DATA-DRIVEN SOFT SENSOR MODELING IN INDUSTRIAL PROCESSES

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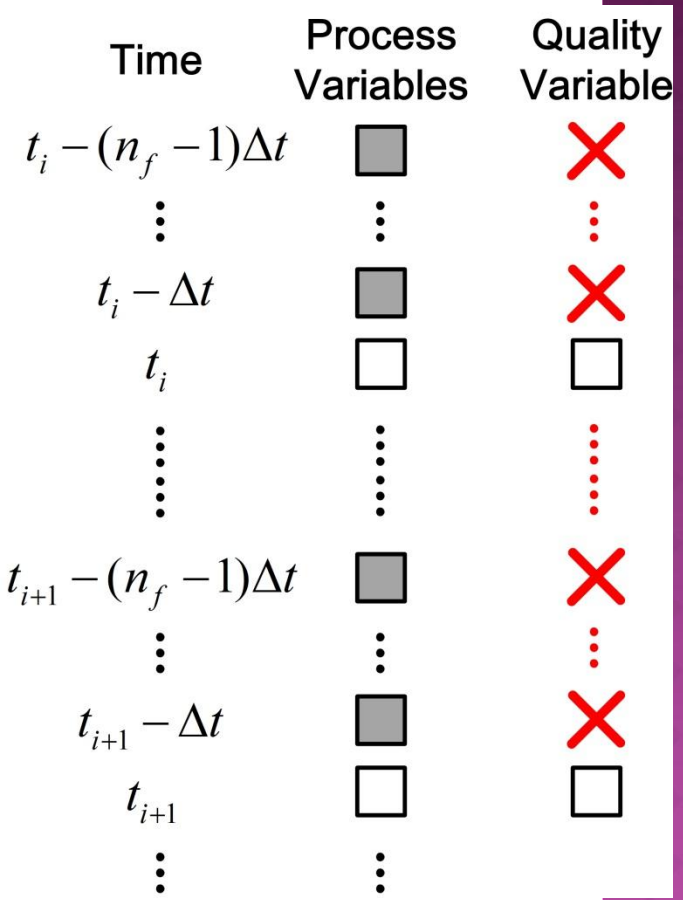
BACKGROUNDS

- Product quality: a central focus in process industries:
  - ✓ Economic interests
  - ✓ Plant operation safety
- Importance of prediction models for product quality:
  - ✓ Real-time estimations for quality control
  - ✓ Mathematical basis for control strategy design and total optimizations

Quality variables: melt index of polythene, boiling temperature of diesel, etc.

BACKGROUNDS

- Difficulties in measuring product quality:
  - ✓ Some qualities can only be measured via laboratory analysis.
  - ✓ Online analyzers: high prices & maintenance costs, low accuracy
  - ✓ Laboratory analysis: scarce & large time delay



Quality variables: melt index of polythene, boiling temperature of diesel, etc.

BACKGROUNDS

- Soft Sensing Technique Brosilow (1978)
  - ✓ Use **fast-sampled** process variables to predict quality
- First-principle vs. Data-driven modeling
  - ✓ Industrial processes are complicated to analyze
  - ✓ Data-driven methods ask for less prior knowledge
- Popularity of **data-driven methods** in soft sensing
  - ✓ Partial Least Squares (PLS)
  - ✓ Neural Networks (NN)
  - ✓ Support Vector Machines (SVM)

Process variables: temperature, pressure, flow rate, liquid level, etc.

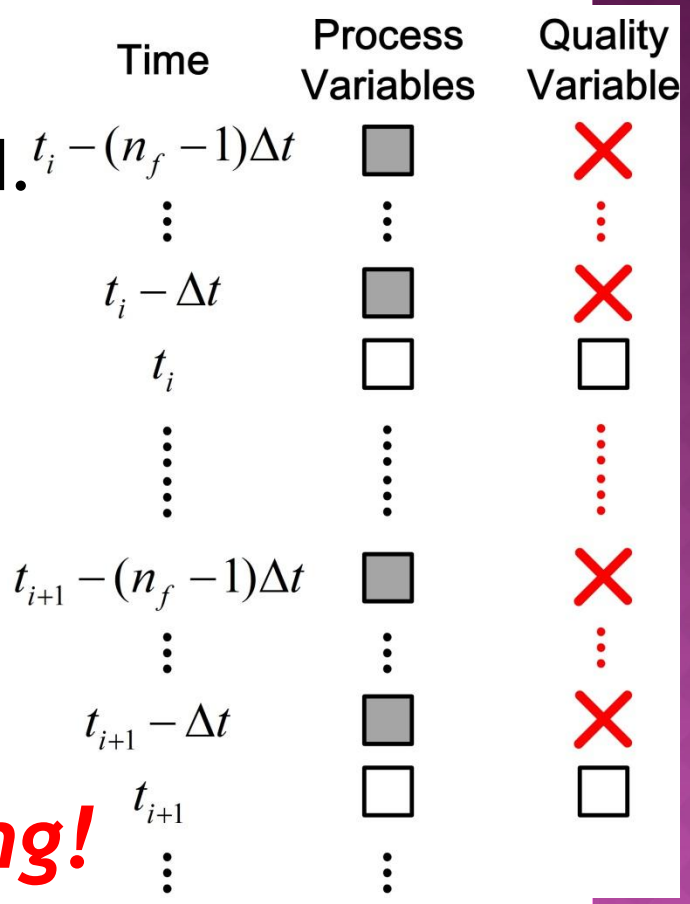
CHARACTERISTICS OF PROCESS DATA

- Data co-linearity:
  - ✓ Data rich but information poor (Dong & McAvoy, 1996)
  - ✓ Redundancy in configurations of sensors
  - ✓ Popular approaches: Latent variable (LV) models with low-dimensional subspaces
    - Principal Component Regression (PCR)
    - PLS
- Irregular sampling of product quality
- Process Dynamics: correlations in temporal proximity

Not fully addressed yet!

IRREGULAR SAMPLING OF PRODUCT QUALITY

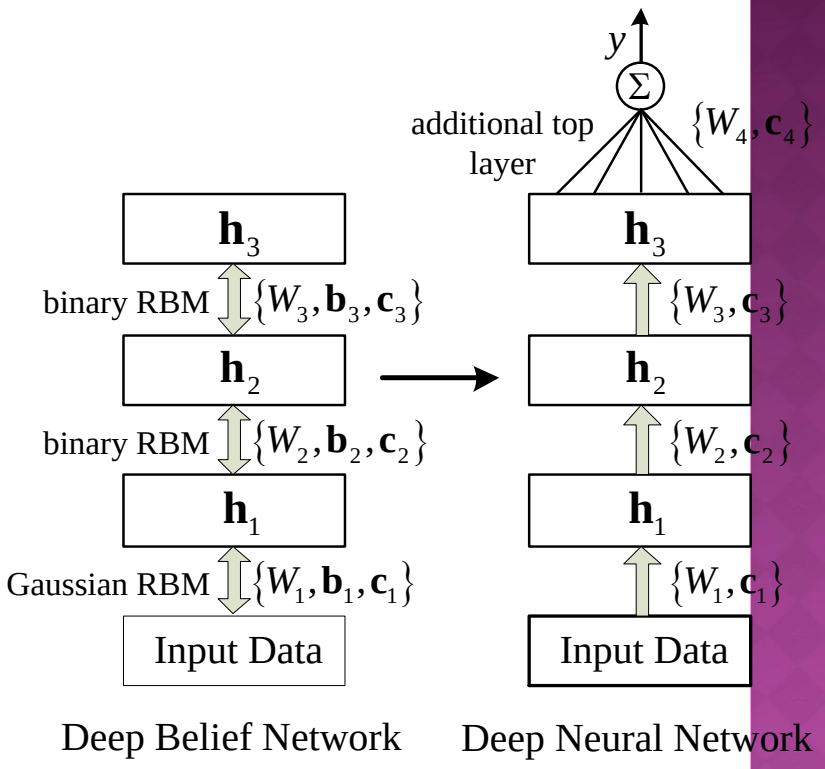
- White boxes □ : only down-sampled process data are used.
- Grey boxes ■ : most process data remain overlooked!



Semi-supervised Learning!

SEMI-SUPERVISED LEARNING

- Deep neural networks: a rising approach in machine learning
  - ✓ Semi-supervised learning
  - ✓ Low-dimensional LVs
  - ✓ Compact nonlinearity description

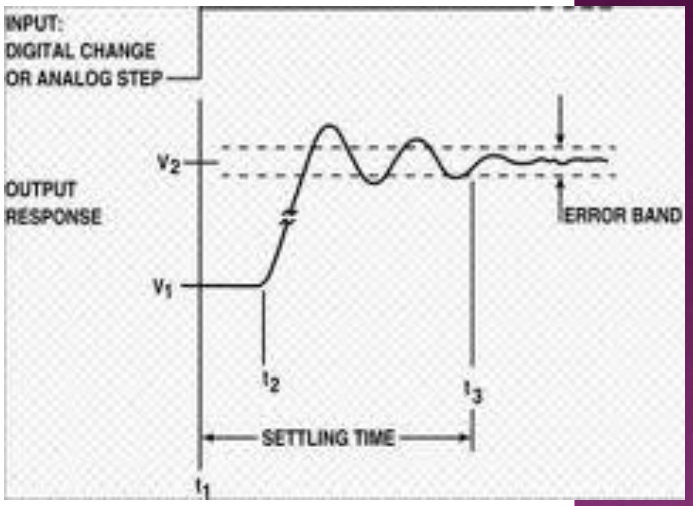


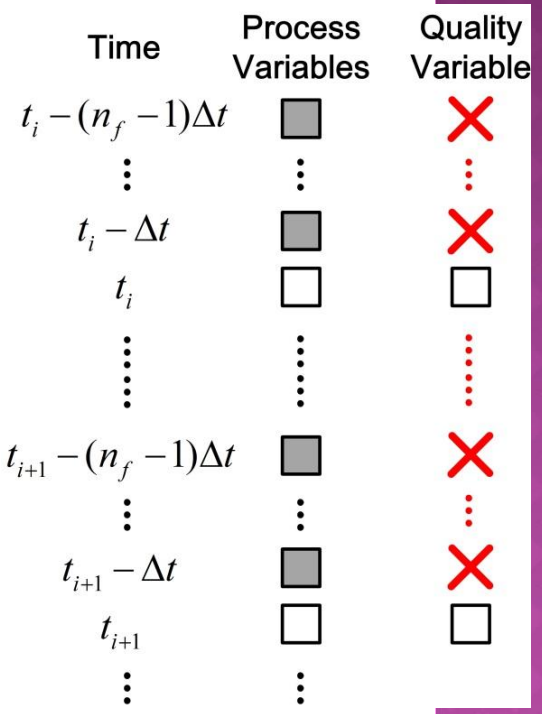
Shang, C., Yang, F., Huang, D., & Lyu, W. (2014). Data-driven soft sensor development based on deep learning technique. *Journal of Process Control*, *24*(3), 223-233.

PROCESS DYNAMICS

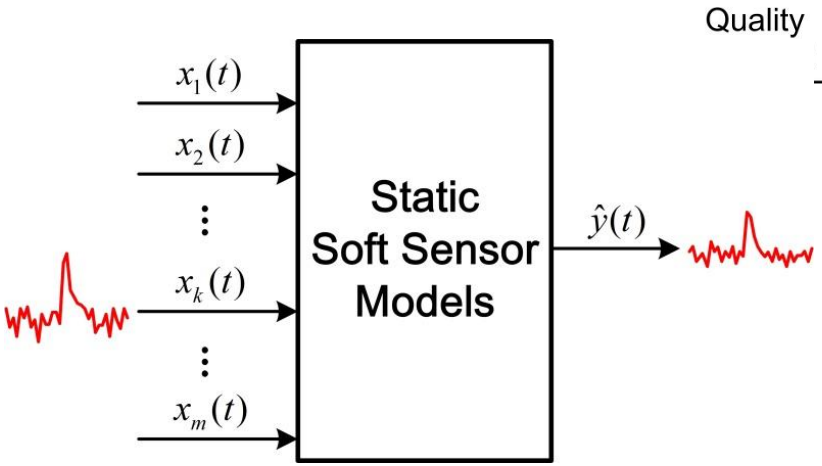
- Evident dynamics of processes
  - ✓ Settling time
  - ✓ Several hours in some cases
- Product quality is related to
  - ✓ Process samples at time t_i ***Static!***
  - ✓ Historical samples at time

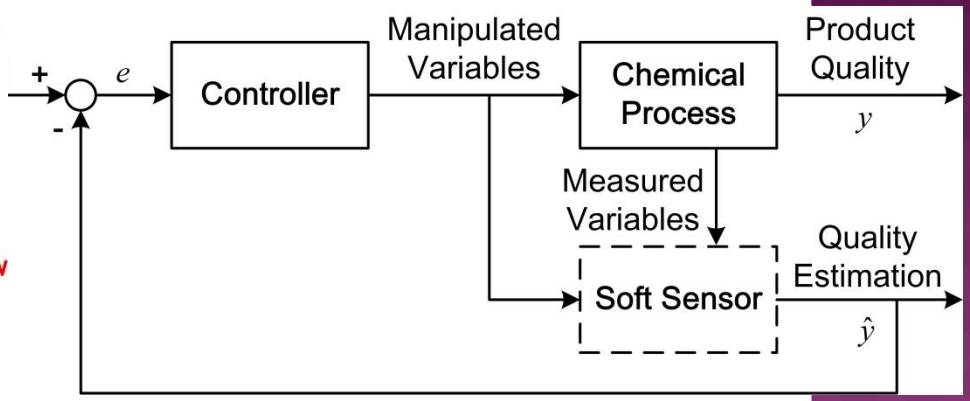
$$t_i - \Delta t, t_i - 2\Delta t, \cdots$$

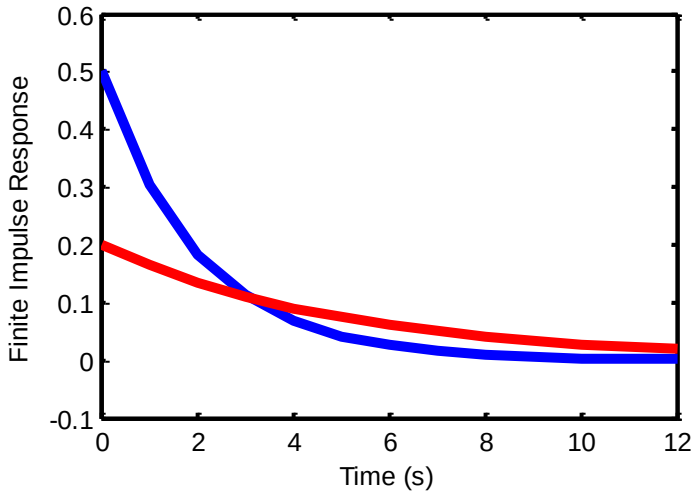


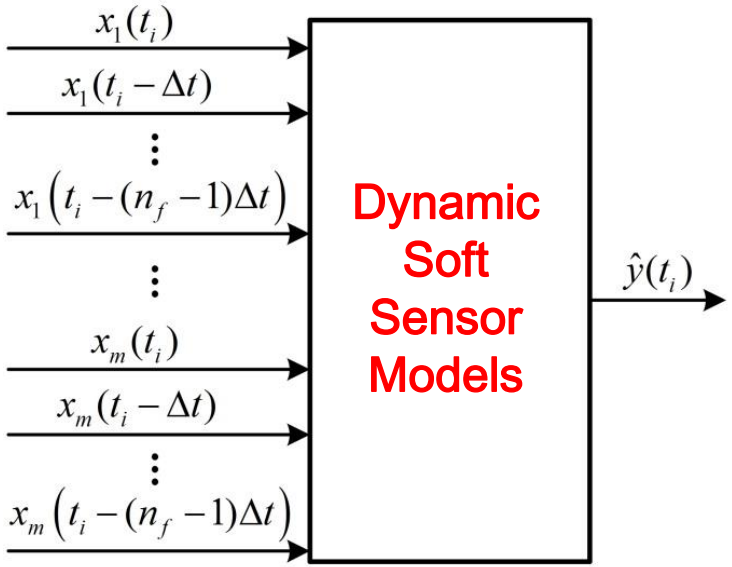


PROCESS DYNAMICS



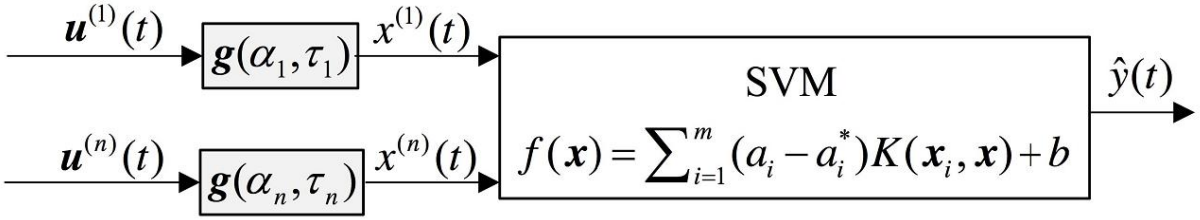




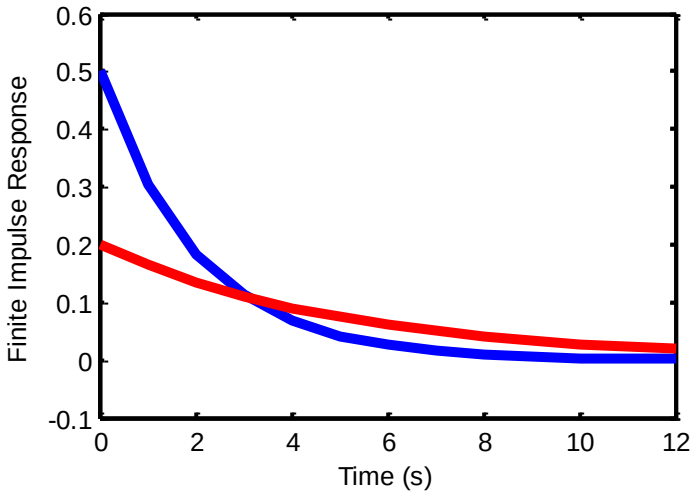


DYNAMIC LATENT FEATURES

- A Wiener Structure



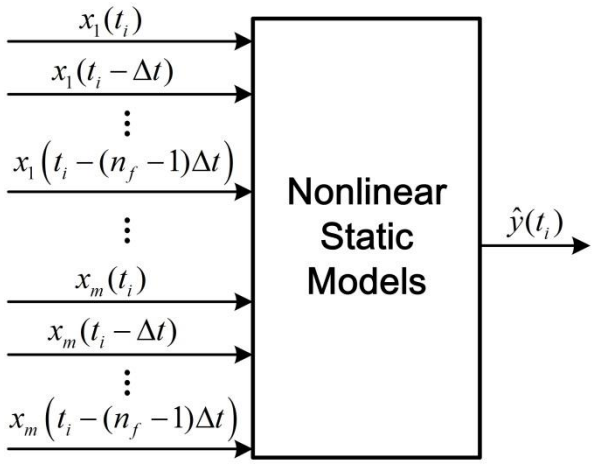
- ✓ First filter data to contain dynamic information
- ✓ Then feed filtered data to traditional static models
- ✓ Optimized within Bayesian framework
- ✓ Easy to use in practice



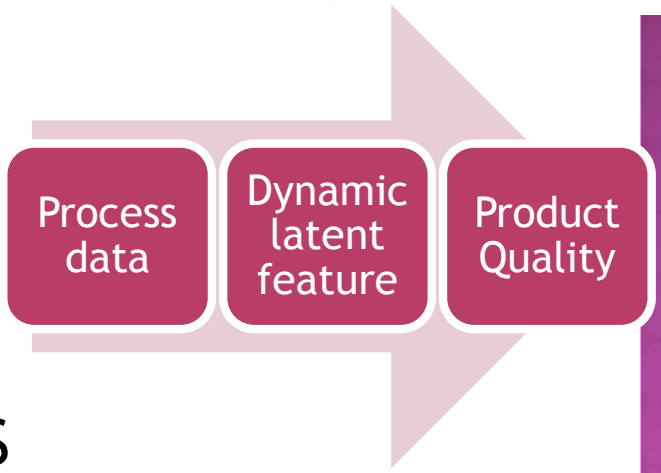
Shang, C., Gao, X., Yang, F., & Huang, D. (2014). Novel Bayesian Framework for Dynamic Soft Sensor Based on SVM with FIR. *IEEE Transactions on Control Systems Technology*, 22(4), 1550-1557.

DYNAMIC LATENT FEATURES

- Alternative: direct inclusion of lagged data into models
  - ✓ Drawbacks: increasing parameters leads to over-fitting with limited data



- Temporal Smoothness Regularization:
  - ✓ Smooth the **impacts** of proximal lagged variables on LVs
  - ✓ Combined with dynamic PLS



Shang, C. et al. (2014). Enhancing Dynamic Soft Sensors based on DPLS: a Temporal Smoothness Regularization Approach, To be submitted.

DYNAMIC PLS WITH TEMPORAL SMOOTHNESS

- Ordinary PLS:

$$\mathbf{X} = \mathbf{T}\mathbf{P}^{\mathrm{T}} + \mathbf{E}$$
$$\mathbf{Y} = \mathbf{T}\mathbf{Q}^{\mathrm{T}} + \mathbf{F}$$

- Score variables (LV)

$$t_j(i) = \sum_{k=1}^{m}\sum_{l=1}^{n_f} x_k(t-(l-1)\Delta t)w_{j,k}(l)$$

$$\min_{\vec{w}_{j,k}} \left[w_{j,k}(l+1) - w_{j,k}(l) \right]^2$$

- Modified optimization problem:

$$\max_{\mathbf{w}_j} \mathbf{w}_j^{\mathrm{T}} \left(\mathbf{X}_j^{\mathrm{T}}\mathbf{Y}_j\mathbf{Y}_j^{\mathrm{T}}\mathbf{X}_j\mathbf{w}_j - \alpha||\mathbf{X}_j^{\mathrm{T}}\mathbf{Y}_j||^2\mathbf{K} \right) \mathbf{w}_j$$

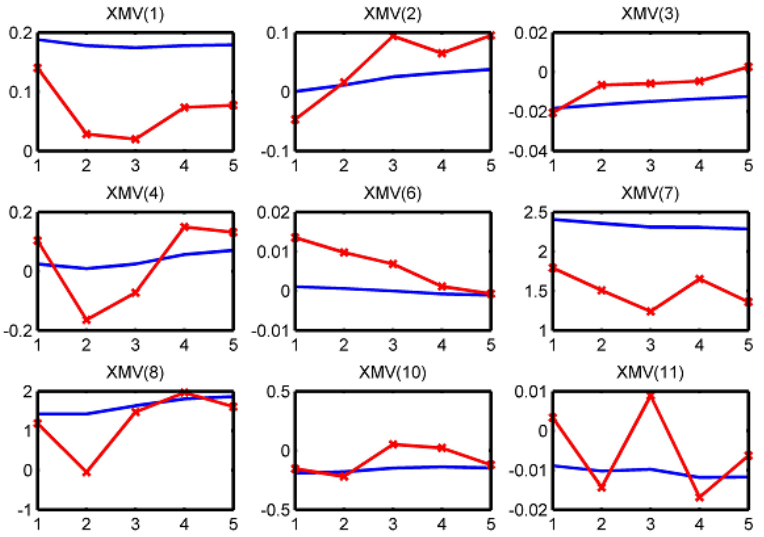
$$\text{s.t. } \mathbf{w}_j^{\mathrm{T}}\mathbf{w}_j = 1$$

$$\mathbf{K} = \mathbf{I}_m \otimes \mathbf{J}^{\mathrm{T}}\mathbf{J}. \quad \mathbf{J} = \begin{bmatrix} 1 & -1 & & \\ & \ddots & \ddots & \\ & & 1 & -1 \end{bmatrix} \in \mathbb{R}^{(n_f-1)\times n_f}$$

Shang, C. et al. (2014). Enhancing Dynamic Soft Sensors based on DPLS: a Temporal Smoothness Regularization Approach, To be submitted.

DYNAMIC PLS WITH TEMPORAL SMOOTHNESS

- Tennessee Eastman process
- Quality Variable: Product B in Stream 9
- Process Variables: manipulated & measured variables



- A(# of LVs)=2 for DPLS
- A=4 for DPLS-TS

	DPLS-TS	DPLS
Cross-validation RMSE	0.1122	0.1137
Prediction RMSE	0.1083	0.1160
Smoothness Loss	0.0003	0.0353

Shang, C. et al. (2014). Enhancing Dynamic Soft Sensors based on DPLS: a Temporal Smoothness Regularization Approach, To be submitted.

FUTURE WORK AND CONCLUSION

- Dynamic feature extraction should be integrated with semi-supervised learning.
  - ✓ At present limited to supervised learning
  - ✓ Semi-supervised learning helps extract dynamic features from massive process data.
- Soft sensor models in future should handle:
  - ✓ Data correlations (LV model)
  - ✓ Nonlinearity (in some cases)
  - ✓ Process Dynamics (Dynamic feature extraction)
  - ✓ Irregular Sampling (Semi-supervised learning)
  - ✓ Practical usability

FUTURE WORK AND CONCLUSION

- Additional Issues in Practical Implementations:
  - ✓ Process Variable Selection
  - ✓ Missing Data & Outliers
  - ✓ Soft Sensor Model Maintenance:
    - Real-time Performance Monitoring
    - Online Updating Scheme
  - ✓ Piecewise Linear Modeling for Optimization
  - ✓ MPC design based on Dynamic Latent Features

THANKS FOR YOUR ATTENTIONS!