Run-to-run optimization of fed-batch processes with unfold-PLS

IFPAC 2009

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Batch Process Optimization

Outline

- Objectives: maximize production, improve quality, improve safety conditions, reduce costs, etc.
- Extremely hard task
  - Uncertainties
  - Lack of critical measurements
  - Non-linear nature
  - Slow response
  - …
- Fundamental knowledge ➔ quality of the model or the assumptions assumed.
- Repetitive nature ➔ **Useful for optimization**

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Optimization Method

Outline

- Run-to-run (R2R) optimization
  - Learn from the past batches to improve the performance of the current one
- Three ideas: ★

a) The batch-wise unfolding : X(I, J, K) → X(I, JK)

b) A PLS model → gradient of the optimization function

c) Non-linearities and Non-convexity → adaptive PLS model + heuristic rules (CV).

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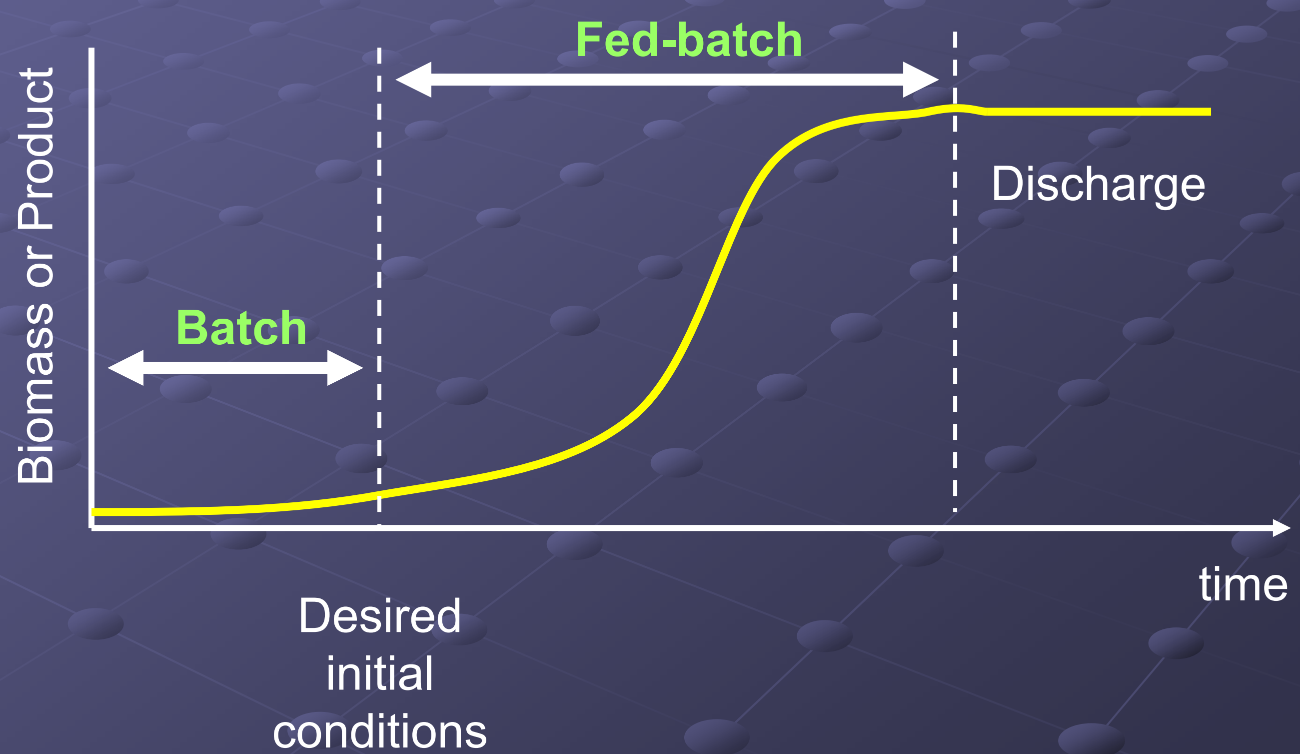
Optimization Method

Outline

- Illustrative example: Fermentation process.



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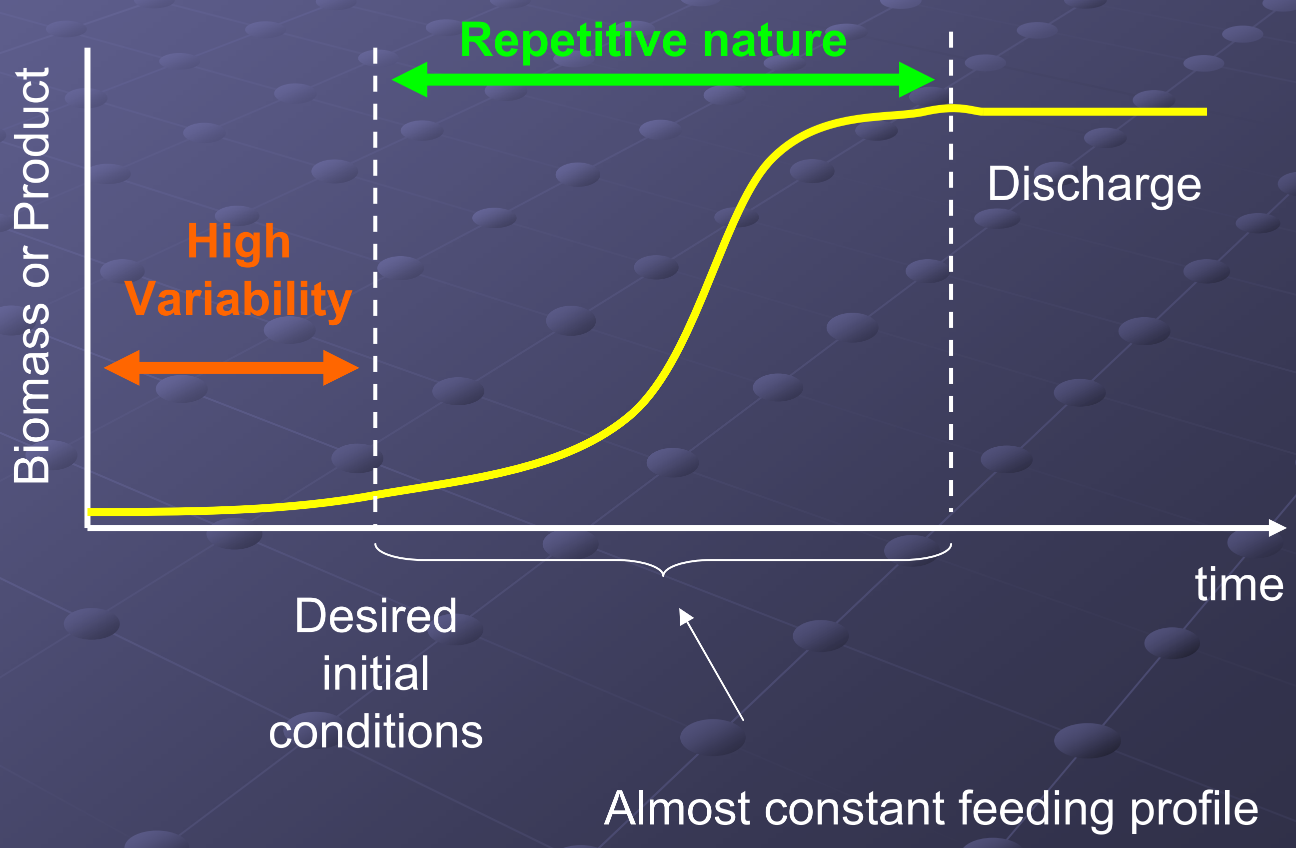

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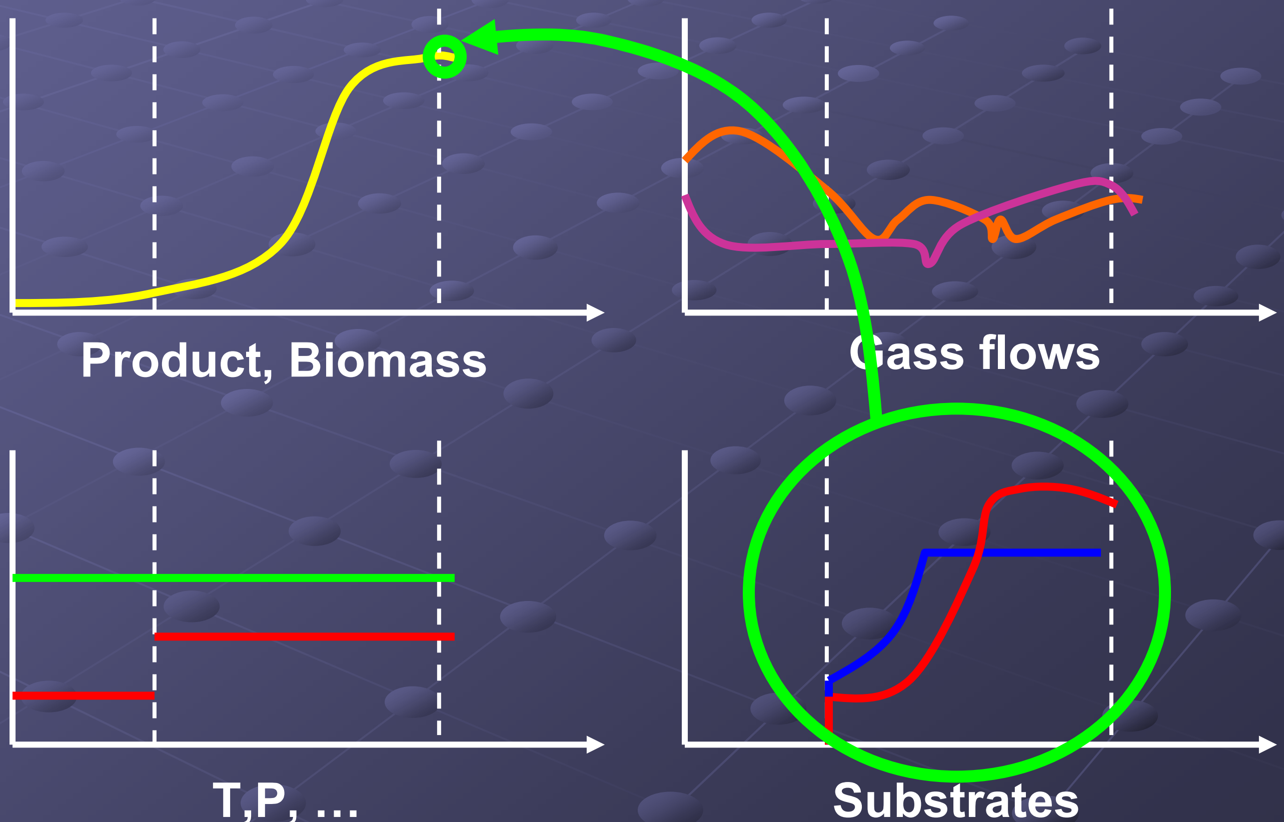

Objective: Select the feeding profile of substrate to maximize final product or biomass .

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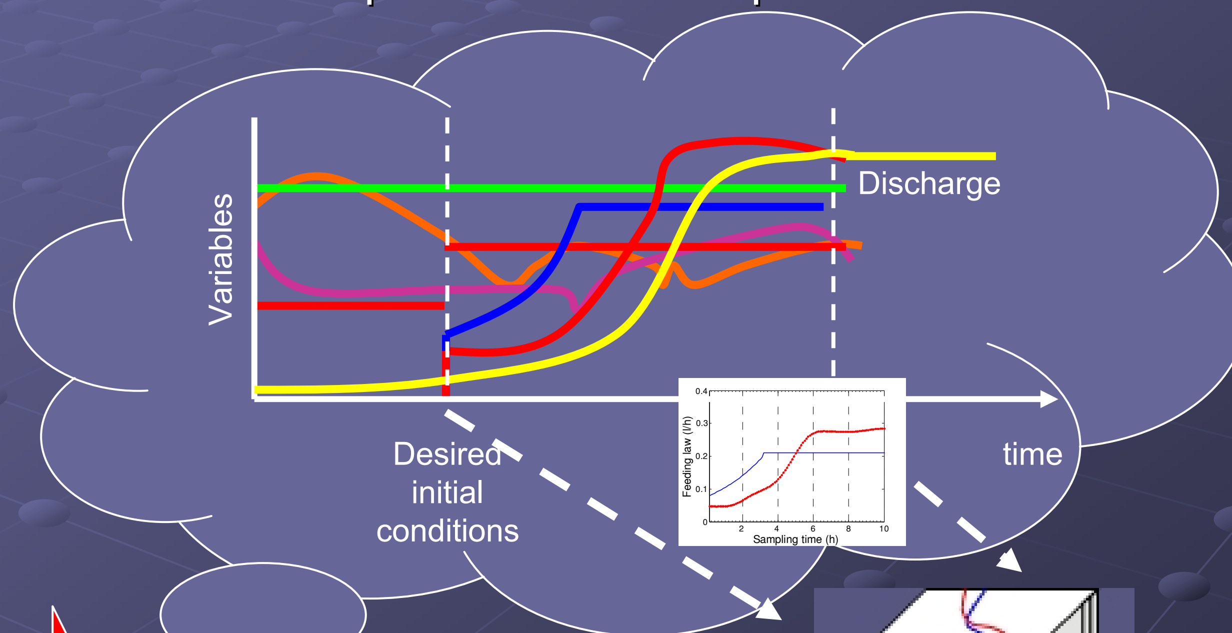
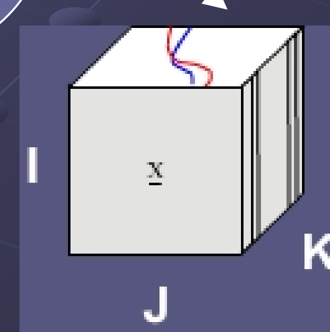
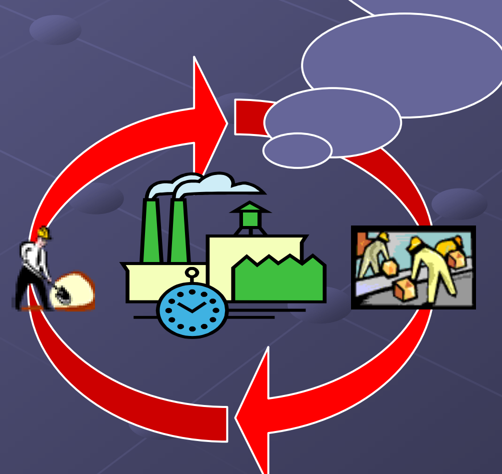




I batches
J variables (substrates)
K intervals



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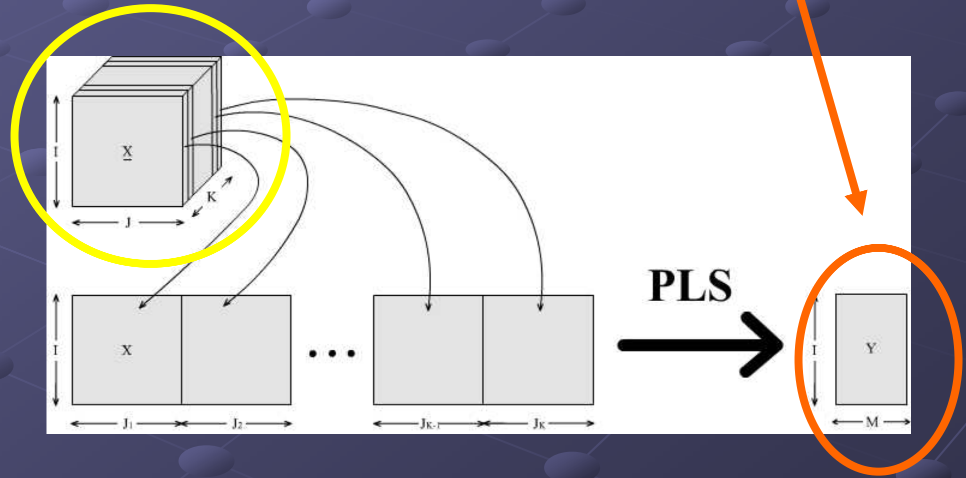
Optimization Method

Outline

- Three ideas: ⭐

Fed-batch data

Optimization index (quality variables, energy consumption, etc..)



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⭐ J. Camacho, J. Picó and A. Ferrer. *Self-tuning run to run optimization of fed-batch processes using unfold-PLS*, AIChE Journal, 53(7):1789-1804 (2007).

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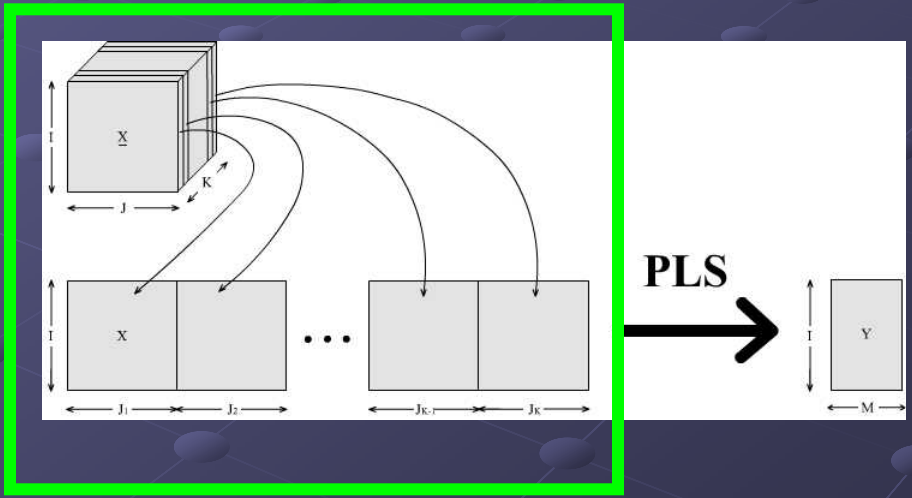

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Optimization Method

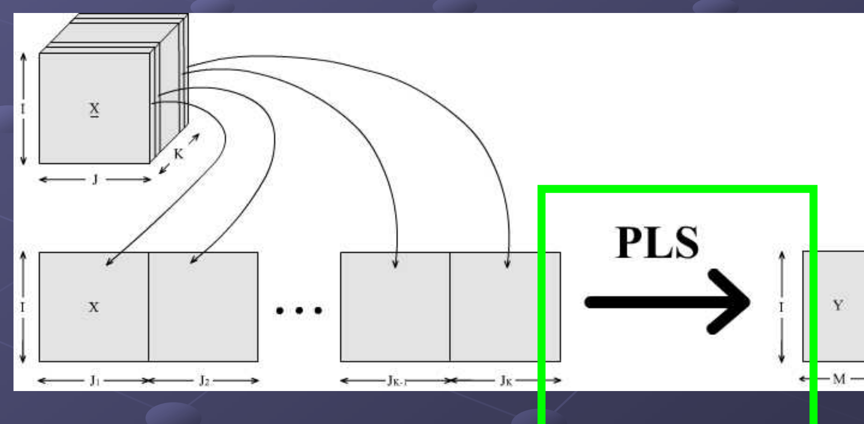
Outline

1. Batch Process Optimization
2. **Optimization Method**
3. Case Study: Simulation
4. Extensions
5. Conclusions

- Three ideas: ★

  a) The batch-wise unfolding : X(I, J, K) ➔ X(I, JK)

  b) A PLS model ➔ gradient of a function



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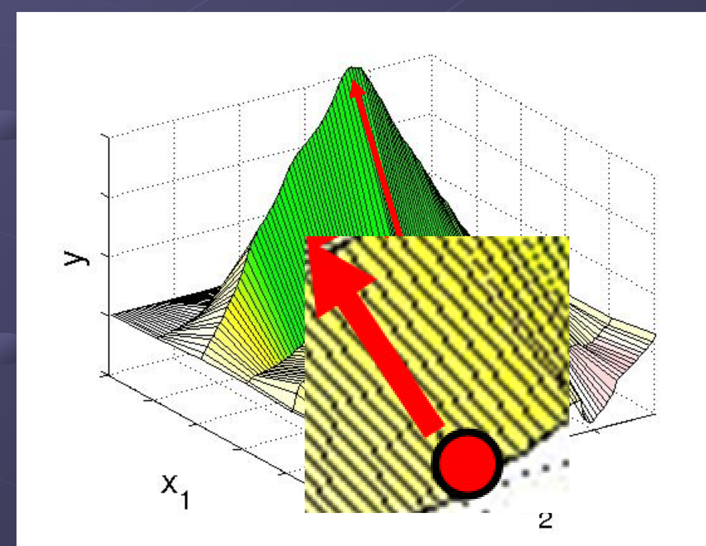
Gradient-based optimization:

X = [x1,x2] ➔ Y

$$X_{k+1} = X_k + c \cdot \frac{dy}{dX}$$

We need to estimate the gradient!!!



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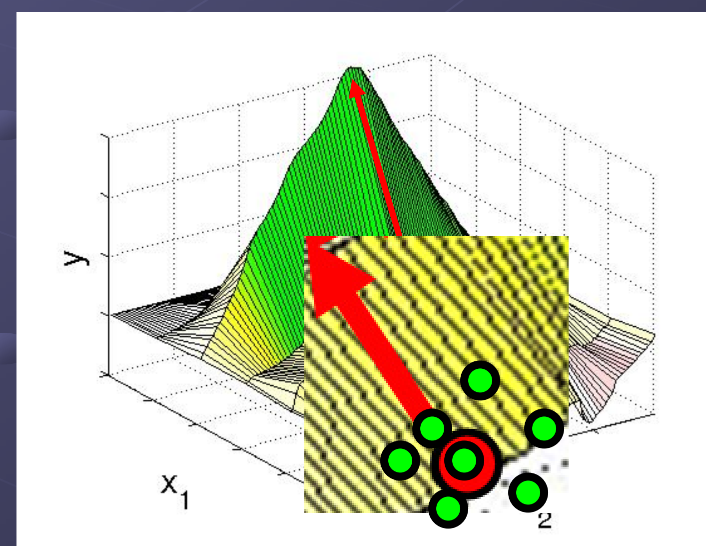

At least as many samples as process variables

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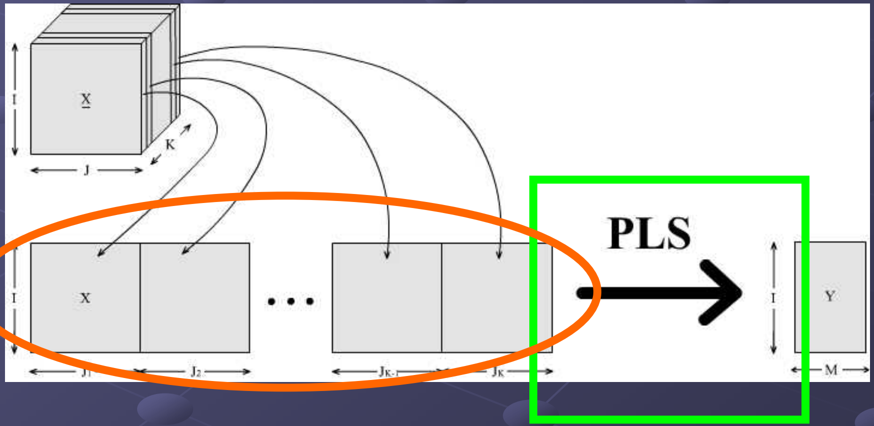

High number of process variables #Var(X) = J·K

PLS ➔ Fast Gradient-based Optimization !!!

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c) Non-linearities and Non-convexity ➔ adaptive PLS model + heuristic rules (CV).

- Construct the PLS model with the last N batches

- Only trust the model with a certain degree:

Confidence degree [0,1] by cross-validation.

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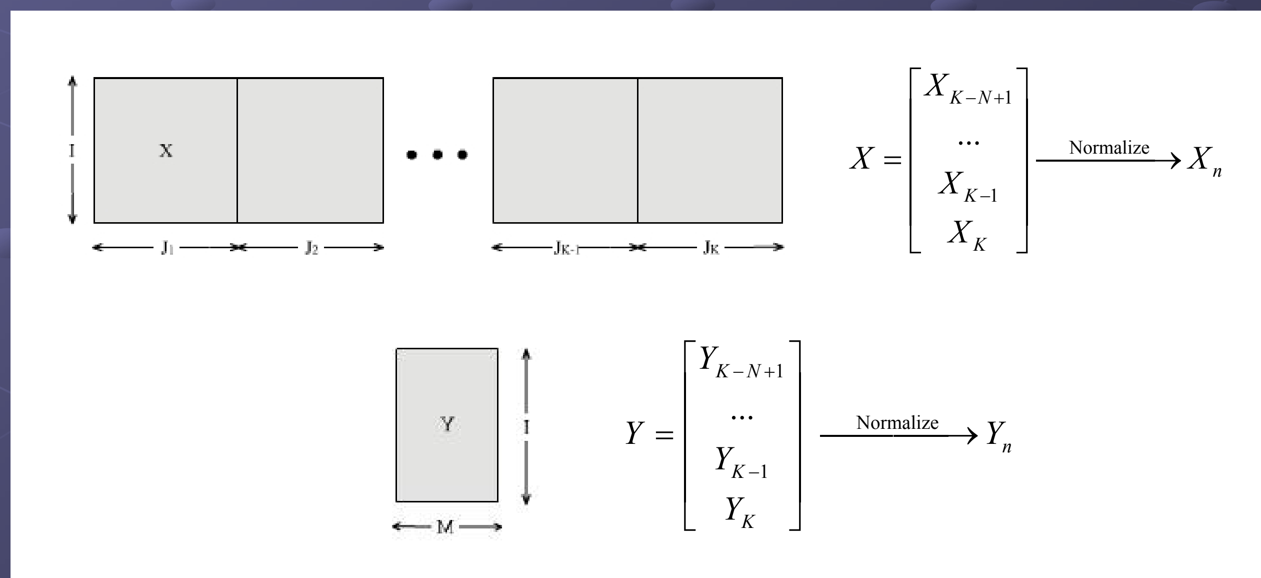
Optimization Method

Outline

- Self-tuning algorithm:
  - Step 1: Process a new batch *k* with feeding law X_k and obtain the output Y_k.

Take last N batches



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- Self-tuning algorithm:
  - Step 1: Process a new batch *k* with feeding law X_k and obtain the output Y_k.
  - Step 2: Rebuild the BW-PLS model with the data of batch i.

$$Y_n = \hat{B}_{PLS} \cdot X_n + E$$
$$\hat{B}_{PLS} = W \cdot (P^T \cdot W)^{-1} \cdot Q^T$$

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  - Step 3: Compute the gradient and the next feeding law.

$$\frac{d\hat{Y}}{dX} = \frac{\sigma_y}{\sigma_x} \cdot W \cdot (P^T \cdot W)^{-1} \cdot Q^T$$

Heuristics (CV)

$$X_{k+1} = X_k + c_k \cdot \frac{d\hat{Y}}{dX} + \rho_k$$

Excitation

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  - Step 3: Compute the gradient and the next feeding law.
  - Step 4: Increment the counter $k = k+1$ and loop back to Step 1.

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Case Study: Simulation

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2. Optimization Method
3. **Case Study: Simulation**
4. Extensions
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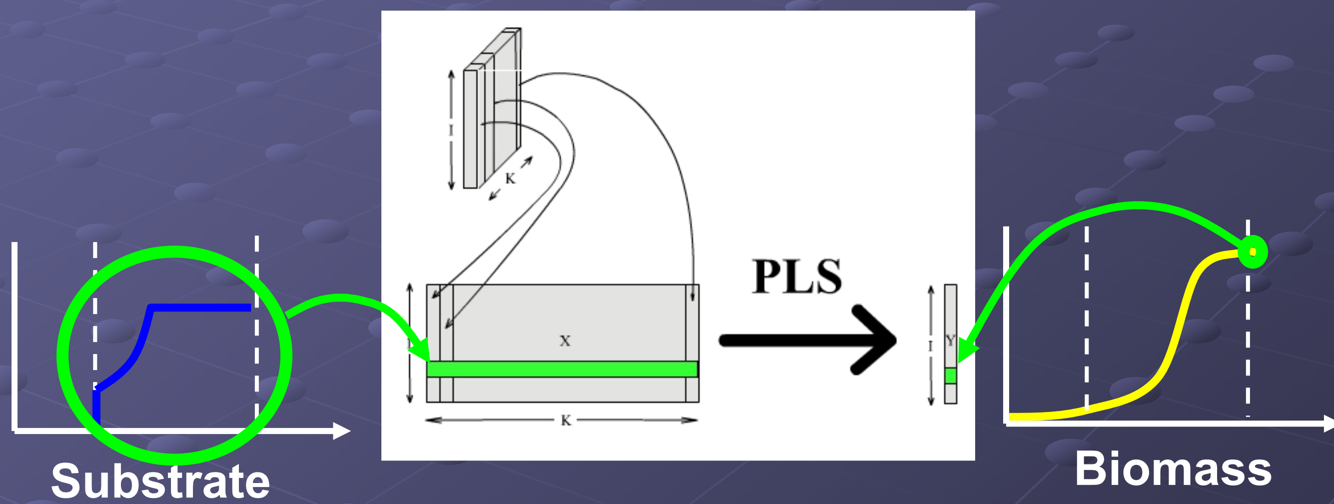
- Saccharomyces cerevisiae fed-batch cultivation



Input: Feeding profile of substrate

Ouput: Biomass concentration

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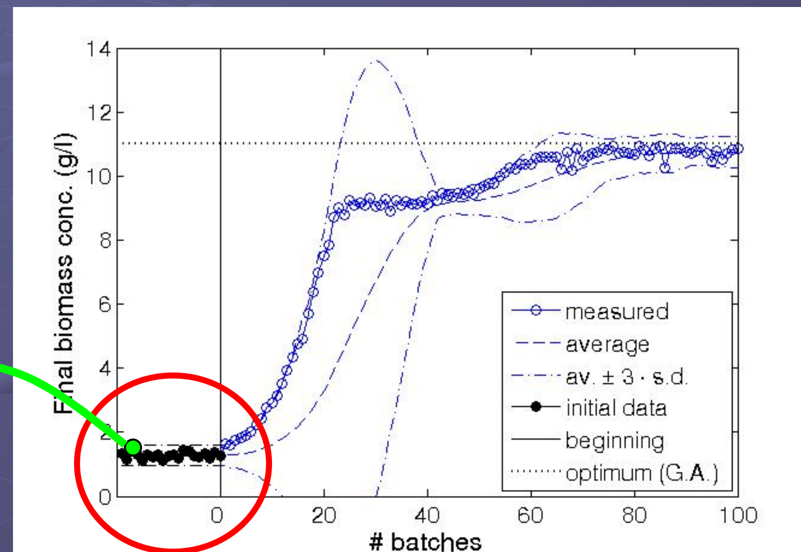

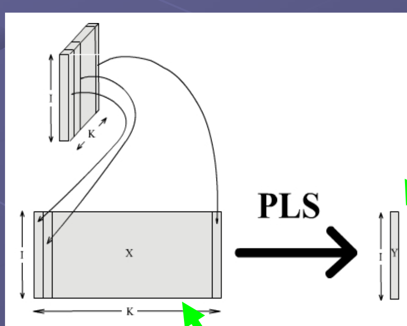

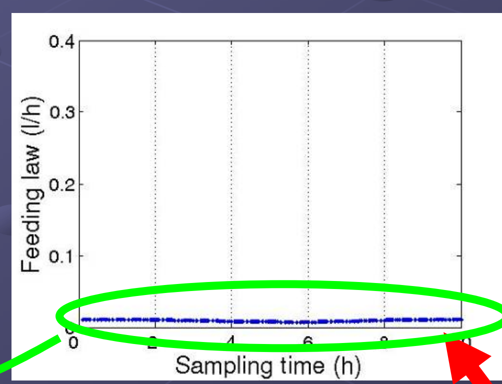

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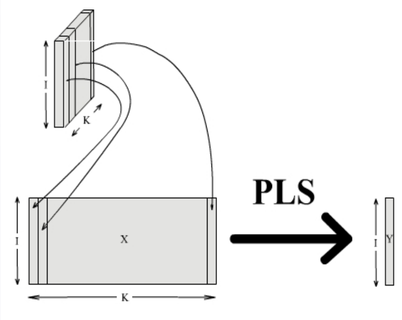

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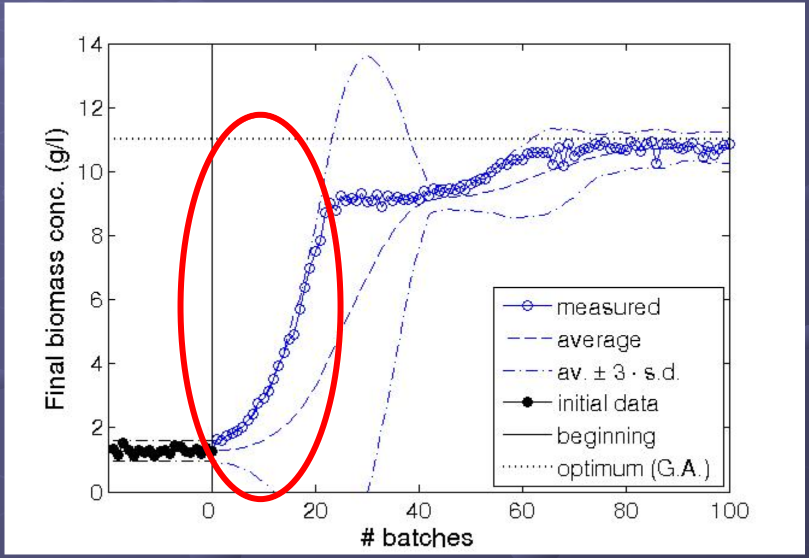

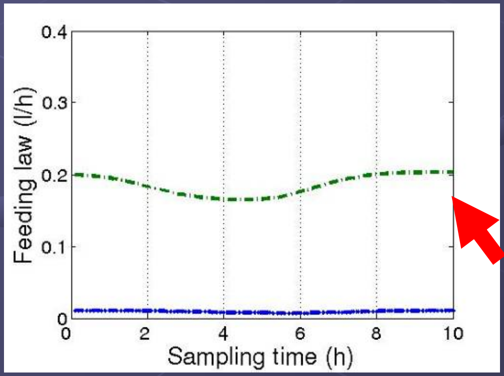

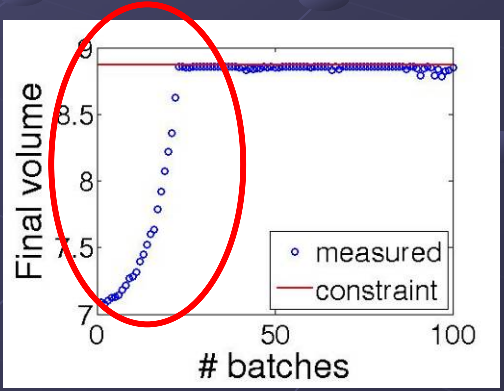

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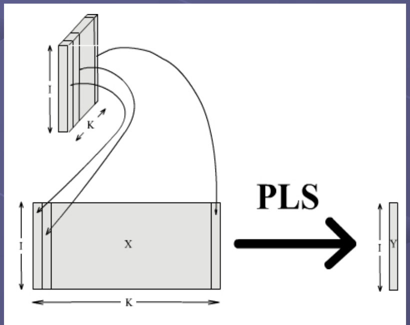

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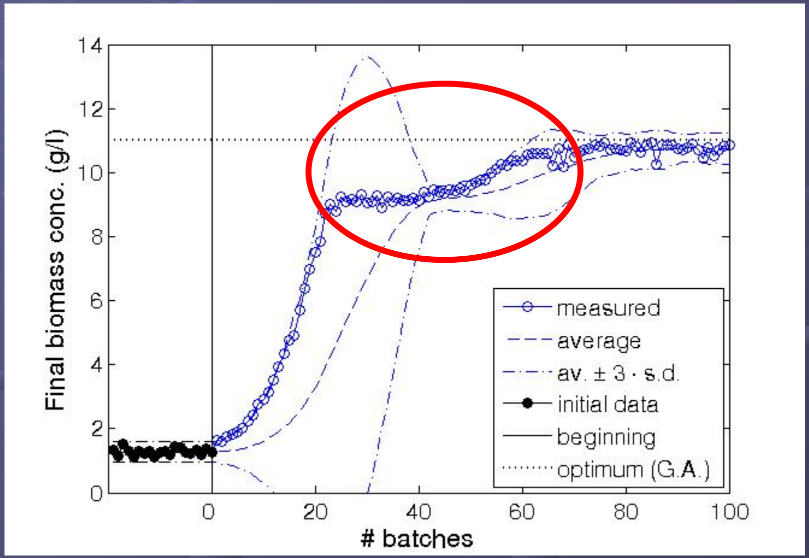

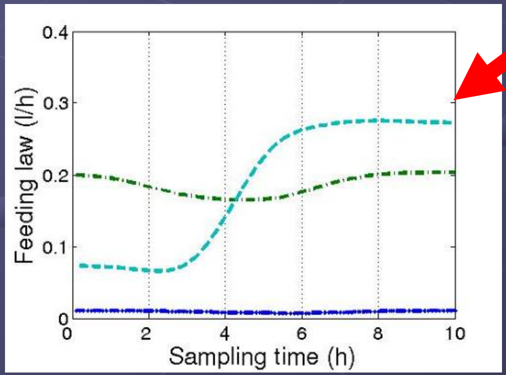

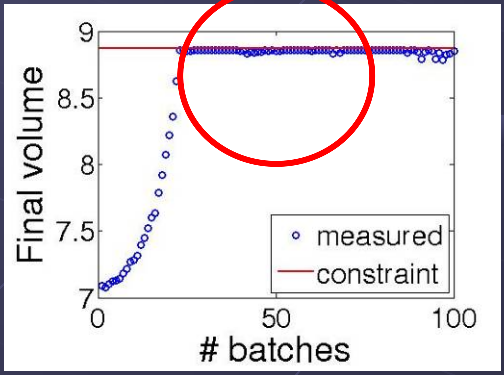

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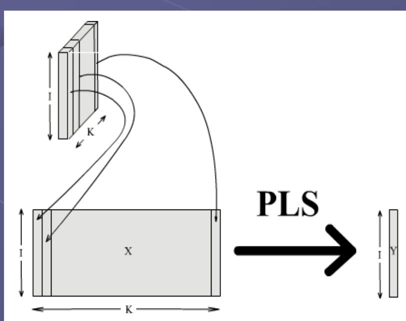

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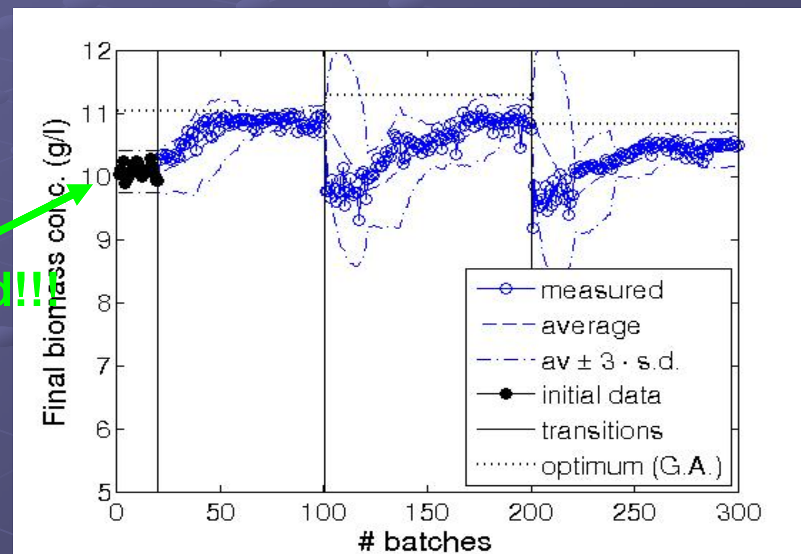
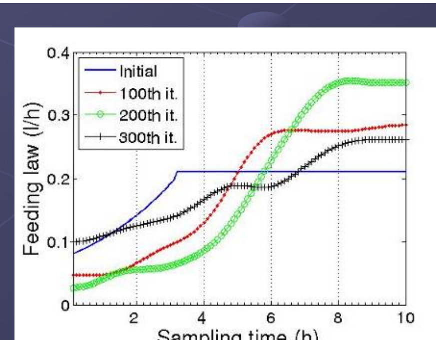
- Saccharomyces cerevisiae cultivation

The one suggested!!!





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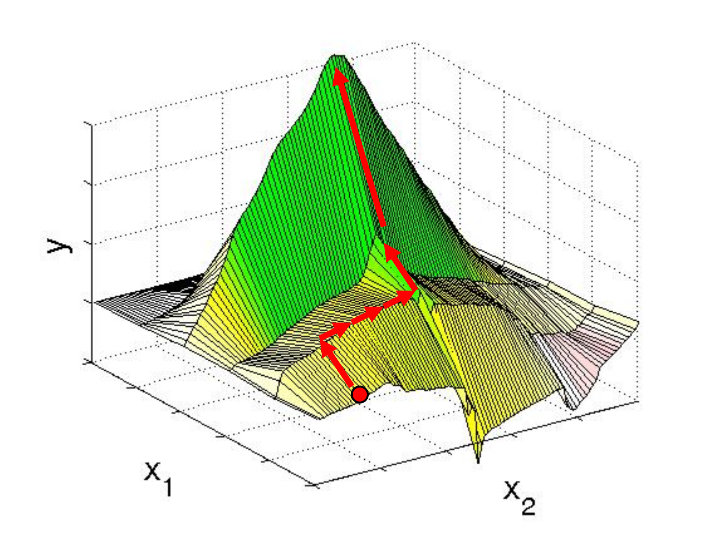

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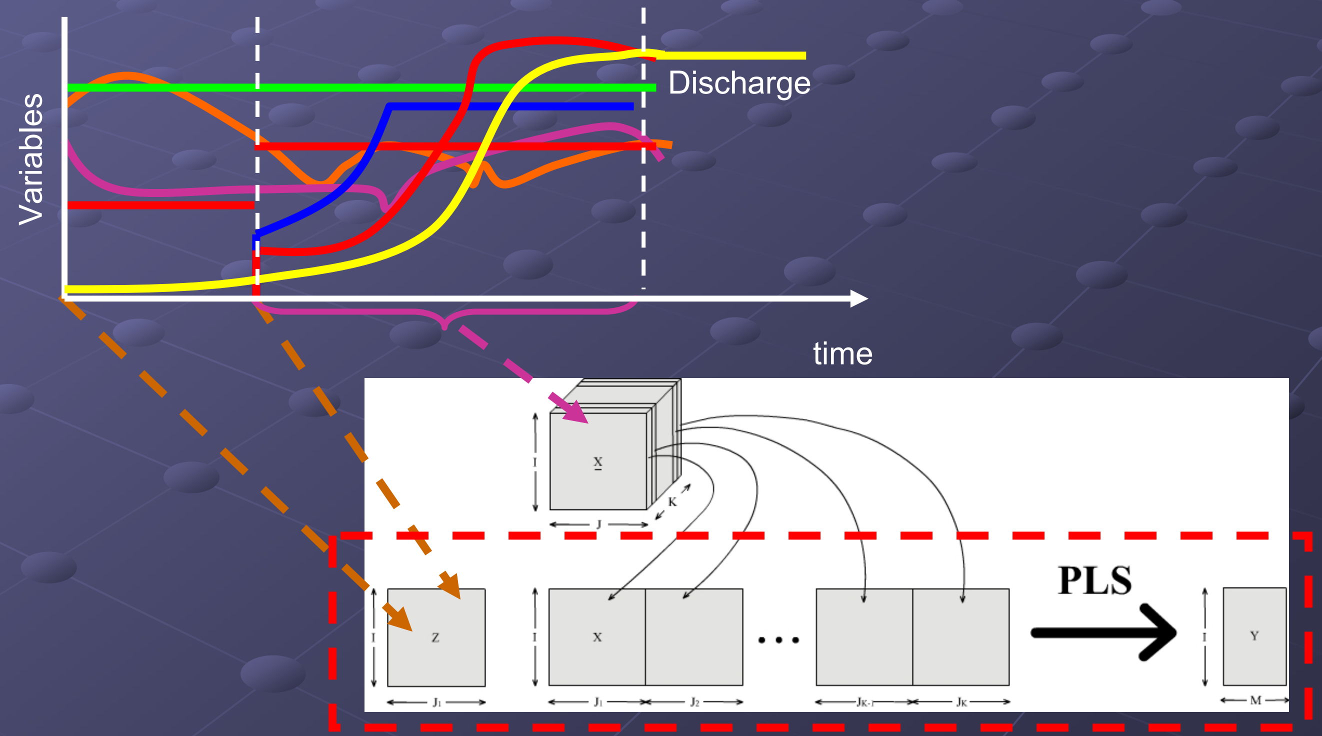
Extensions

Outline

- Straightforward use of additional information:

  e.g. initial conditions + process variables



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Extensions

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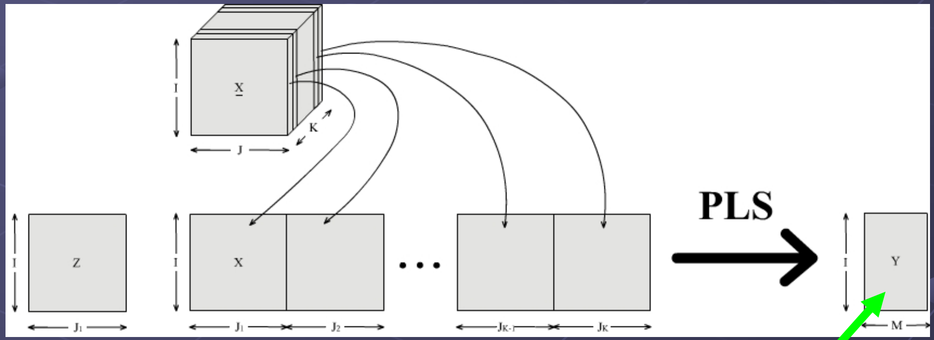
- Straightforward use of additional information:
- Straightforward extension to multi-criteria:

  e.g. maximize biomass while reducing final volume



Multiple Y variables

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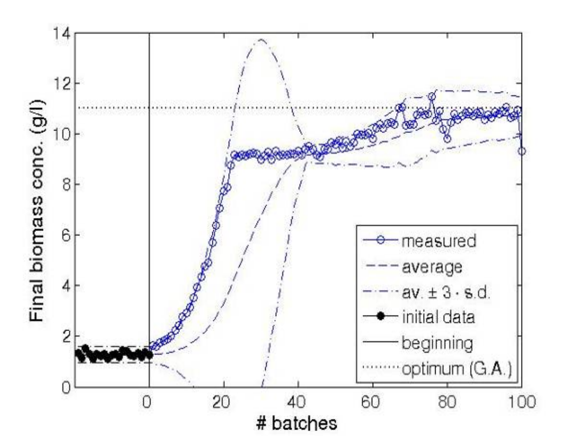
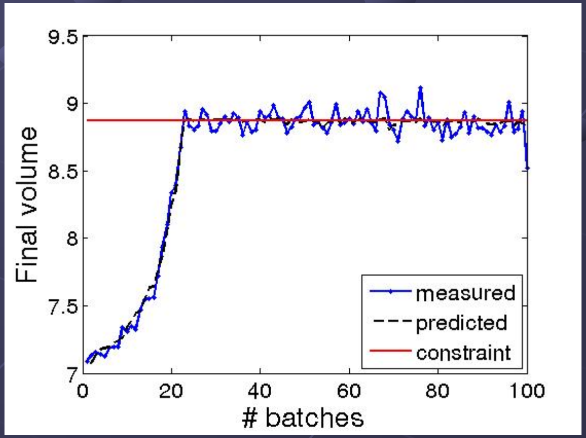
- Straightforward use of additional information:
- Straightforward extension to multi-criteria:
- Soft constraints on Y can be handled by using PLS estimations.

e.g. constraint final volume





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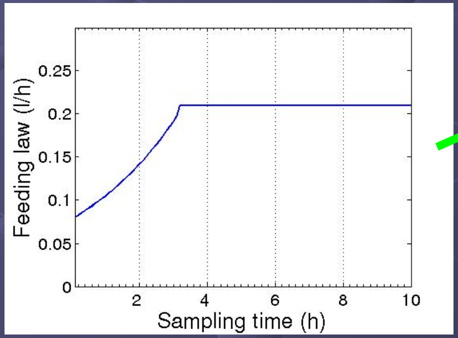
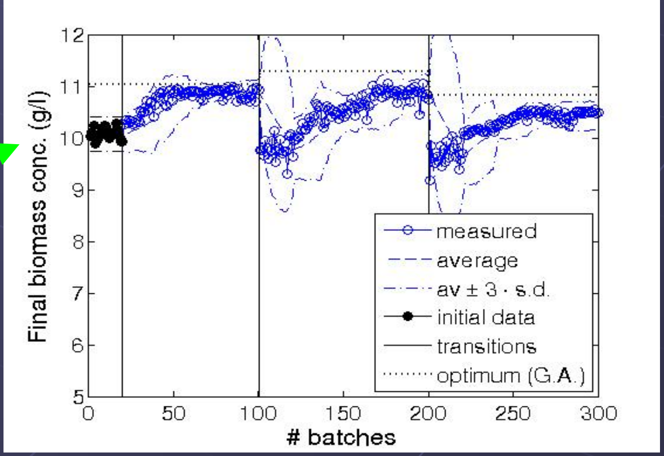
- Straightforward use of additional information:
- Straightforward extension to multi-criteria:
- Soft constraints on Y can be handled by using PLS estimations.
- Possible combination with fundamental knowledge.





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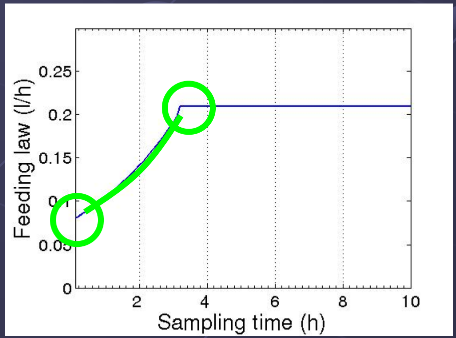
e.g. parameterization of the feeding profile.

a) Data-based ➔ divide in 100 intervals and optimize (100 parameters)

b) Grey approach ➔ 3 parameters



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Conclusions

Outline

- Advantages:
  - No fundamental knowledge is required but can be used.
  - The only requirement is to measure the performance index.
  - Applicable to any batch process.
  - High degree of discretization of the input.
  - Any other measurement can be integrated straightforwardly.
  - Extension to several performance indices.
  - Extension to constraints handling.

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