# Quality-Relevant Process Monitoring

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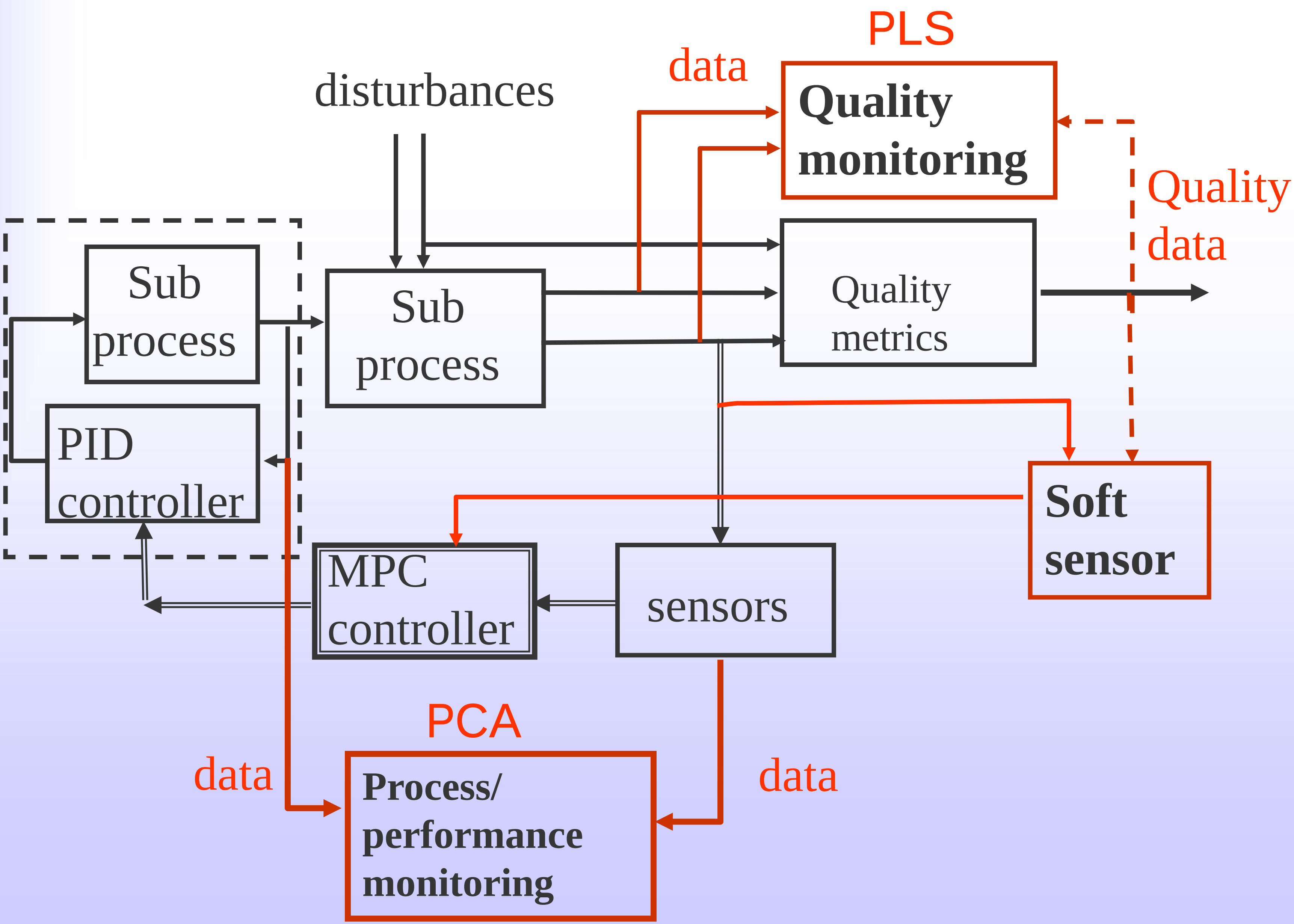
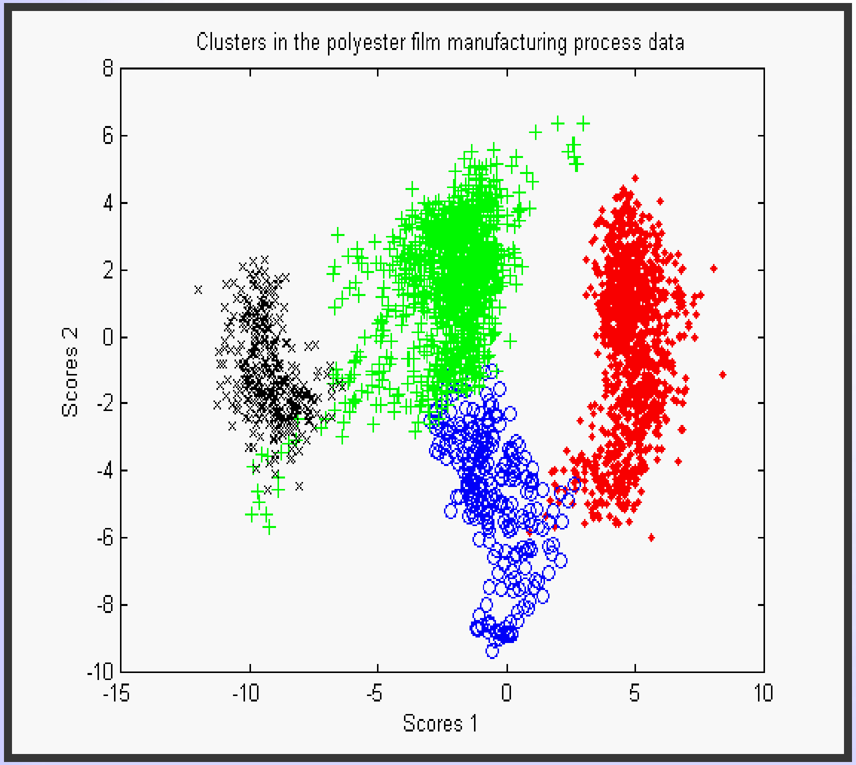
# Data-driven process monitoring

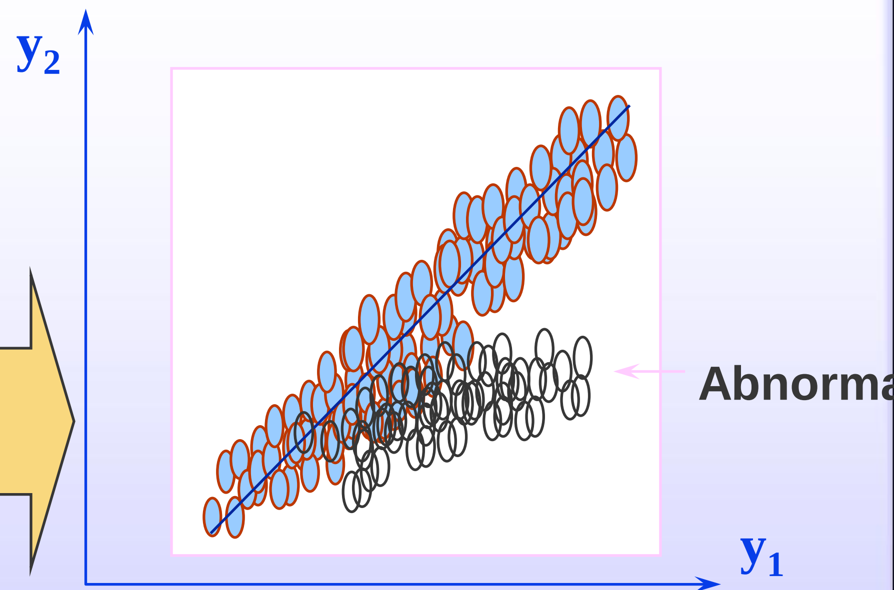


# Process and Quality variables

## Process data

## Quality data




PCA monitoring: X alone

PLS monitoring: X guided by Y

- PCA based monitoring focuses on process data variation only
  - ‘unsupervised’ analysis of process data
  - Nuisance alarms
- PLS based monitoring monitors process data by its co-variation with quality data
  - ‘supervised’ analysis of process data
  - removes nuisance alarms cased by PCA

# PCA diagnosis methods

- Currently applied in many areas
  - Fault detection: SPE, T2, or combined
  - Fault diagnosis: contribution plots; fault identification via reconstruction
- Recent progress
  1. Understand the weakness of contribution plots
  2. Unifying many diagnosis methods and suggest relative contributions to be used
  3. Kernel methods for nonlinear data monitoring

# Unifying many diagnosis methods

- Carlos Alcala and S. Joe Qin (2010). Analysis and Generalization of Fault Diagnosis Methods for Process Monitoring. Revised for *J. of Process Control*. (Special Issue in honor of T.J. McAvoy)
  - Most contribution plot methods do not have statistically equal contributions when no fault is present
  - Suggest relative contributions which posses this property

# Nonlinear, Kernel PCA methods

- C. Alcala and S.J. Qin (2010). Reconstruction-based Contribution for Process Monitoring with Kernel Principal Component Analysis, to appear in *I&EC Research*. (Special Issue in honor of T.F. Edgar)

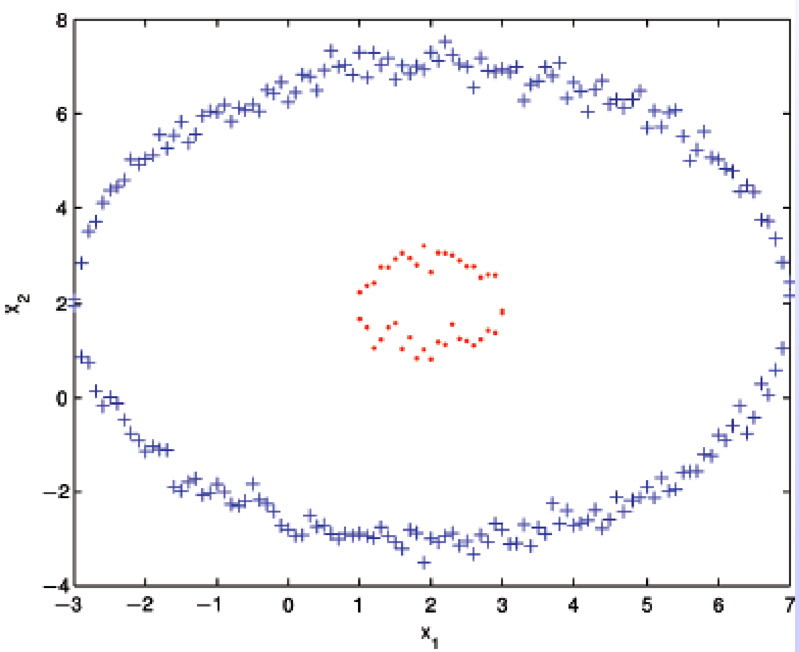



**Figure 1.** Normal and faulty data in a bidimensional space.

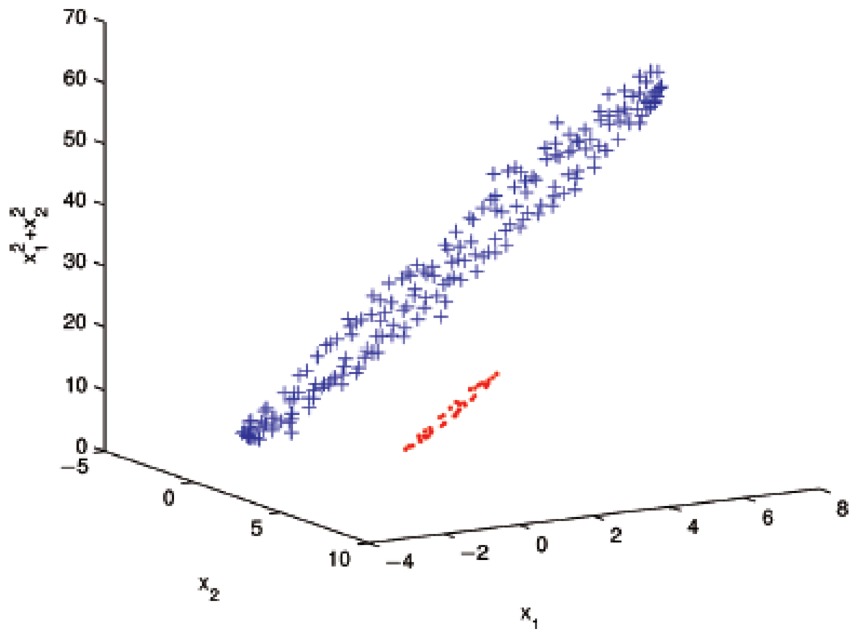
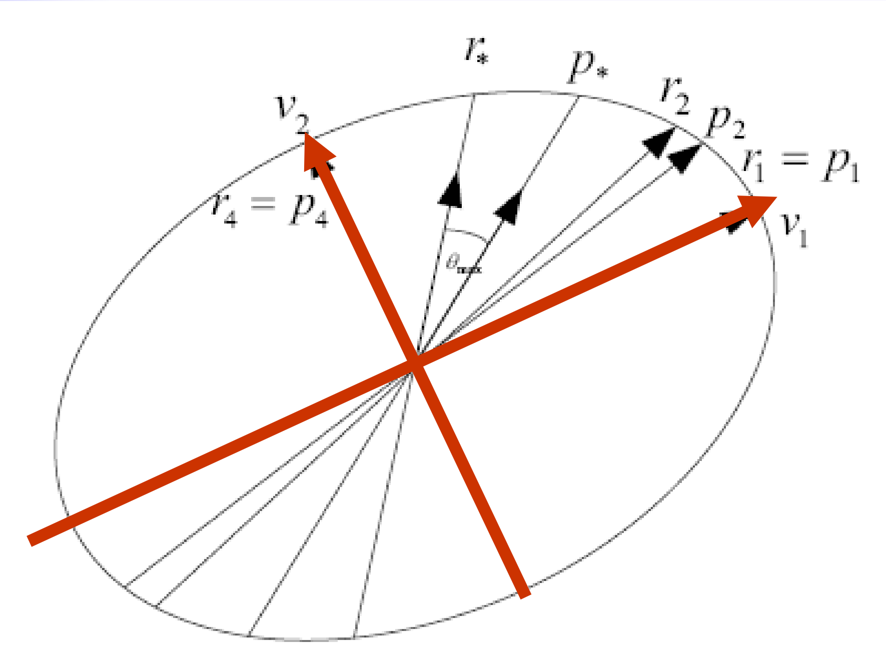
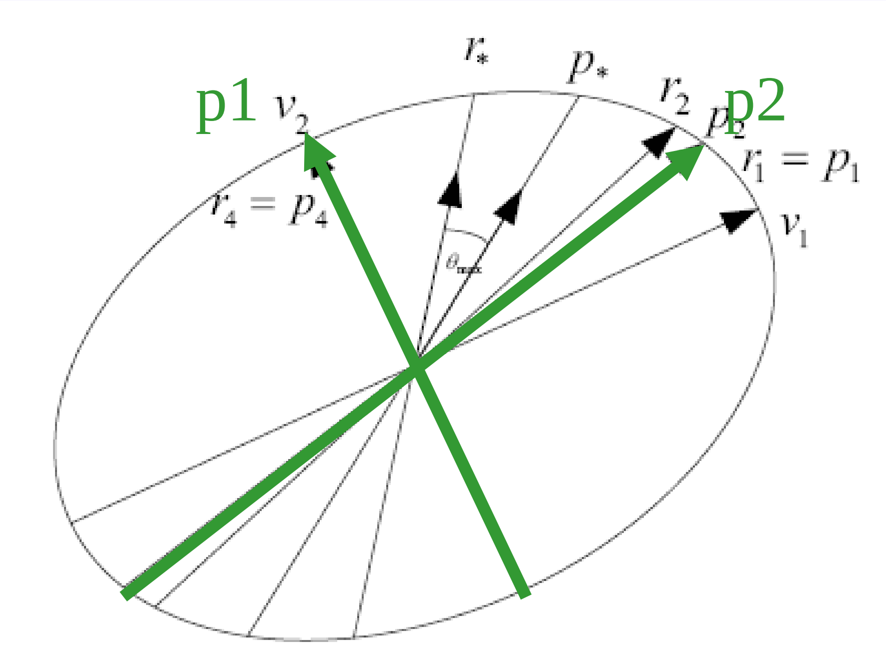



**Figure 2.** Normal and faulty data in a tridimensional space.

# PLS: Impact of Y on X-space Decomposition

- PLS partition of X, depending on whether Y lines up with the major X directions or not



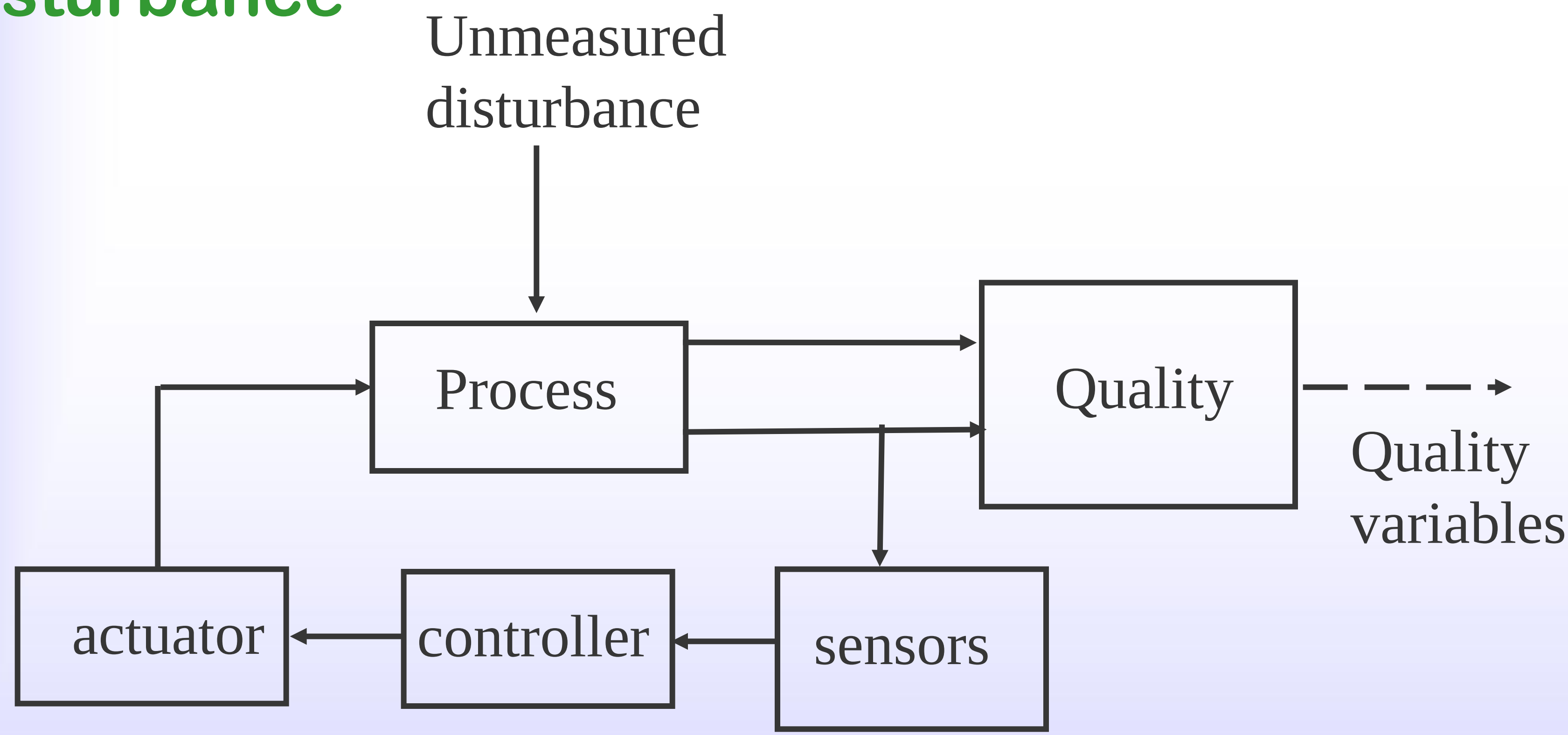




**PCA directions** **PLS directions**

## PCA-like, Unsupervised Monitoring

- Pros: plenty of process data, easy to use given normal data
- Cons: need normal data to define 'normal'
- Cons: out-of-control in process data does not always point to a 'quality' problem
- Cons: Measured variables being normal does not guarantee the quality is normal because of unmeasured contributors to quality

# Example: Controller responds to unmeasured disturbance




- Tracking measured variables alone would signal an alarm even though the control does it job to reject the unmeasured disturbance

# PLS-Based Process Monitoring

- PLS-based monitoring uses quality data Y to guide the partition of process data X, which is different from PCA partition of X-space
- Impact of Y on the structural modeling of X-space
  - PLS is the de facto method for modeling X and Y
  - PLS factors and residuals are interpreted in the same way as PCA factors and residuals
  - Lack of understanding of the impact of Y on the decomposition of X-space

## Recent work

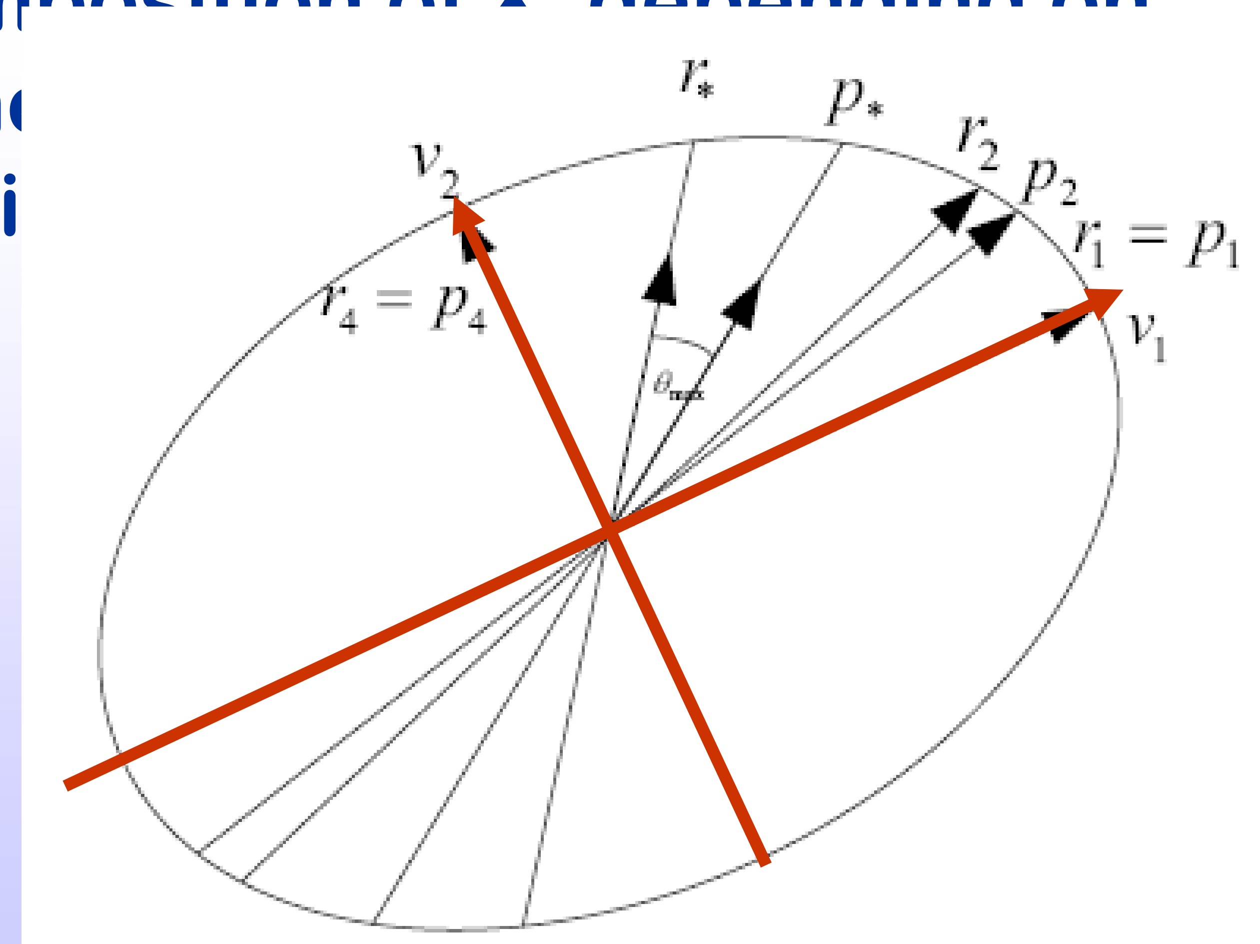
- Gang Li, S. Joe Qin, and Donghua Zhou (2008). Geometric properties of partial least squares for process monitoring, submitted to *Automatica*.
  - Gives a fairly thorough understanding of X-space decomposition guided by Y
- Donghua Zhou, Gang Li, and S. Joe Qin (2008). Total projection to latent structures for process monitoring, accepted by *AIChE Journal*.
  - PCA-like interpretation of PLS partition is not adequate. Additional projections (i.e.,

# PCA vs. PLS for monitoring

| | |
|---|---|
| PCA model<br>$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E}$ **T=XP** | PLS model<br>$\mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E}$<br>$\mathbf{Y} = \mathbf{T}\mathbf{Q}^T + \mathbf{F}$ $\mathbf{T} = \mathbf{X}\mathbf{R}$ |
| PCA projection<br>**P=R** | PLS projection<br>$\mathbf{x} = \hat{\mathbf{x}} + \tilde{\mathbf{x}}$<br>$\hat{\mathbf{x}} = \mathbf{P}\mathbf{R}^T\mathbf{x} \in S_p \equiv Span\{\mathbf{P}\}$<br>$\tilde{\mathbf{x}} = (\mathbf{I} - \mathbf{P}\mathbf{R}^T)\mathbf{x} \in S_r \equiv Span\{\mathbf{R}\}^{\perp}$ |
| PCA monitoring<br>$T^2 = \mathbf{t}^T\mathbf{\Lambda}^{-1}\mathbf{t} \sim \frac{A(n^2-1)}{n(n-A)}F_{A,n-A,\alpha}$<br>$Q = \|\tilde{\mathbf{x}}\|^2 \sim g\chi^2_{h,\alpha}$ | PLS monitoring<br>$T^2 = \mathbf{t}^T\mathbf{\Lambda}^{-1}\mathbf{t} \sim \frac{A(n^2-1)}{n(n-A)}F_{A,n-A,\alpha}$<br>$Q = \|\tilde{\mathbf{x}}\|^2 \sim g\chi^2_{h,\alpha}$ |
| | **PLS residual not always 'small'** |
| | **PLS scores not all related to Y**<br>**PLS residual 'faults' can affect Y** |

# Impact of Y on X-space Decomposition

- **PLS partition of X departs from PCA decomposition of X, depending on whethe directi**




PCA directions

# Total PLS for Monitoring

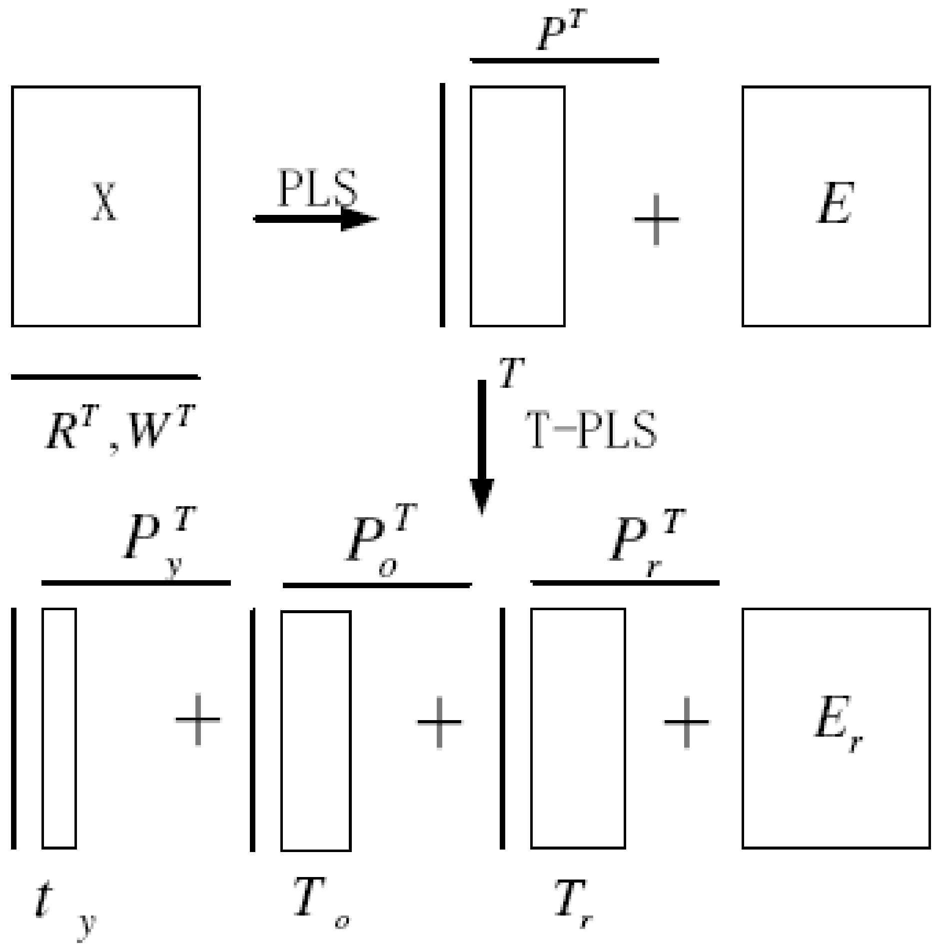



Fig. 1. T-PLS structure

# Four subspaces – Total PLS

1. Two related to scores
   1. subspace of X-space that is solely responsible in predicting Y
   2. subspace of X-space that is explored by the PLS objective but does not predict Y
2. Two related to residuals
   1. subspace of X-space that is not ‘useful’ for the PLS objective, but has significant variation or excitation in X-space
   2. subspace of X-space that is not excited in the X-space of the data
3. Detail will be presented by Carlos Alcala

# PLS-based monitoring papers

- Gang Li, S. Joe Qin, and Donghua Zhou (2010). Geometric properties of partial least squares for process monitoring, *Automatica*, 46, 204-210.
- Donghua Zhou, Gang Li, and S. Joe Qin (2010). Total projection to latent structures for process monitoring, *AIChE Journal*, 56, 168-178.
- Gang Li, S. Joe Qin, and Donghua Zhou (2010). Output relevant fault reconstruction and fault subspace extraction in Total PLS models. Accepted by *I&EC Research*.