Approaches to the optimization of batch processes in the presence of model uncertainty

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Bachelors

Location of the 30 NITs. Green indicates existing NITs and red indicates upcoming campuses.

REC Warangal

One among Top 20 technical universities in India

Chemical Engineering
1998 - 2002

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Masters

NUS National University of Singapore

Department of Chemical *and* Biomolecular Engineering

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Statistics

(as of August 2007)

Our Community		
Students	**Class of 2007**	**Faculty & Staff**
Undergraduate: 1080 • BEng (Chemical): 1080 **Graduate: 335** • MSc: 106 • MEng: 32 • PhD: 190 • NUS-UIUC Jt PhD: 7	• BEng degrees: 252 • MSc degrees: 54 • MEng degrees: 9 • PhD degrees: 30 • NUS-UIUC Jt PhD: 1	• Faculty Members: 41 • Visiting Faculty: 4 • Instructor: 4 • Research Staff: 24 • Administrative Staff: 11 • Laboratory Staff: 31

Our Accolades

AWARDS FOR ACADEMIC EXCELLENCE

AWARDS FOR ChBE STAFF

AWARDS FOR RESEARCH INNOVATION & ENTERPRISE

National University of Singapore

Chemical Engineering
2002 – 2004

Process Control

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Honeywell

Honeywell Technology Solutions Lab Pvt Ltd
Bangalore
Automation Team, Research &Technology Group
Sep 2004 –Jan 2008 (3 year 5 month)

Senior Research Scientist

Job

NTNU

Started PhD in Jan 2008 in

Norwegian University of Science & Technology
Trondheim, Norway
Department of Chemical Engineering

PhD

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Presentation outline

- Batch process challenges
- Modeling
- Uncertainty and its characterization
- Batch process optimization problem
- Nominal optimization approaches
- Optimization with uncertain models
  - Stochastic optimization
  - Measurement-based optimization
- Conclusions

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Batch process challenges

Process

- Low volume and high value products
- Unsteady-state operation
- Inter – and Intra - batch variation

Instrumentation

- No or Infrequent or less accurate measurements

Modeling

- Good kinetic models are rare
- Poor models
- Reproducibility less than 5 %

Optimization objectives

- Economic objective $\Longrightarrow$ Modeling and engineering effort should pay off
- Guarantee high reproducibility and high yield despite of the uncertainties
- Incorporate safety constraints without losing significant optimization potential

Terwiesch et al., 1994

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Modeling

- ❖ First principle modeling
  - Mass, energy & momentum balance equations
    - ➢ Require physical insight
    - ➢ Valid over a wide range with better predictability
    - ➢ Modeling and maintenance are both time and resource intensive
- ❖ Emperical modeling
  - input – output data
    - ➢ Valid over a short range
    - ➢ Poor predictability
- ❖ Hybrid Modeling
  - Combination of both modeling methods
    - ➢ Minimum modeling effort
    - ➢ Covers a range of operation

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Uncertainties and their characterization

Simplifications and inaccuracies in modeling and disturbances result in variations from the real plant

Mathematically these variations are treated as uncertainties

Uncertainties are treated as random variables that follow a specific probability distribution

Characterization: involves the selection of probability distribution function and their associated parameters, for example, for a normally distributed random variable, mean and variance are the parameters

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Terwiesch et al., 1994

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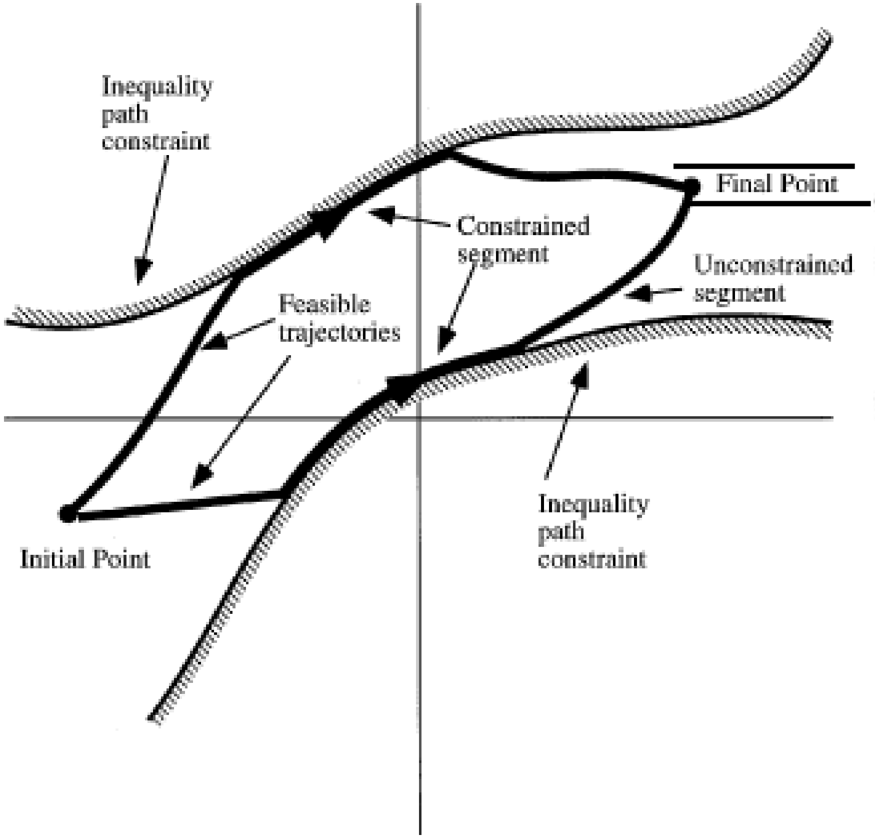
Batch process optimization : Problem formulation

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

$$s.t. \quad \dot{x} = F(x,u) \qquad x(0) = x_0$$

$$S(x,u) \le 0 \qquad T(x(t_f)) \le 0$$



Srinivasan et al., 2003
Feehery and Barton, 1998

Batch process optimization : Pontryagin Maximum Principle

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

$$s.t. \quad \dot{x} = F(x,u) \qquad x(0) = x_0$$

$$S(x,u) \le 0 \qquad T(x(t_f)) \le 0$$

Reformulation using Pontryagin Maximum Principle
with adjoint variables λ and Lagrange multipliers μ,ν

$$\min_{t_f, u(t)} H(t) = \lambda^T F(x,u) + \mu^T S(x,u)$$

$$s.t. \; \dot{x} = F(x,u) \qquad x(0) = x_0$$

$$\dot{\lambda}^T = -\frac{\partial H}{\partial x} \qquad \lambda^T(t_f) = \left.\frac{\partial \phi}{\partial x}\right|_{t_f} + \nu^T \left.\frac{\partial T}{\partial x}\right|_{t_f}$$

$$\mu^T S = 0 \qquad \nu^T T = 0$$

require solving Two Point Boundary Value Problem

Srinivasan et al., 2003

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Nominal optimization: Numerical solution approaches

- Piecewise constant u(t) –

  Control vector iteration (CVI)

  decision variables : discretized u in the intervals

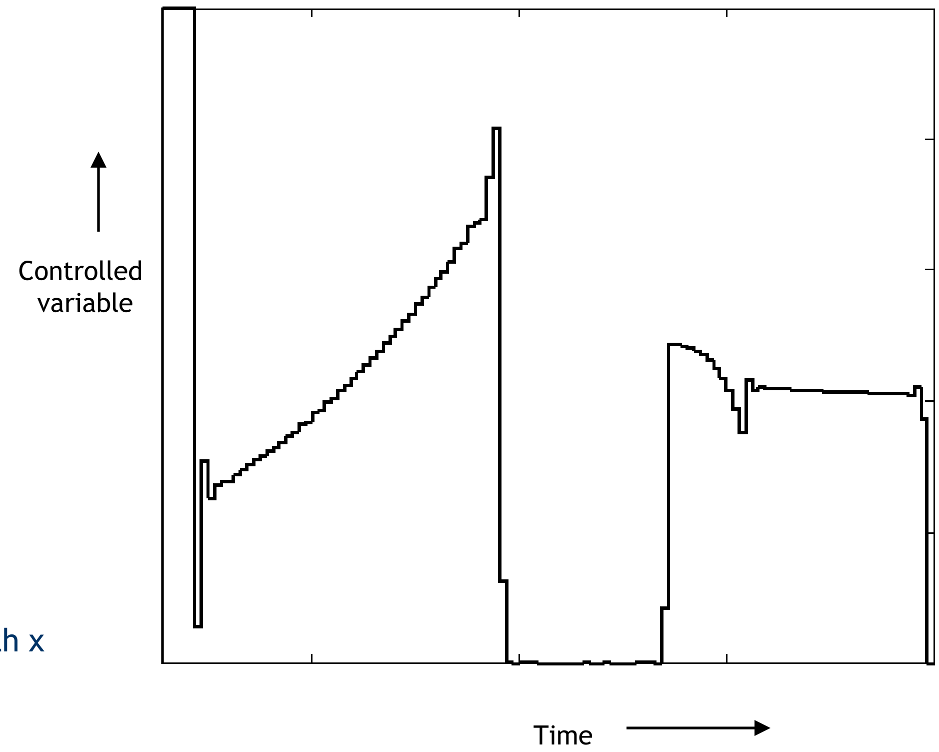
- Polynomial u(t) or u(x)

  Control vector parameterization (CVP)

  decision variables : polynomial coefficients

- Polynominal x(t) and u(t)

  decision variables : polynominal coefficients of both x and u



Bryson and Ho, 1969; Hicks and Ray, 1971; Ray, 1981; Biegler, 1984; Vassiliadis et al., 1994

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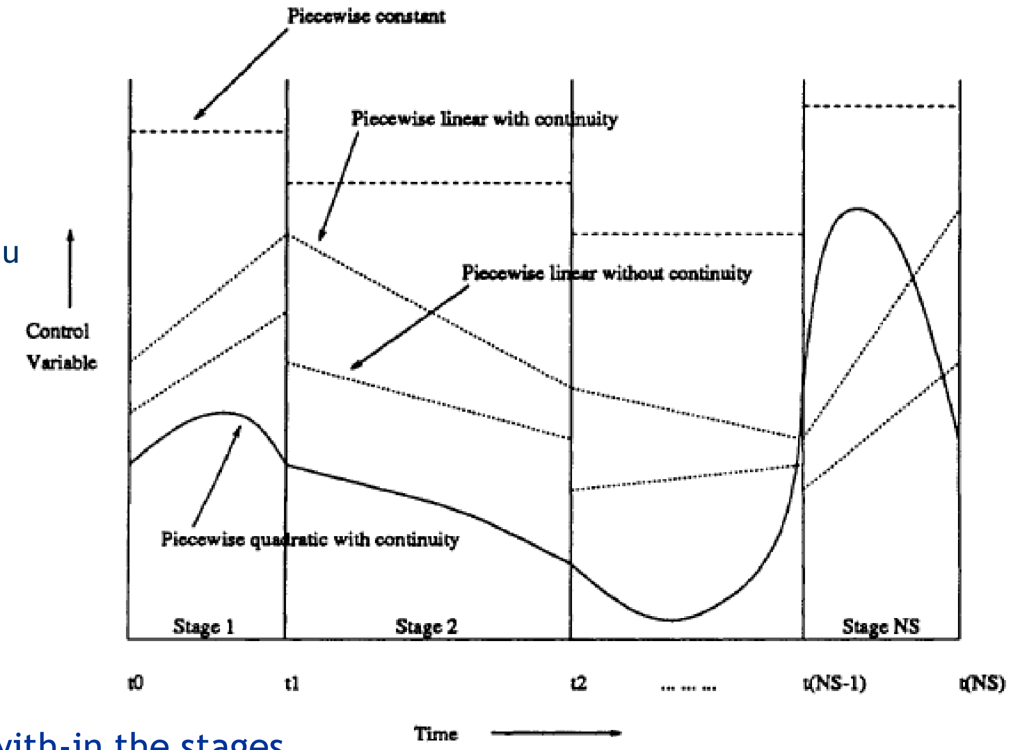
Nominal optimization: Numerical solution approaches

- Piecewise polynomial x(t) and u(t)

  decision variables: polynominal coefficients of x and u in each stage

- Discrete charges u_i

  decision variables: stage end times, discrete jumps in u



Path constraints cannot be handled with-in the stages

In addition to parameterization, numerical integration is also replaced with polynominal approximations to reduce computational burden

Bryson and Ho, 1969; Hicks and Ray, 1971; Ray, 1981; Biegler, 1984; Vassiliadis et al., 1994

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Nominal optimization: Numerical solution approaches

State and input handling	Problem formulation	
	Direct	PMP
States—parameterized Inputs—parameterized	Simultaneous approach (NLP)	State and adjoint parameterization (NR, QL)
States—continuous Inputs—parameterized	Sequential approach (CVP)	Gradient method (CVI)
States—continuous Inputs—continuous	Analytical parameterization approach	Shooting method (BCI)

PMP : pontryagin maximum principle
BCI : boundary condition iteration
NR : newton –raphson

QL : quasi-linearization

Srinivasan et al., 2003

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Summary of numerical solution approaches

Numerical approaches accuracy α # of stages, # of coefficients

Adaptive control vector parameterization techniques are developed by including stage times also as decision variables in optimization

Terwiesch et al., 1994
Schlegel, 2005

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Interpretation optimal solution

	Path	Terminal
Constraints	$\mu^T S(x, u) = 0$	$\nu^T T(x(t_f)) = 0$
Sensitivities	$\lambda^T(\partial F/\partial u) + \mu^T(\partial S/\partial u) = 0$	$\lambda^T(t_f) - (\partial \phi/\partial x)\vert_{t_f} - \nu^T(\partial T/\partial x)\vert_{t_f} = 0, \quad H(t_f) = 0$

Lagrange multipliers μ and ν capture the cost deviations in not meeting the active constraints

$$\delta J = \int_0^{t_f} \mu^T \delta S \, dt + \nu^T \delta T$$

The cost in not meeting sensitivity constraints $\delta J = H_u S_u = 0$ as $H_u = 0$

Uncertainties are inevitable in the modeling and optimization, methods that handle uncertainties are needed

Srinivasan et al., 2003

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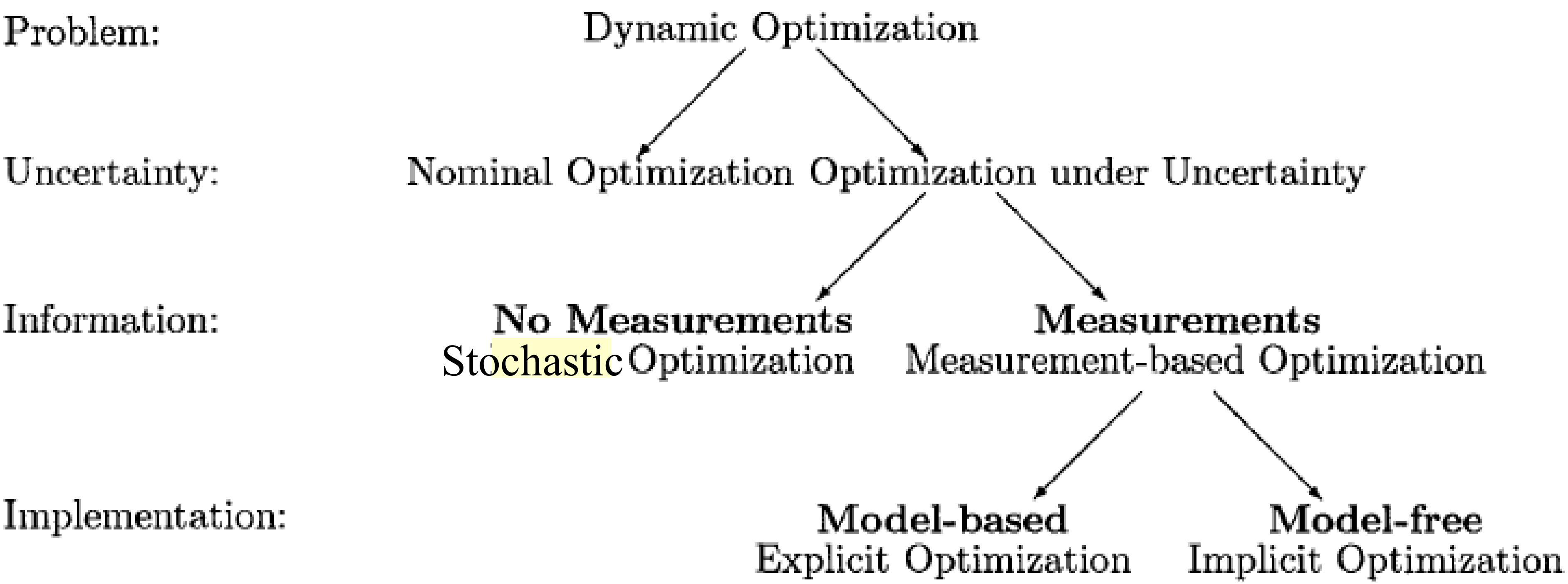
Classification of Batch process optimization approaches



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Srinivasan et al., 2002

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  - ❖ **Stochastic optimization**
  - ❖ Measurement-based optimization
- ❖ Research opportunities
- ❖ Conclusions

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Optimization with uncertain models

Stochastic optimization

Offline optimization

Given uncertain parameters θ

M – model with uncertain parameters θ
Q – specified product quality
g – product quality requirements
α – specified level of confidence for quality

Best expected value	$\max_u E(J(M))$
Minimum variance	$\min_u E\{[Q-\bar{Q}]^2\}$
Threshold	$\max_u P(g(u,\theta)) \le 0$
Variable threshold	$\max_u P(g(u,\theta)) \le \alpha$
Best worst case	$\max_u \min_M J$
Best best case	$\max_u \max_M J$

No need for measurements
Typically conservative

Terwiesch et al., 1994

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Optimization with uncertain models in parameters θ

Online optimization approaches

Dealing uncertainty through feedback - Measurements are used to estimate x and θ

1. Online reoptimization
2. Optimal singular feedback control
3. Optimal nonsingular feedback control
4. Necessary conditions of optimality tracking

Explicit uncertainty accounting - Measurements are used to estimate x, θ, P(θ)

1. Minimum effort for specified confidence of feasible operation
   - Final state uncertainty is predicted by propogating the covariance of uncertain parameters through system equations and α-confidence ellipsoid is constructed
   - u(t) is optimized to locate the desired x_{set} at the centre of confidence ellipsoid
   - does not account for future parameter estimation accuracy
2. Dual control
   - also accounts for future parameter estimation accuracy
3. Differential Game

   Two player game
   - Engineer vs Nature
   - Iu[u(t),v(t)] Iv[u(t),v(t)]

   Super structure of stochastic optimization

Reduces conservatism and improves performance

Bryson and Ho, 1969; Palanki et al., 1993; Terwiesch et al., 1994
Astroom and Wittenmark, 1989; Meadows and Rawlings, 1991;
Gupta and Leondes, 1981

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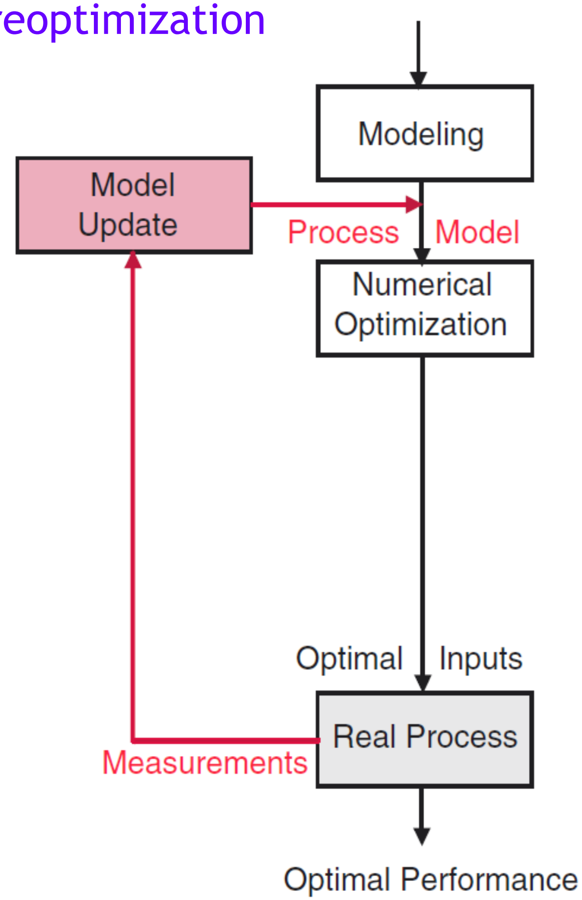
Optimization approach 1

Dealing uncertainty through feedback

Online reoptimization



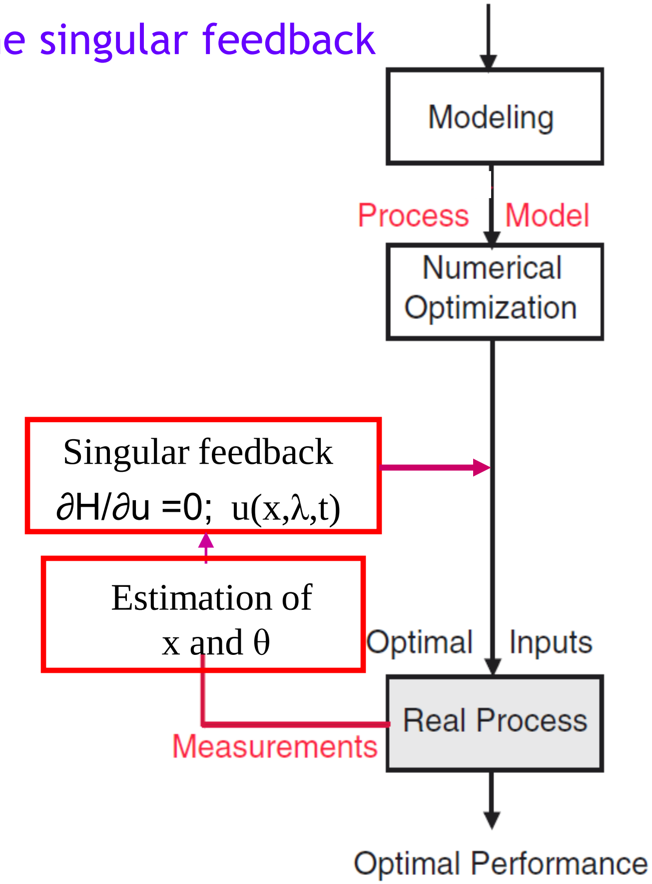
- model is updated at each sampling instant
- re-optimization is performed at each sampling instant
- computationally intensive and require high effort in modeling

Welz et al., 2008
Würth et al., 2009

Optimization approach 2

Dealing uncertainty through feedback

Online singular feedback



- Optimal control problem is singular when Hamiltonian is linear in control u.
- In singular feedback control u(x,λ,t) is a function of adjoint variables λ on singular arcs, which are solutions of TPBVP
- For practical purpose λ is replaced with λ_{nom}
- It is shown to work well practically but cannot always guarantee better performance with uncertainties

Terwiesch et al., 1994

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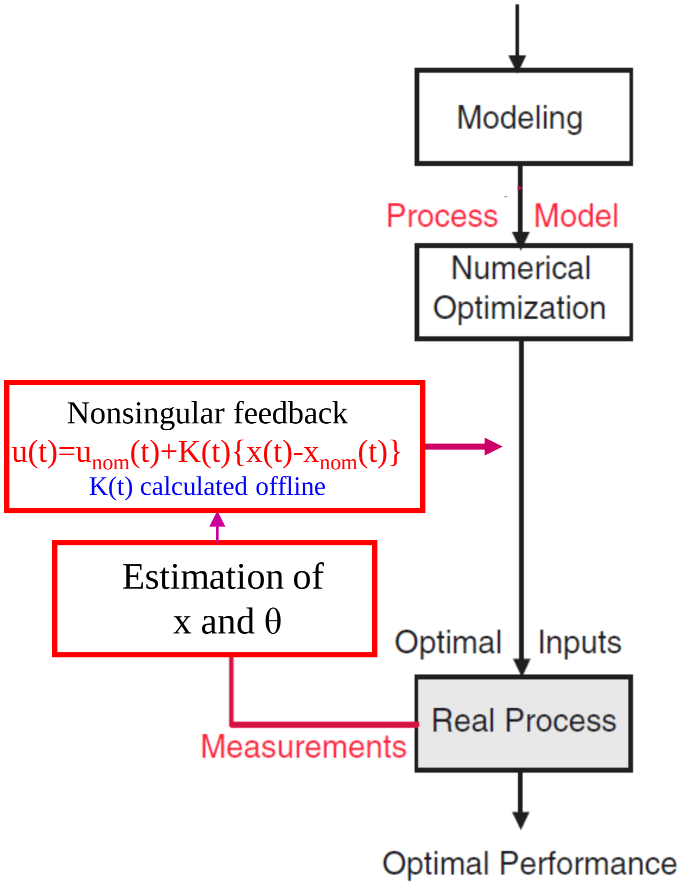
Optimization approach 3

Dealing uncertainty through feedback

Online nonsingular feedback



- It requires online computation effort of a P controller
- time-variant corrector gains K(t) is performed offline
- dynamic feedback can also be used
- guarantees optimality in case of small uncertainties
- large uncertainties are handled with multiple nominal profiles and time-variant corrector gains

Terwiesch et al., 1994

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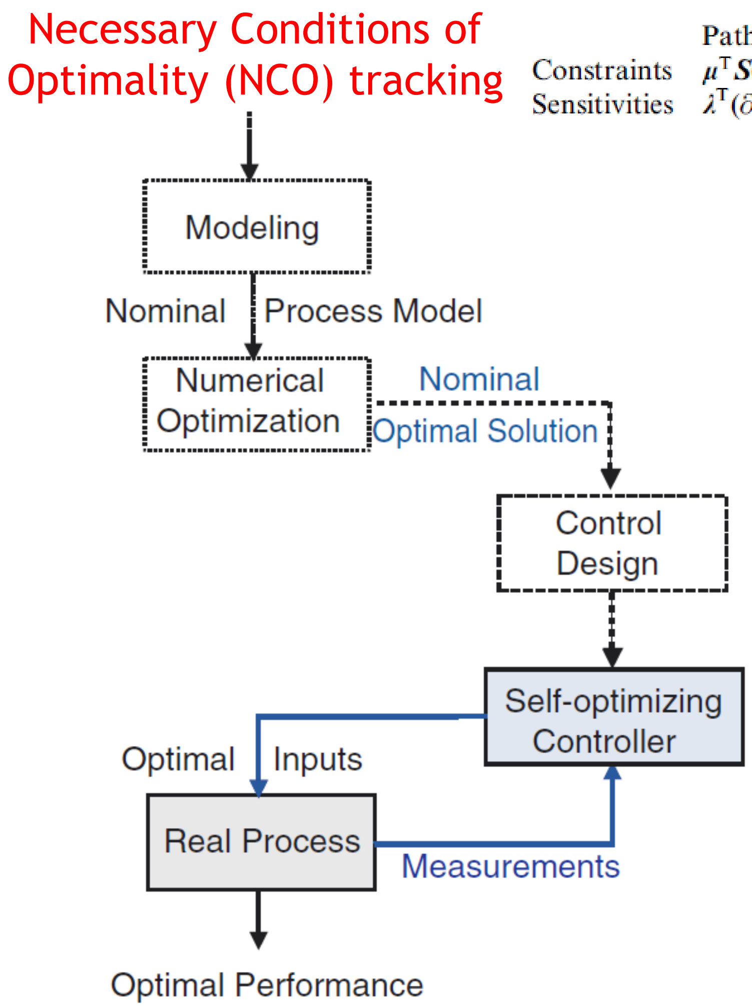
Optimization approach 4: Necessary conditions of optimality tracking



	Path	Terminal
Constraints	$\mu^{T} S(x, u) = 0$	$\nu^{T} T(x(t_f)) = 0$
Sensitivities	$\lambda^{T}(\partial F/\partial u) + \mu^{T}(\partial S/\partial u) = 0$	$\lambda^{T}(t_f) - (\partial \phi/\partial x)\vert_{t_f} - \nu^{T}(\partial T/\partial x)\vert_{t_f} = 0, \quad H(t_f) = 0$

- Optimal inputs are partitioned as arcs η(t) for constraints and parameters π for sensitivities
- Solution model is developed as the sequence of arcs
- Control laws are developed to adjust the arcs η(t) and parameters π to meet the NCO conditions
- Large uncertainties are dealt by including switching times of arcs as new decision variables in optimization

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Welz et al., 2008

NCO illustration on a fed-batch bioreactor

S – substrate concentration
X – biomass concentration
P – product concentration
u – feed rate
μ_m, v_m, K_m, K_i, K_0
- Kinetic parameters
Yx, Yp –yield coefficients

Reactions

$$S \rightarrow X$$
$$S \xrightarrow{X} P$$

$$J = \max_{u(t)} P(t_f)$$

Model equations

$$\dot{X} = \mu X - \frac{u}{V} X, \quad X(0) = X_0,$$
$$\dot{S} = -\frac{\mu X}{Y_x} - \frac{v X}{Y_p} + \frac{u}{V}(S_{in} - S), \quad S(0) = S_0,$$
$$\dot{P} = v X - \frac{u}{V} P, \quad P(0) = P_0,$$
$$\dot{V} = u, \quad V(0) = V_0,$$

with

$$\mu(S) = \frac{\mu_m S}{K_m + S + \frac{S^2}{K_i}},$$
$$v(S) = \frac{v_m S}{S + K_0},$$

Kadam et al., 2007

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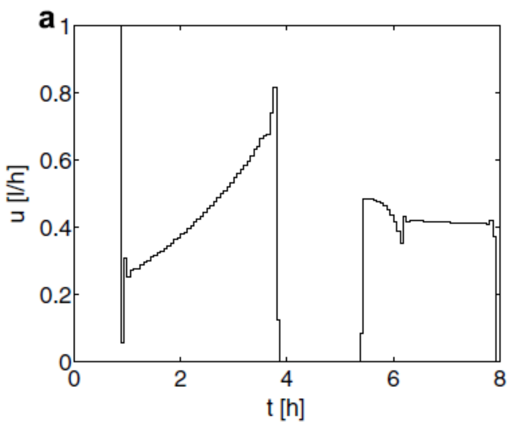
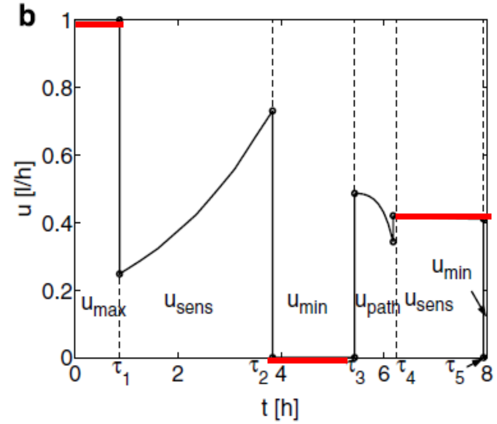
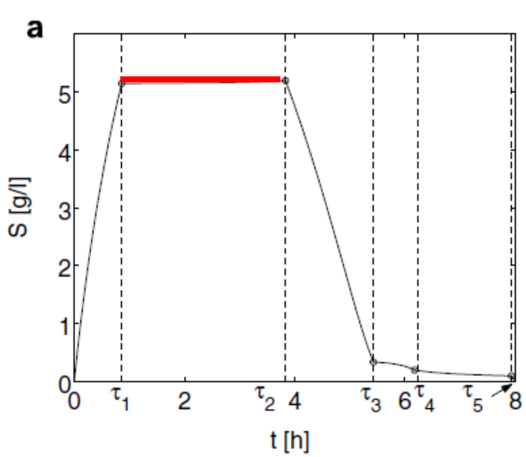
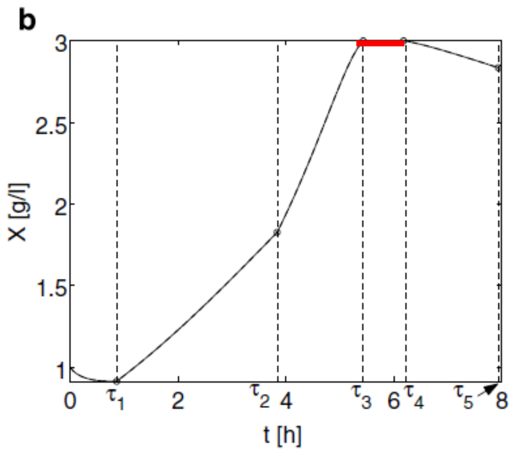
	Path	Terminal
Constraints	$\mu^T S(x, u) = 0$	$\nu^T T(x(t_f)) = 0$
Sensitivities	$\lambda^T(\partial F/\partial u) + \mu^T(\partial S/\partial u) = 0$	$\lambda^T(t_f) - (\partial \phi/\partial x)\vert_{t_f} - \nu^T(\partial T/\partial x)\vert_{t_f} = 0, \quad H(t_f) = 0$

NCO illustration









$$u(t) = \begin{cases} u_{max}, & 0 \leqslant t < \tau_1, \\ \mathcal{N}_2(S, S_{ref,2}), & \tau_1 \leqslant t < \tau_2, \\ u_{min}, & \tau_2 \leqslant t < \tau_3, \\ \mathcal{K}_4(X, X_{max}), & \tau_3 \leqslant t < \tau_4, \\ \mathcal{N}_5(S, S_{ref,5}), & \tau_4 \leqslant t < \tau_5, \\ u_{min}, & \tau_5 \leqslant t \leqslant t_f, \end{cases}$$

$$\tau_1 = t \quad \text{s.t. } S(t) = S_{ref,2},$$

$$\tau_2 = t \quad \text{s.t. } X_{pred}(t) = 0.95 X_{max},$$

$$\tau_3 = t \quad \text{s.t. } X(t) = X_{max},$$

$$\tau_4 = t \quad \text{s.t. } S(t) = S_{ref,5},$$

$$\tau_5 = 7.93,$$

$$X_{pred}(t) = X(t) - \alpha(1.25 S_{ref,2} - S(t)),$$

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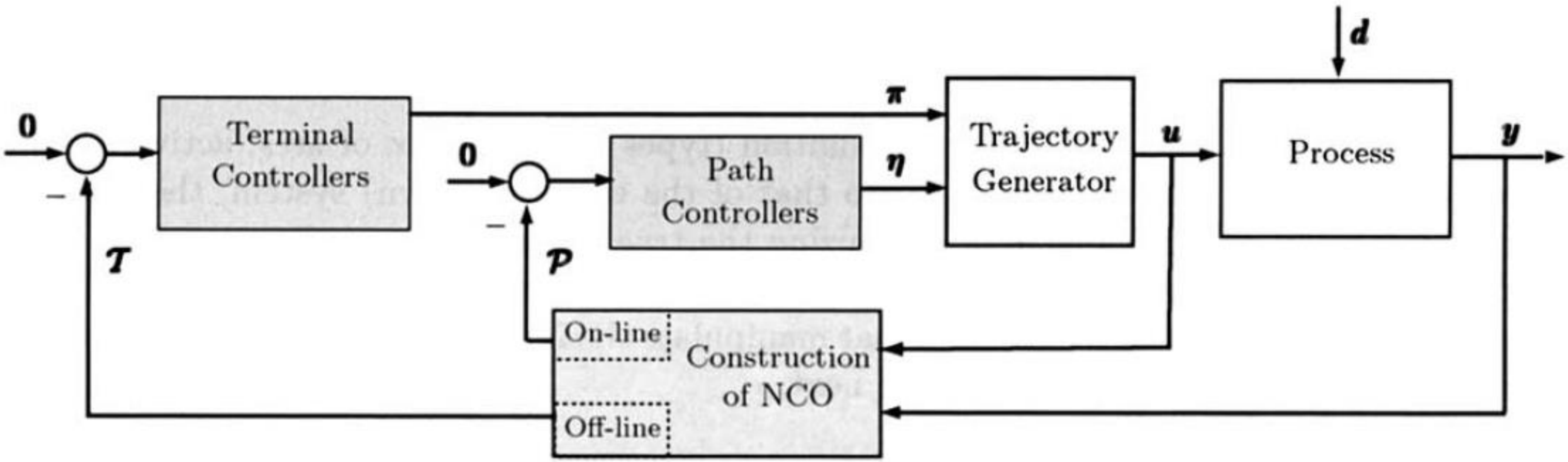
NCO tracking implementation



Path and terminal controllers can be either decentralized PI or Multivariable controllers

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Conclusions

- Batch process challenges and numerical solution approaches for nominal optimization are discussed

- Stochastic methods for optimization under uncertainty are presented

- Measurement based optimization approaches are described

- NCO tracking is illustrated on an example

Research opportunities

- Better technique for estimation of states and parameters for a given parameter probability distribution is vital as extended kalman filter is sub-optimal for non-gausian random variables

- Developing methods that quantify the lost economic value with various approaches

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Thank You

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