Loss Method: A Static Estimator Applied for Product Composition Estimation From Distillation Column Temperature Profile

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Motivation

- Some process variables can not be measured frequently
  - Example: Composition measurement using online analyzers (like Gas Chromatograph)
    - Large measurement delays
    - High investment/maintenance costs
    - Low reliability

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  - Pressure
  - Flow rate
  - etc.

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An estimator attempts to approximate the unknown parameters using the measurements

Outline

1. Introduction
   - Estimation
   - Partial Least Squares
2. Loss Method
   - Optimal estimators for different scenarios
   - Necessary data for the task of estimation
3. Examples

Estimators

Different categories: Static / Dynamic, Data-based / Model-based, Open-loop / Close-loop

- Static Estimators

- Dynamic Estimators

[1] R. Weber, C. Brosilow, The Use of Secondary Measurements to Improve Control, AIChE J., 18, 3, p. 614-623

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  - Model-based
    - Example: Brasilow estimator[1]
    - Our method is in this category
  - Data-based
    - Example: Partial Least Square (PLS)
- Dynamic Estimators

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- Static Estimators
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  - Data-based
    - Example: Partial Least Square (PLS)
- Dynamic Estimators
  - Model-based
    - Example: Kalman filter
  - Data-based
    - Time variant reliability analysis of existing structures using data

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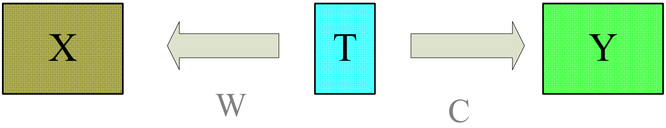
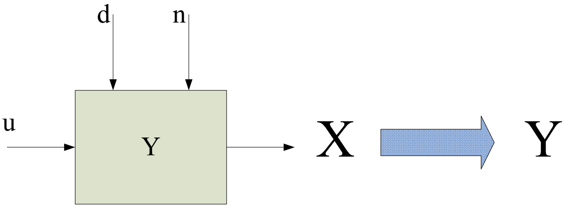
Partial Least Squares

- PC regression = weights are calculated from the covariance matrix of the predictors
- PLS = weights reflect the covariance structure between predictors and response – mostly requires a complicated iterative algorithm



- Nipals and SIMPLS algorithms probably most common
- The goal is to maximize the correlation between the response(s) and component scores
- PLS can extends to multiple outcomes and allows for dimension reduction
- No collinearity – Independence of observations not required

PLS



$$\hat{Y} = BX$$

- PLS: is not optimal for any particular problem
- Loss method: optimal for certain well-defined problems

Loss Method

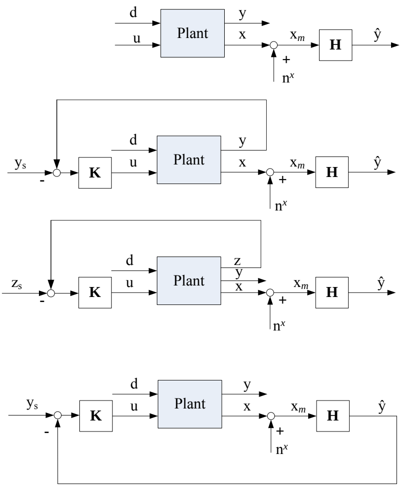
OBJECTIVE

The main objective is to find a linear combination of measurements such that keeping these constant indirectly leads to nearly accurate estimation with a small loss L in spite of unknown disturbances, d, and measurement noise, n^x.

$$\min_{\mathbf{H}} \|e\|_2 = \|\mathrm{y} - \hat{\mathrm{y}}\|_2$$

Loss Method

- "Open-loop" (for the purpose of Monitoring):
  1. No control (u is a free variable)
  2. Primary variables y are controlled (u is used to keep $y = y_s$).
  3. Secondary variables z are controlled (u is used to keep $z = z_s$).
- "Close-loop" (for the purpose of Control)



Loss Method

Assumption: Linear models for the primary variables y, measurements x, and secondary variables z

$$\mathrm{y} = \mathbf{G}_y \mathrm{u} + \mathbf{G}_y^d \mathrm{d} \qquad \mathrm{x} = \mathbf{G}_x \mathrm{u} + \mathbf{G}_x^d \mathrm{d} \qquad \mathrm{z} = \mathbf{G}_z \mathrm{u} + \mathbf{G}_z^d \mathrm{d}$$

$$\mathbf{G}_y = \left(\frac{\partial \mathrm{y}}{\partial \mathrm{u}}\right)_{\mathrm{d}}, \quad \mathbf{G}_y^d = \left(\frac{\partial \mathrm{y}}{\partial \mathrm{d}}\right)_{\mathrm{u}} \qquad \mathbf{G}_x = \left(\frac{\partial \mathrm{x}}{\partial \mathrm{u}}\right)_{\mathrm{d}}, \quad \mathbf{G}_x^d = \left(\frac{\partial \mathrm{x}}{\partial \mathrm{d}}\right)_{\mathrm{u}} \qquad \mathbf{G}_z = \left(\frac{\partial \mathrm{z}}{\partial \mathrm{u}}\right)_{\mathrm{d}}, \quad \mathbf{G}_z^d = \left(\frac{\partial \mathrm{z}}{\partial \mathrm{d}}\right)_{\mathrm{u}}$$

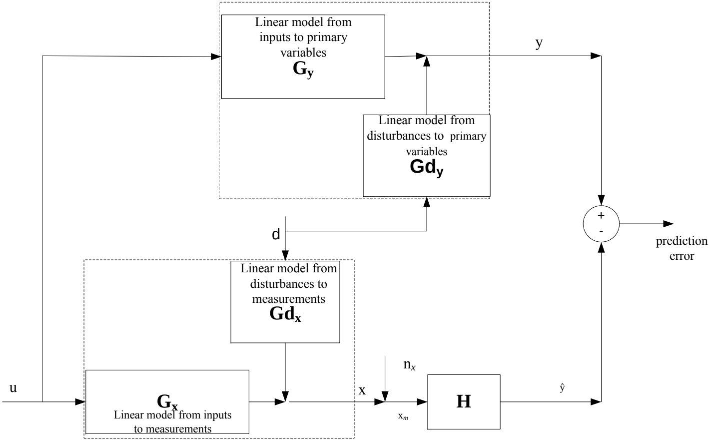
The actual measurements x_m, containing measurement noise n^x is

$$\mathrm{x}_m = \mathrm{x} + \mathrm{n}^x$$

The linear estimator is of the form

$$\hat{\mathrm{y}} = \mathbf{H} \mathrm{x}_m$$

Loss Method


Linear model from inputs to primary variables
Gy
y
Linear model from disturbances to primary variables
Gdy
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+
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prediction error
Linear model from disturbances to measurements
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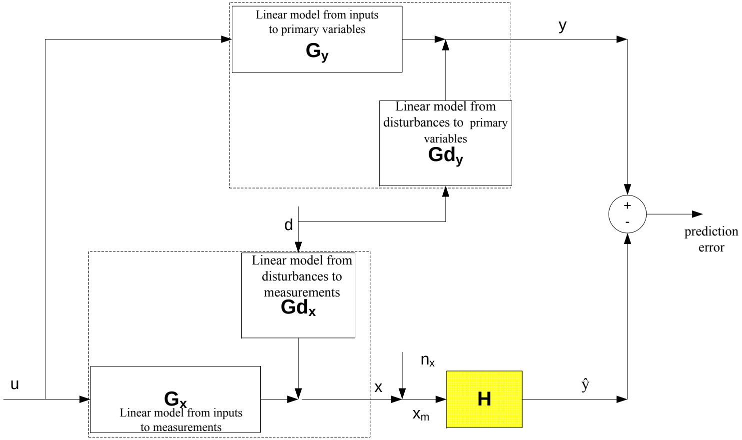
Loss Method


Linear model from inputs
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Optimal estimators for different scenarios (Loss Method)

"Open-loop" 1

$$\mathbf{H}_1 = \mathbf{Y}_1 \mathbf{X}_1^{\dagger}$$
$$\mathbf{Y}_1 = \left[\begin{array}{ccc} \mathbf{G}_y \mathbf{W}_u & \mathbf{G}_y^d \mathbf{W}_d & 0 \end{array}\right]$$
$$\mathbf{X}_1 = \left[\begin{array}{ccc} \mathbf{G}_x \mathbf{W}_u & \mathbf{G}_x^d \mathbf{W}_d & \mathbf{W}_{n^x} \end{array}\right]$$

"Open-loop" 2

$$\mathbf{H}_2 = \mathbf{Y}_2 \mathbf{X}_2^{\dagger}$$
$$\mathbf{Y}_2 = \left[\begin{array}{ccc} \mathbf{W}_{y_s} & 0 & 0 \end{array}\right]$$
$$\mathbf{X}_2 = \left[\begin{array}{ccc} \mathbf{G}_x^{cl} \mathbf{W}_{y_s} & \mathbf{F}\mathbf{W}_d & \mathbf{W}_{n^x} \end{array}\right]$$

"Open-loop" 3

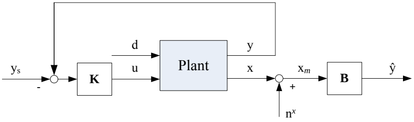
$$\mathbf{H}_3 = \mathbf{Y}_3 \mathbf{X}_3^{\dagger}$$
$$\mathbf{Y}_3 = \left[\begin{array}{ccc} \mathbf{G}_y^{cl} \mathbf{W}_{z_s} & \mathbf{F}'_y \mathbf{W}_d & 0 \end{array}\right]$$
$$\mathbf{X}_3 = \left[\begin{array}{ccc} \mathbf{G}_x^{cl} \mathbf{W}_{z_s} & \mathbf{F}'_x \mathbf{W}_d & \mathbf{W}_{n^x} \end{array}\right]$$

"Closed-loop"

$$\min_{\mathbf{H}} \left\| \mathbf{H} \left[\begin{array}{cc} \mathbf{F}\mathbf{W}_d & \mathbf{W}_{n^x} \end{array}\right] \right\|_F$$
$$\text{s.t. } \mathbf{H}\mathbf{G}_x = \mathbf{G}_y$$

* All subject to the constraint of independent variables values

Optimal "open-loop" estimator, when y=ys (Loss Method)



$$\mathbf{H}_2 = \mathbf{Y}_2 \mathbf{X}_2^{\dagger}$$

$$\mathbf{Y}_2 = \begin{bmatrix} \mathbf{W}_{y_s} & 0 & 0 \end{bmatrix}$$

$$\mathbf{X}_2 = \begin{bmatrix} \mathbf{G}_x^{cl}\mathbf{W}_{y_s} & \mathbf{F}\mathbf{W}_d & \mathbf{W}_{n^x} \end{bmatrix}$$

Initial Equations

$$y = \mathbf{G}_y u + \mathbf{G}_y^d d$$
$$x = \mathbf{G}_x u + \mathbf{G}_x^d d$$
$$x_m = x + n^x$$
$$\hat{y} = \mathbf{H} x_m$$

$$u = \mathbf{G}_y^{-1} y_s - \mathbf{G}_y^{-1}\mathbf{G}_y^d d$$

$$\hat{y} = \mathbf{H}\left[\mathbf{G}_x \mathbf{G}_y^{-1} y_s + \left(\mathbf{G}_x^d - \mathbf{G}_x \mathbf{G}_y^{-1}\mathbf{G}_y^d\right) d + n^x\right]$$

$$e = \underbrace{\begin{bmatrix} (\mathbf{I} - \mathbf{H}\mathbf{G}_x^{cl})\mathbf{W}_{y_s} & -\mathbf{H}\mathbf{F}\mathbf{W}_d & -\mathbf{H}\mathbf{W}_{n^x} \end{bmatrix}}_{\mathbf{M}_{ol}(\mathbf{H})} \begin{bmatrix} y'_s \\ d' \\ n^{x'} \end{bmatrix}$$

$$\|e(\mathbf{H})\|_2 = \frac{1}{2}\|\mathbf{M}_{ol}(\mathbf{H})\|_F^2$$

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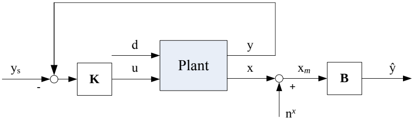

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$$\hat{\mathrm{y}} = \mathbf{H}\mathrm{x}_m$$

$$\mathrm{u} = \mathbf{G}_y^{-1}\mathrm{y}_s - \mathbf{G}_y^{-1}\mathbf{G}_y^d \mathrm{d}$$

$$\hat{\mathrm{y}} = \mathbf{H}\left[\mathbf{G}_x\mathbf{G}_y^{-1}\mathrm{y}_s + \left(\mathbf{G}_x^d - \mathbf{G}_x\mathbf{G}_y^{-1}\mathbf{G}_y^d\right)\mathrm{d} + \mathrm{n}^x\right]$$

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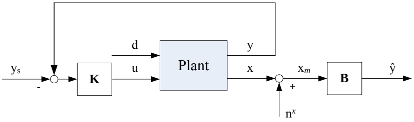
Optimal "open-loop" estimator, when y=ys (Loss Method)



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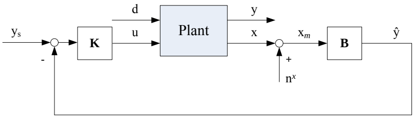
$$\tilde{d} = \left\| \begin{bmatrix} \mathrm{u}' \\ \mathrm{d}' \\ \mathrm{n}^{x'} \end{bmatrix} \right\| \sim \mathcal{N}\left(0, \mathbf{I}_{n_u+n_d+n_x}\right)$$

$$\|e(\mathbf{H})\|_{2,exp} = \frac{1}{2}\mathrm{E}\left[\mathrm{tr}\left(\mathbf{M}\tilde{\mathrm{d}}\tilde{\mathrm{d}}^T\mathbf{M}^T\right)\right] = \frac{1}{2}\mathrm{tr}\left(\mathbf{M}^T\mathbf{M}\mathrm{E}\left[\tilde{\mathrm{d}}\tilde{\mathrm{d}}^T\right]\right)$$

$$\mathrm{E}\left[\tilde{\mathrm{d}}\tilde{\mathrm{d}}^T\right] = Cov\left(\tilde{\mathrm{d}},\tilde{\mathrm{d}}\right) + \mu\mu^T$$

$$\min_{\mathbf{H}} \left\| \begin{bmatrix} \mathbf{W}_{y_s} & 0 & 0 \end{bmatrix} - \mathbf{H}\begin{bmatrix} \mathbf{G}_x^{cl}\mathbf{W}_{y_s} & \mathbf{F}\mathbf{W}_d & \mathbf{W}_{n^x} \end{bmatrix} \right\| = \min_{\mathbf{H}} \|\mathbf{Y}_2 - \mathbf{H}\mathbf{X}_2\|$$

Optimal "close-loop" estimator (Loss Method)



$$\min_{\mathbf{H}} \left\| \mathbf{H} \begin{bmatrix} \mathbf{F}\mathbf{W}_d & \mathbf{W}_{n^x} \end{bmatrix} \right\|_F$$
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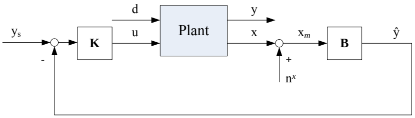
$$u = -(\mathbf{H}\mathbf{G}_x)^{-1}\mathbf{H}\left(\mathbf{G}_x^d d + n^x\right) + (\mathbf{H}\mathbf{G}_x)^{-1} y_s$$

$$y = -\mathbf{G}_y(\mathbf{H}\mathbf{G}_x)^{-1}\mathbf{H}\left[\left(\underbrace{\mathbf{G}_x^d - \mathbf{G}_x\mathbf{G}_y^{-1}\mathbf{G}_y^d}_{F}\right) d + n^x\right] + \mathbf{G}_y(\mathbf{H}\mathbf{G}_x)^{-1} y_s$$

$$e = y - \hat{y} = y - y_s = -\mathbf{G}_y(\mathbf{H}\mathbf{G}_x)^{-1}\mathbf{H}(\mathbf{F}d + n^x) + \left[\mathbf{G}_y(\mathbf{H}\mathbf{G}_x)^{-1} - \mathbf{I}\right] y_s$$

Optimal "close-loop" estimator (Loss Method)



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Optimal "close-loop" estimator (contd.)

The prediction error e

$$\mathrm{e} = \mathrm{y} - \hat{\mathrm{y}} = \mathrm{y} - \mathrm{y}_s = -\mathbf{G}_y(\mathbf{H}\mathbf{G}_x)^{-1}\mathbf{H}(\mathbf{F}\mathrm{d} + \mathrm{n}^x) + \left[\mathbf{G}_y(\mathbf{H}\mathbf{G}_x)^{-1} - \mathbf{I}\right]\mathrm{y}_s$$

Introducing the normalized variables:

$$\mathrm{e} = \underbrace{-\mathbf{G}_y(\mathbf{H}\mathbf{G}_x)^{-1}\mathbf{H}\begin{bmatrix} \mathbf{F}\mathbf{W}_d & \mathbf{W}_{n^x} \end{bmatrix}\begin{bmatrix} \mathrm{d}' \\ \mathrm{n}^{x'} \end{bmatrix}}_{\mathrm{e}_1} + \underbrace{\left[\mathbf{G}_y(\mathbf{H}\mathbf{G}_x)^{-1} - \mathbf{I}\right]\mathrm{y}_s}_{\mathrm{e}_2}$$

Degree of Freedom

$$\mathrm{e}_1(\mathbf{H}) = \mathrm{e}_1(\mathbf{D}\mathbf{H})$$

Optimal "close-loop" estimator (contd.)

If $\tilde{\mathbf{F}} = \begin{bmatrix} \mathbf{F}\mathbf{W}_d & \mathbf{W}_{n^x} \end{bmatrix}$ is full rank, **which is always the case if we include independent measurement noise**, then [2]

$$\mathbf{H} = \mathbf{D}\left(\left(\mathbf{X}_{opt}\mathbf{X}_{opt}^T\right)^{-1}\mathbf{G}_x\right)^T$$

where

$$\mathbf{D} = \mathbf{G}_y\left(\mathbf{G}_x^T\left(\mathbf{X}_{opt}\mathbf{X}_{opt}^T\right)^{-1}\mathbf{G}_x\right)^{-1}$$

[2] Alstad et al. (2009), Optimal measurement combinations as controlled variables, J. Proc. Control, 19 (1), 138-148

Necessary data for the task of estimation (Model-based)

Model-Based Estimation

$$\mathbf{Y}_{all} = \begin{bmatrix} \mathbf{Y} \\ \mathbf{X} \end{bmatrix} = \begin{bmatrix} \mathbf{G}_y & 0 \\ \mathbf{G}_x & \mathbf{X}_{opt} \end{bmatrix} \text{ where } \mathbf{X}_{opt} = \begin{bmatrix} \mathbf{FW}_d & \mathbf{W}_{n^x} \end{bmatrix}$$

$$\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_{non-opt} & 0 \end{bmatrix}$$
$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_{non-opt} & \mathbf{X}_{opt} \end{bmatrix}$$

Necessary data for the task of estimation (Data-based)

Theorem

Closed Loop Regressor (CLR) [a]*. The data matrices can be transformed to the "optimal – non-optimal" structure by*

1. *Performing a singular value decomposition on the data matrix* $\mathbf{Y}$
2. *Multiplying the data matrices* $\mathbf{X}$ *and* $\mathbf{Y}$ *with the unitary matrix* $\mathbf{V}$

$$\mathbf{YV} = \begin{bmatrix} \mathbf{Y}_{non-opt} & 0 \end{bmatrix}$$
$$\mathbf{XV} = \begin{bmatrix} \mathbf{X}_{non-opt} & \mathbf{X}_{opt} \end{bmatrix}$$

[a] Skogestad et al (2011). Selected Topics on Constrained and Nonlinear Control Workbook

Necessary data for the task of estimation (Data-based)

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Proof.

Since $\mathbf{V}$ is unitary, so $\|\mathbf{YV} - \mathbf{HXV}\|_F = \|\mathbf{Y} - \mathbf{HX}\|_F$
Writing the unitary matrix $\mathbf{U}$ in block form as $\mathbf{U} = \begin{bmatrix} \mathbf{U}_1 & \mathbf{U}_2 \end{bmatrix}$, we will have

$$\mathbf{YV} = \mathbf{U}\Sigma = \begin{bmatrix} \mathbf{U}_1 & \mathbf{U}_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 \\ 0 \end{bmatrix} = \begin{bmatrix} \mathbf{U}_1\Sigma_1 & 0 \end{bmatrix}$$

Example 1: Results

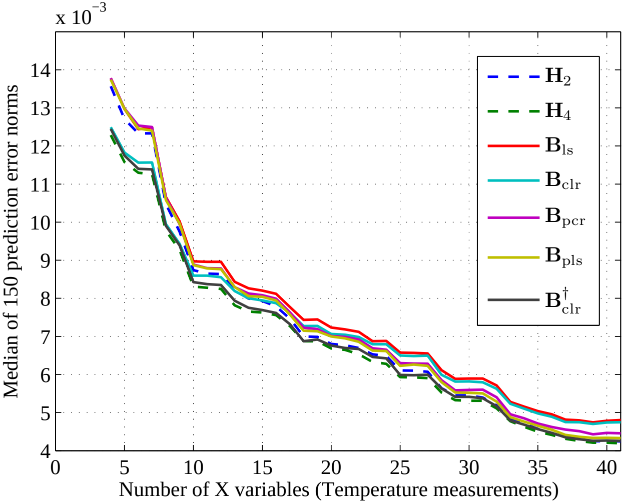
- Binary Distillation (Col. A), 41 trays, 8 measurements
- Secondary variables: Reflux, temperature in 25th tray

The mean prediction error of the model-based estimators applied to four operation scenarios

Validation Data (columns) / Calibration Data (rows)

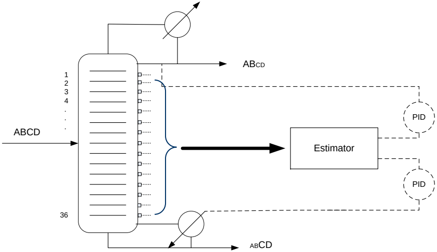
	S1	S2	S3	S4
S1	0.0085	0.2749	0.0215	0.0506
S2	0.0591	0.0093	0.0104	0.0104
S3	0.0599	0.0166	0.0098	0.0132
S4	0.0099	0.0099	0.0099	0.0099

Example 1: Results



Median prediction error for 150 data set with 200 samples

Example 2: Multi-component distillation



$$u = y = \begin{bmatrix} x_{C_3\, in\, D} & x_{C_2\, in\, B} \end{bmatrix}$$

$$G_y = I$$

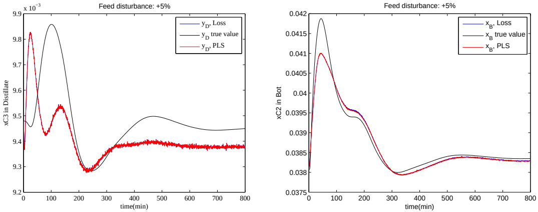
$$G_x^d = F$$

$$G_y^d = 0$$

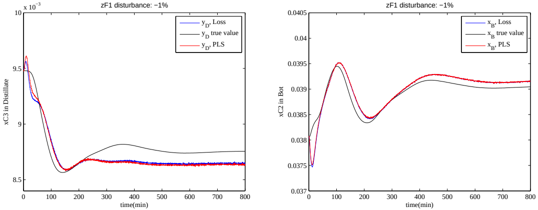
Example 2: Results

$$\mathbf{H} = \begin{bmatrix} 0.0004 & 0.0014 \\ 0.0081 & -0.0045 \\ -0.005 & 0.0074 \\ -0.0047 & 0.0006 \\ 0.0062 & -0.0104 \\ -0.003 & 0.0126 \\ -0.0013 & 0.0051 \\ 0.0024 & -0.0162 \\ -0.0028 & 0.0042 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} 0.0002 & 0.0013 \\ 0.0087 & -0.0041 \\ -0.006 & 0.0068 \\ -0.0051 & 0.0003 \\ 0.0077 & -0.0096 \\ -0.0034 & 0.0124 \\ -0.0016 & 0.0049 \\ 0.0026 & -0.016 \\ -0.0031 & 0.004 \end{bmatrix}$$

Example 2: Results

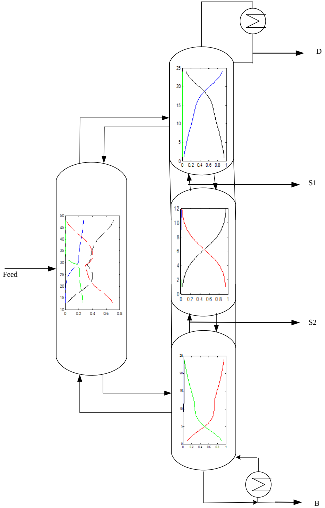


(a) +5% disturbance in feed flow



(b) -1% disturbance in Feed composition $z_{1,F}$

Example 3: Kaibel distillation column



DoF

$$u = \left[\; R_L \quad R_V \quad L \quad V \quad S_1 \quad S_2 \; \right]$$

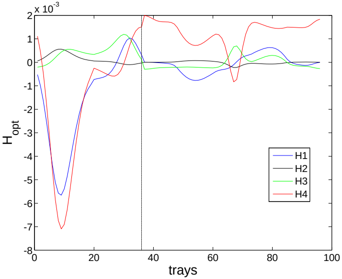
Extra Degrees of Freedom:

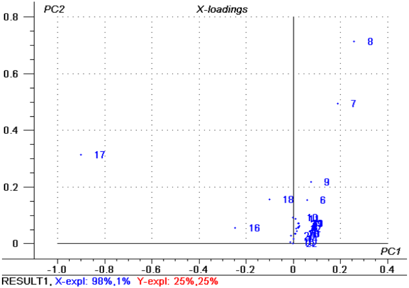
- Vapor Split (R_V)
- Liquid Split (R_L)

Disturbances:

- Feed flowrate, composition and quality
- Column Pressure
- Setpoints for splits

Example 3: Results





Possible Improvement for Loss method: Structured H^3

3 Yelchuru et al., MIQP formulation for Controlled Variable Selection in Self Optimizing Control

Conclusion

- Loss method is more systematic method to design soft-sensor compared to PLS
- For the example we showed, PLS and Loss method show almost the same result although two different approaches are used

Comment on PLS

- Shrinkage properties[4]

$$MSE = E(b-\beta)' S (b-\beta) = \underbrace{\Sigma_i \lambda_i (\mathrm{E} a_i - \alpha_i)^2}_{Bias\ term} + \Sigma_i \lambda_i Var(a_i)$$

$$a_i = f(\lambda_i)\, a_i^0$$

$f(\lambda_i) = 0\, or\, 1$ for OLS, PCR, Ridge
Butler et al.: PLS is not a shrinkage method. PLSR nearly always can be improved

[4] Butler et al, The peculier shrinkage properties of partial least squares regression, J. R. Stat. Soc., B 62 (2000) 585-593