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Optimal output selection for batch processes

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Outline

- Batch optimization
- Implementation schemes
- Output selection method
- Reactor case study

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Batch optimization

- Minimum time to given specification
- Minimum energy to given specification
- Maximum product in fixed time

all subject to given constraints

Implementation

- Online optimization: outputs used to update model (MPC)
- Self-optimizing control: controlling "right" outputs give near optimal performance

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Dynamic optimization

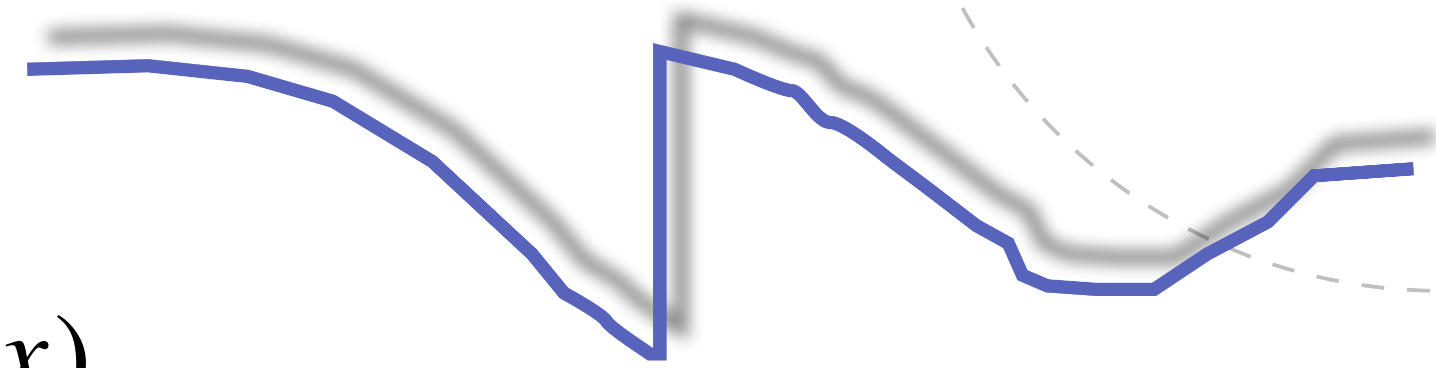
$$\min_{u(t),t_f} J(x(t_f))$$

$$\dot{x} = f(x,u) \quad y = h(x)$$

$$c(x,u) \leq 0$$

$$u(t) \in U[0,T]$$

$$x(t_f) \in X$$



Pontryagin's principle

$$H = \lambda^T f(x,u) + \mu^T c(x,u)$$

$$H(x^*,u^*,\lambda^*) \leq H(x^*,u,\lambda^*)$$

$$\dot{\lambda} = -H_x$$

$$\dot{x} = H_\lambda$$

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Output selection

- Unconstrained degrees of freedom
- Look for outputs that give small loss *L* (deviation from optimality) when controlled at fixed reference, even under disturbances

$$H(t) = \lambda^T f(x,u)$$

$$L(t) = H(t) - H^*(t)$$

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Maximum gain rule

$$L(t) = \underbrace{H_u \delta u}_{0} + \frac{1}{2} \delta u^T H_{uu} \delta u$$

Need to relate variations in inputs to variations in outputs

$$\delta y = \frac{\partial h}{\partial x^T} \frac{\partial x}{\partial u^T} \delta u = G \delta u$$

$$L(t) = \frac{1}{2} \delta y^T G^{-T} H_{uu} G^{-1} \delta y$$

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Maximum gain rule

- Assume the model is scaled such that $\delta y_{max} \approx 1$

Select y's to minimize the following expression along the nominal trajectory

$$\min\left(\int_{t_0}^{t_f} \left\| G^{-T} H_{uu} G^{-1} \right\|_2^2 dt\right)^{1/2}$$

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How to obtain G

- How do variations in inputs map to the states?
- Neighboring optimal control gives $\delta u(t) = K(t)\delta x(t)$
- We estimate G by

$$G \approx \frac{\partial h}{\partial x^T} K^+$$

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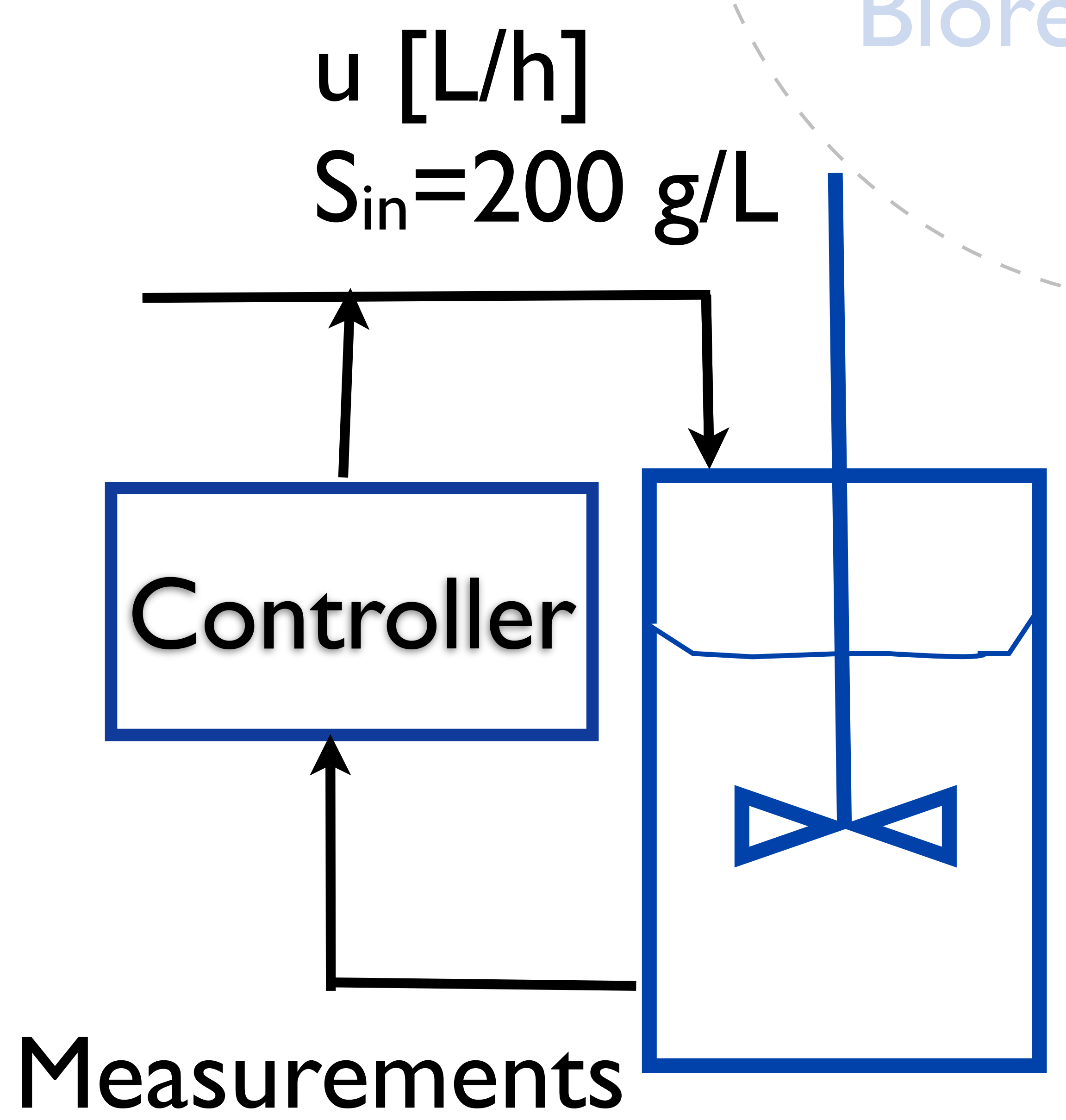
Example: Penicillin

- Fed-batch bioreactor: S → X → P
- Maximize penicillin concentration P
- The biomass concentration is constrained

Srinivasan, B., D. Bonvin, et al. (2002). "Dynamic optimization of batch processes II. Role of measurements in handling uncertainty." Comp. chem. eng. **27**: 27-44.

Example

$X < 3.7$	Biomass concentration
S	Substrate concentration
P	Product concentration
V	Volume
$u < 1$	Substrate feedrate



Example

$$X \xrightleftharpoons[S]{O_2} \alpha X + \beta P$$

Bioreactor

X < 3.7	Biomass concentration
S	Substrate concentration
P	Product concentration
V	Volume
u < 1	Substrate feedrate

$$\dot{X} = \mu(S)X - \frac{u}{V}X$$

$$\dot{S} = -\frac{\mu(S)X}{Y_X} - \frac{\nu X}{Y_P} + \frac{u}{V}\left(S_{\text{in}} - S\right)$$

$$\dot{P} = \nu X - \frac{u}{V}P$$

$$\dot{V} = u$$

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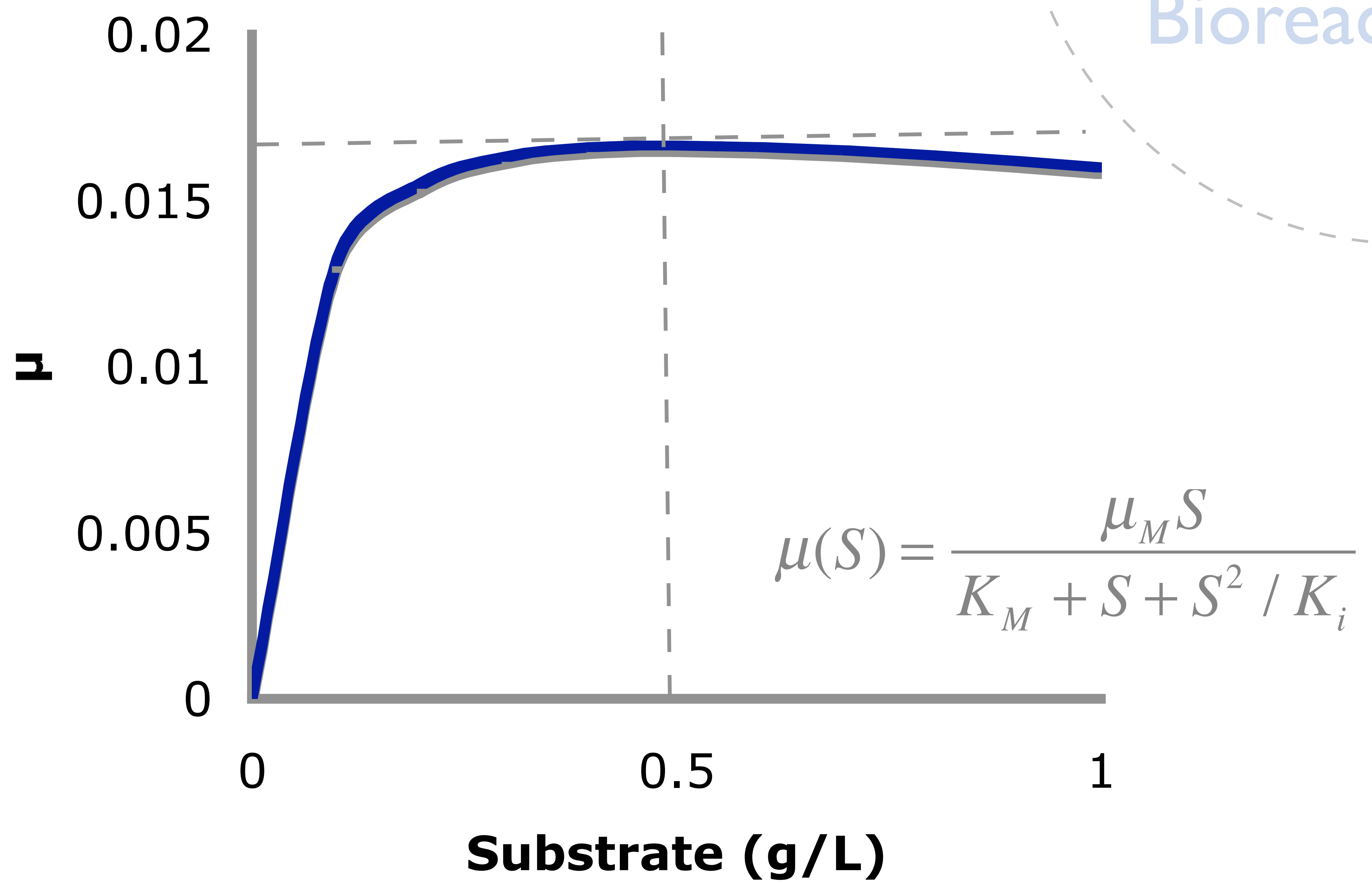
Biomass growth rate μ



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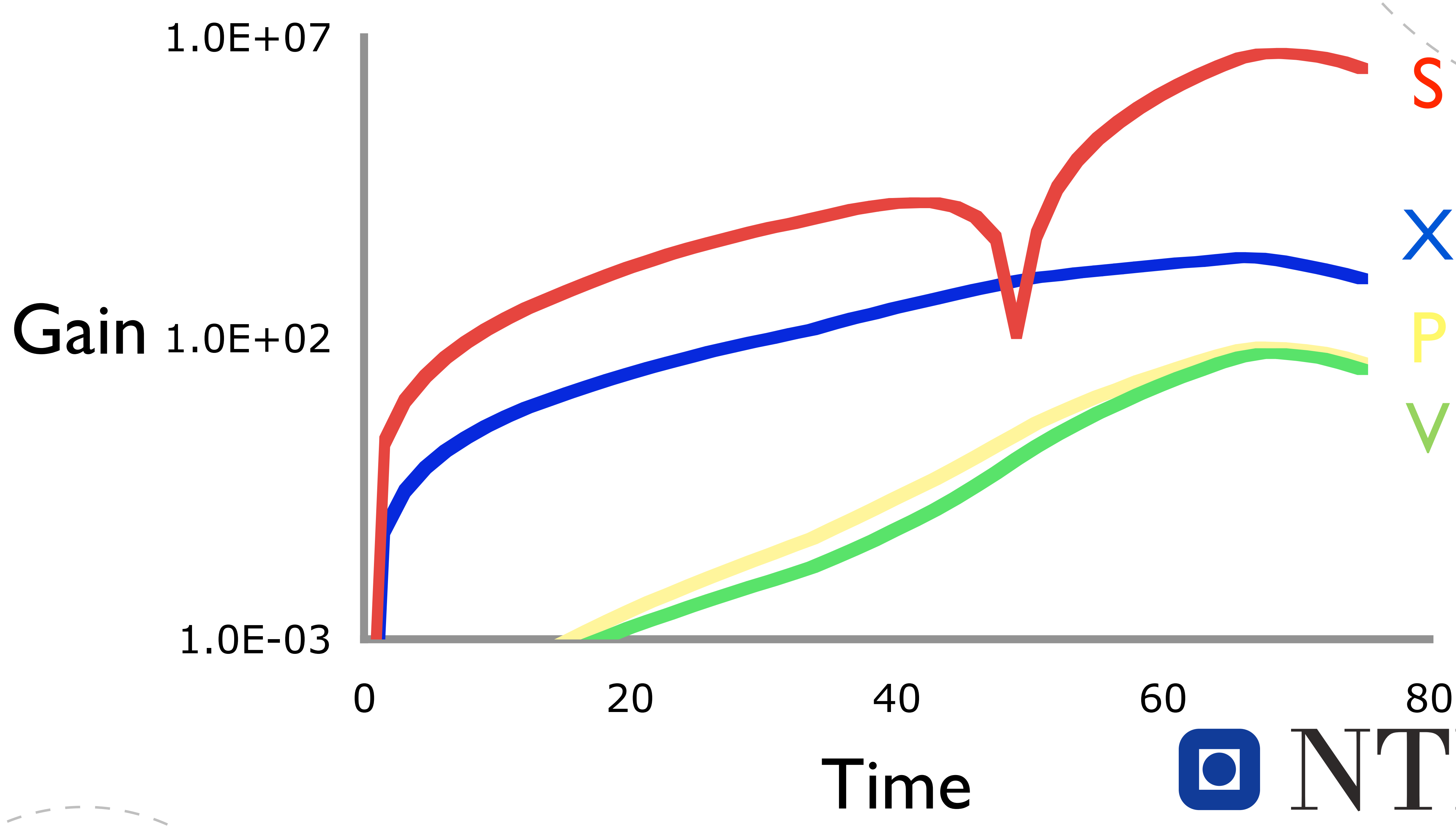
Consider gain magnitude

- Transformation of input: $\xi = \sqrt{u}$
- $H_{\xi\xi}$ is constant

Comparison of gains



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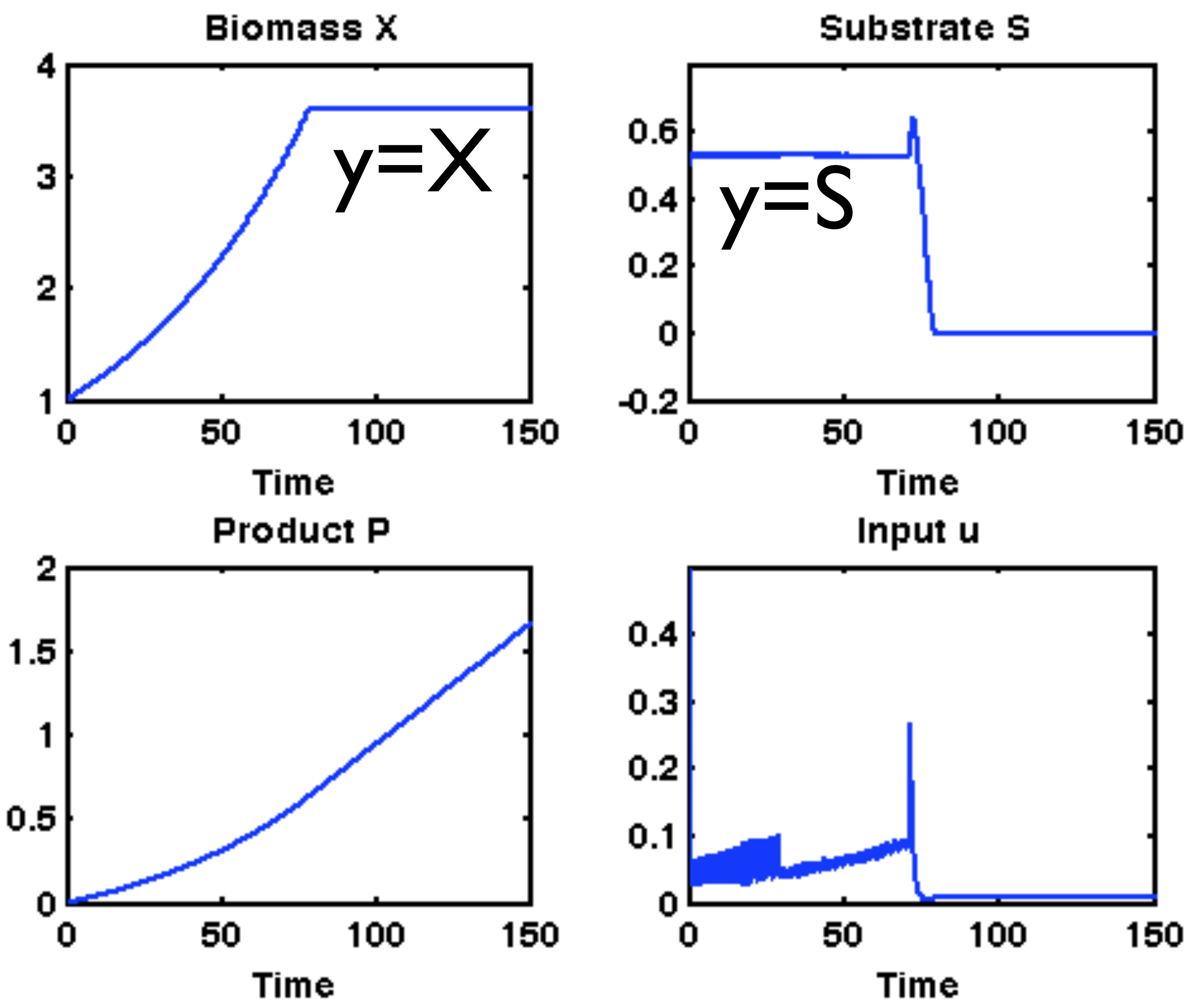
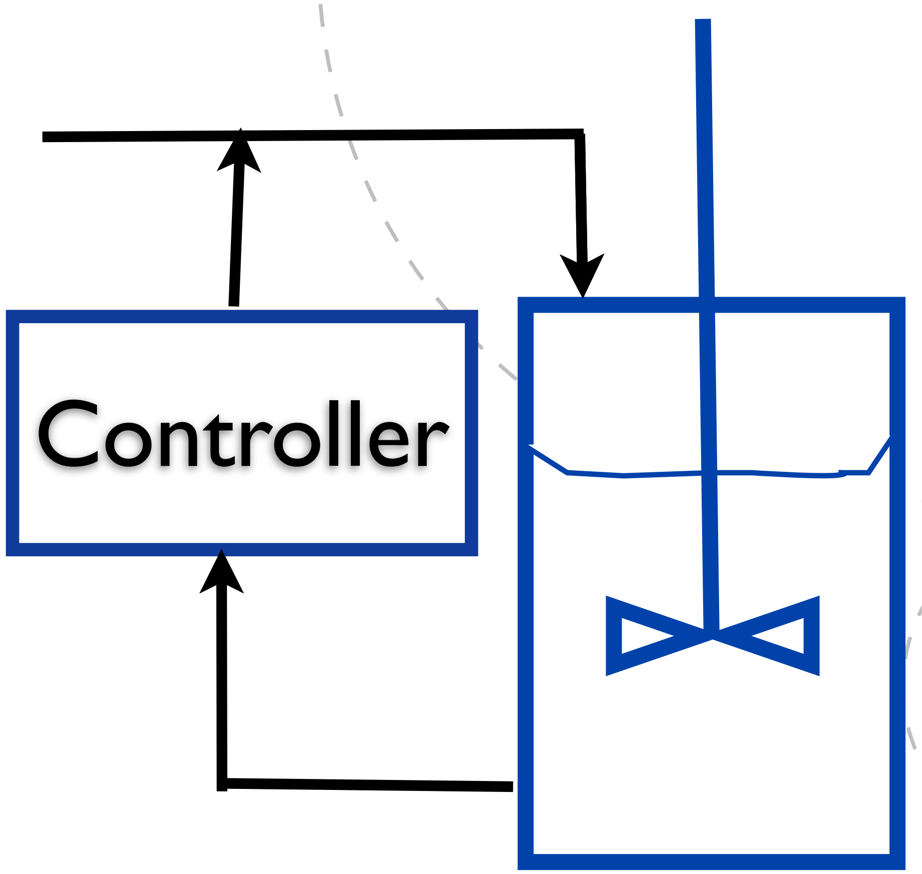
Simulation results





y=S for X ≤ 3.2
y=X for X > 3.2

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Summary: Optimal output selection for batch processes

- Maximum gain rule extended to dynamics
- Variational gain from neighboring optimal control theory
- Method works well for a case study

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