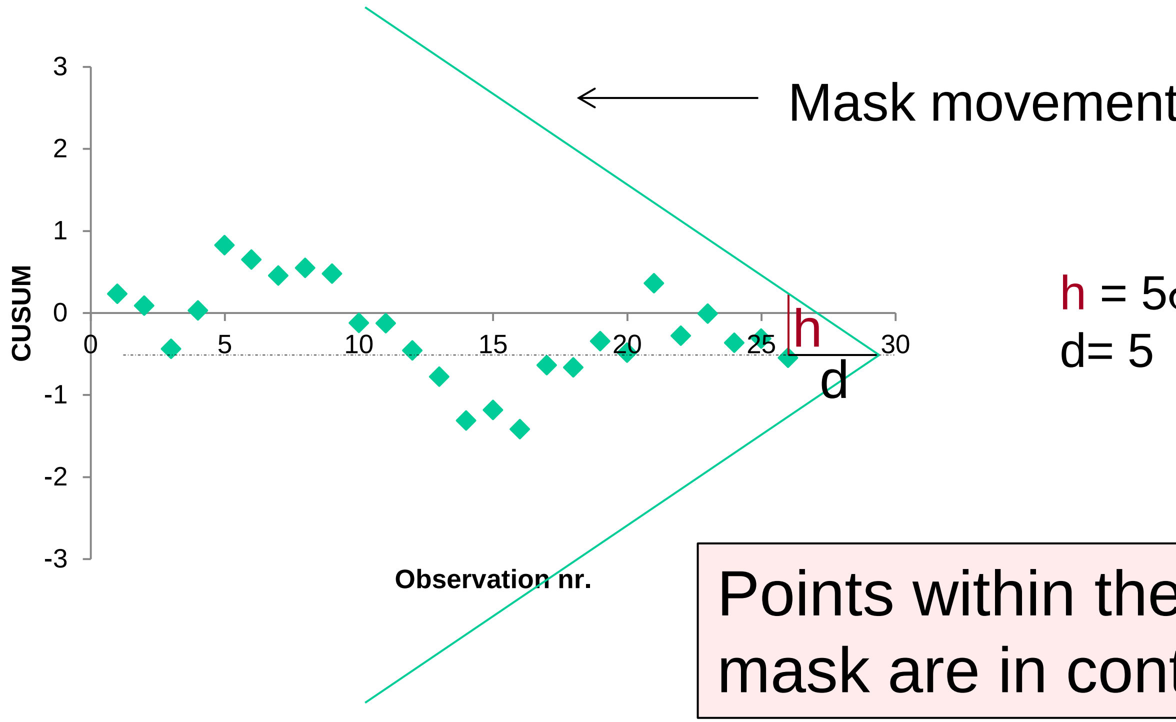
MSPC. Conclusions.

- Takes into account all process and/or quality variables in process control.
- Takes into account the natural correlation among variables.
- Allows process control in real time.
- Helps to check whether process and/or quality variables are IN or OUT of control.
- Helps to detect the end-point of a process (by comparing the observations of an evolving process with a model done with observations related to ‘finished’ processes.

Univariate SPC tools

CUSUM chart (classical visualization)

- Plot of $CUSUM_t$ vs. Observation number. $\mathbf{CUSUM_t} = \sum_{i=1}^{t} (x_i - \bar{x})$
- **Control limits**: set by a V-mask built using k and h limits.
  - ✓ The V-mask was slided from last point and points out of it were out of control.



h = 5σ
d= 5

Points within the mask are in control.

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