Statistical Techniques for Monitoring Industrial Processes

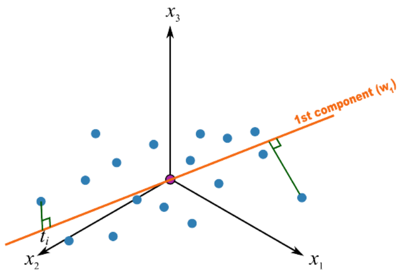
Lecture : PLS – Under the Hood

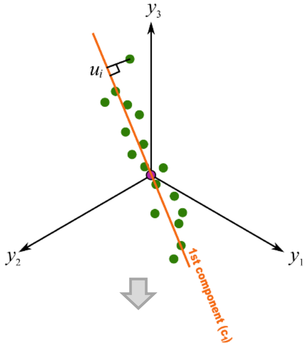
Module : PLS-based MSPM

Course TOC

- Introduction to Statistical Process Monitoring (SPM)
- Python Installation and basics (optional)
- Univariate SPM & Control Charts
  - Shewhart Charts
  - CUSUM Charts
  - EWMA Charts
- Multivariate SPM
  - Principal Component Analysis (PCA)-based MSPM
  - Partial Least Squares (PLS) regression-based MSPM
    - Fault detection & diagnosis (FDD) using PLS
    - Application to a LDPE reactor monitoring
  - Strategies for handling nonlinear, dynamic, multimode systems
- Deploying SPM solutions

PLS Regression: Score / Weight / Loading Vectors





$$t_1 = Xw_1 \qquad u_1 = Yc_1$$

$\boldsymbol{t}_1$ & $\boldsymbol{u}_1$: score vectors
$\boldsymbol{w}_1$ & $\boldsymbol{c}_1$: weight vectors

$$X \approx t_1 p_1^T \qquad Y \approx t_1 q_1^T$$

$\boldsymbol{p}_1$ & $\boldsymbol{q}_1$: loading vectors

repeat for k components

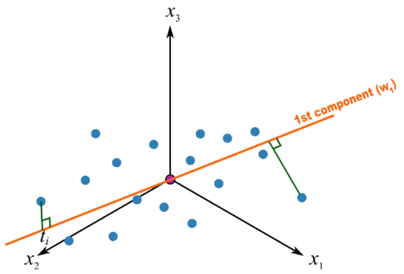
$$X_{new} = X - t_1 p_1^T \qquad Y_{new} = Y - t_1 q_1^T$$

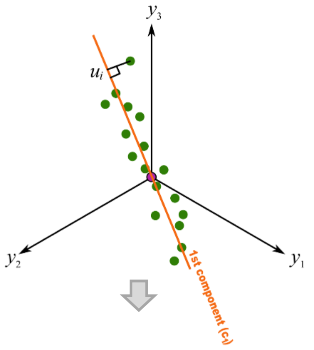
$deflation$ (removes the variability in $\boldsymbol{X}$ and $\boldsymbol{Y}$ that is explained by $\boldsymbol{t}_1$)

$$X = \sum_{i=1}^{k} t_i p_i^T + E \qquad Y = \sum_{i=1}^{k} t_i q_i^T + F$$

PLS decomposition

PLS: Outer and Inner Relations

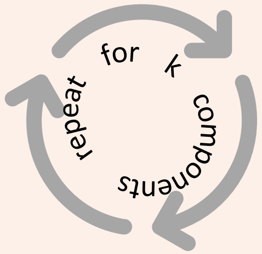




Outer relations

$$\boldsymbol{t}_1 = X\boldsymbol{w}_1 \qquad \boldsymbol{u}_1 = Y\boldsymbol{c}_1$$

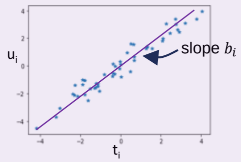
$$\boldsymbol{X} \approx \boldsymbol{t}_1\boldsymbol{p}_1^T \qquad \boldsymbol{Y} \approx \boldsymbol{t}_1\boldsymbol{q}_1^T$$



$$\boldsymbol{X} \leftarrow \boldsymbol{X} - \boldsymbol{t}_1\boldsymbol{p}_1^T \qquad \boldsymbol{Y} \leftarrow \boldsymbol{Y} - \boldsymbol{t}_1\boldsymbol{q}_1^T$$

Inner relations

$$\boldsymbol{u}_i \approx b_i\boldsymbol{t}_i$$



$$\boldsymbol{U} = [\boldsymbol{u}_1, \boldsymbol{u}_2, \cdots, \boldsymbol{u}_k] \approx [b_1\boldsymbol{t}_1, b_2\boldsymbol{t}_2, \cdots, b_k\boldsymbol{t}_k] = \boldsymbol{T}\boldsymbol{B}$$

$$diag([b_1, b_2, \cdots, b_k])$$

helps to estimate $\boldsymbol{U}$ and eventually $\boldsymbol{Y}$ ($\approx \widehat{\boldsymbol{U}}\boldsymbol{Q}^T = \boldsymbol{TBQ}^T$) using only input variables

PLS: Rotation Vectors / Projection Matrix

Can we write: $\boldsymbol{T} \cancel{=} \boldsymbol{XW}$

$$\boldsymbol{t}_i \neq X\boldsymbol{w}_i \;\; ; i > 2$$

Instead, we can write: $\boldsymbol{T} = \boldsymbol{XR}$

$$\boldsymbol{R} = \boldsymbol{W}\left(\boldsymbol{P}^{\boldsymbol{T}}\boldsymbol{W}\right)^{-\boldsymbol{1}}$$

PLS VS PCA: Fault Detection Metrics

PCA

$\boldsymbol{T} = \boldsymbol{X}\boldsymbol{P}$

$T^{\mathbf{2}}$ metrics

$\boldsymbol{E} = \boldsymbol{X} - \widehat{\boldsymbol{X}}$

SPE metrics

PLS

$\boldsymbol{T} = \boldsymbol{X}\boldsymbol{R}$

$T^{\mathbf{2}}$ metrics

Captures systematic variations

$\boldsymbol{E}_x = \boldsymbol{X} - \widehat{\boldsymbol{X}}$

SPE_x metrics

Captures noise in input variables

$\boldsymbol{E}_y = \boldsymbol{Y} - \widehat{\boldsymbol{Y}}$

SPE_y metrics

Captures noise in output variables

Statistical Techniques for Monitoring Industrial Processes

Next Lecture : PLS Modeling of LDPE Reactor

Module : PLS-based MSPM