A Two-Stage Algorithm for Multi-Scenario Dynamic Optimization Problem

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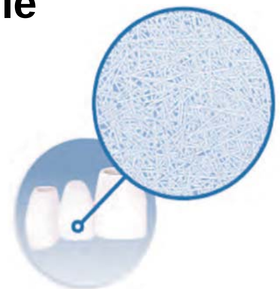
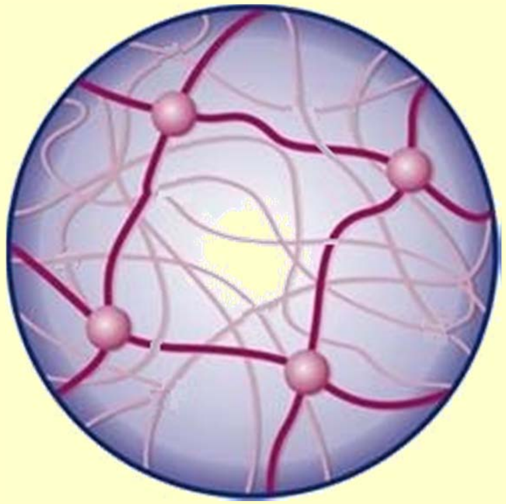
Outline

- Project review and problem introduction
- A Two-stage Algorithm
  - Parameter estimation from multiple data sets
  - Optimization under uncertainty with multi-scenario formulation
- An Illustrative example
- Current direction
- Summary

Project Review (1)

Strong & flexible

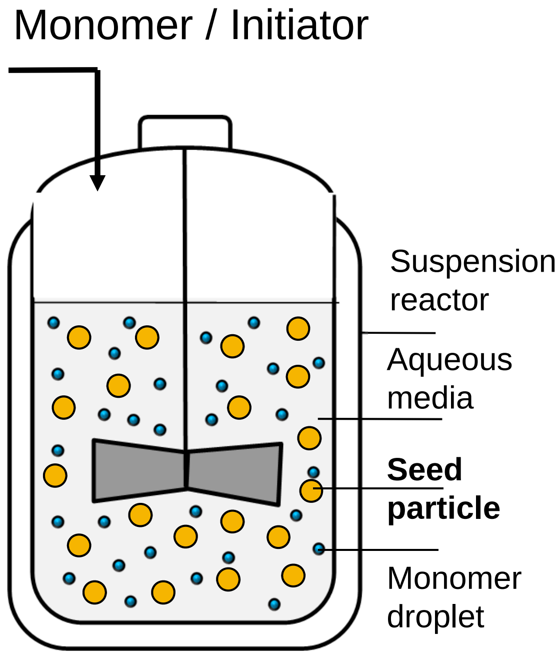




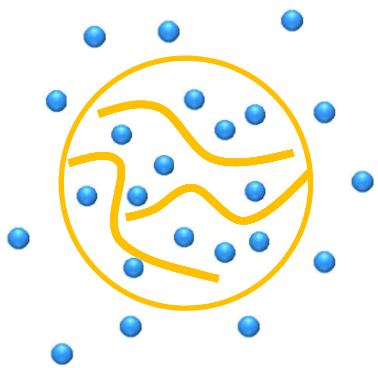
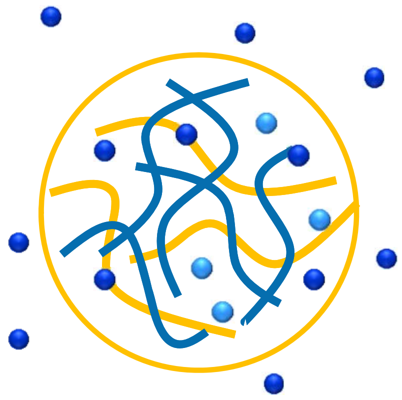
SIPN

(**S**emi-**I**nterpenetrating **P**olymer **N**etwork)

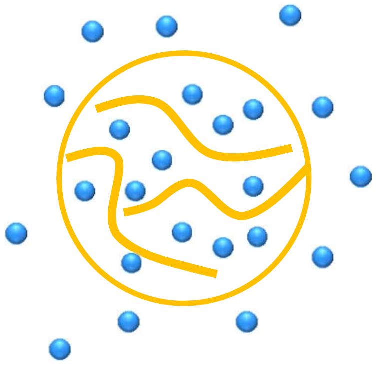
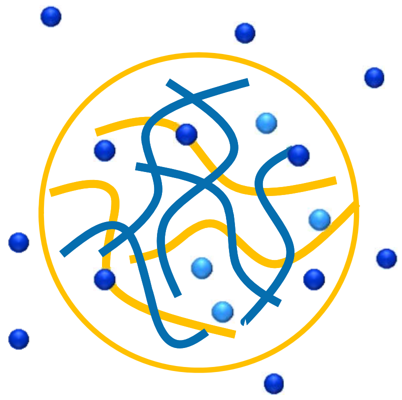
Low productivity & difficult to control



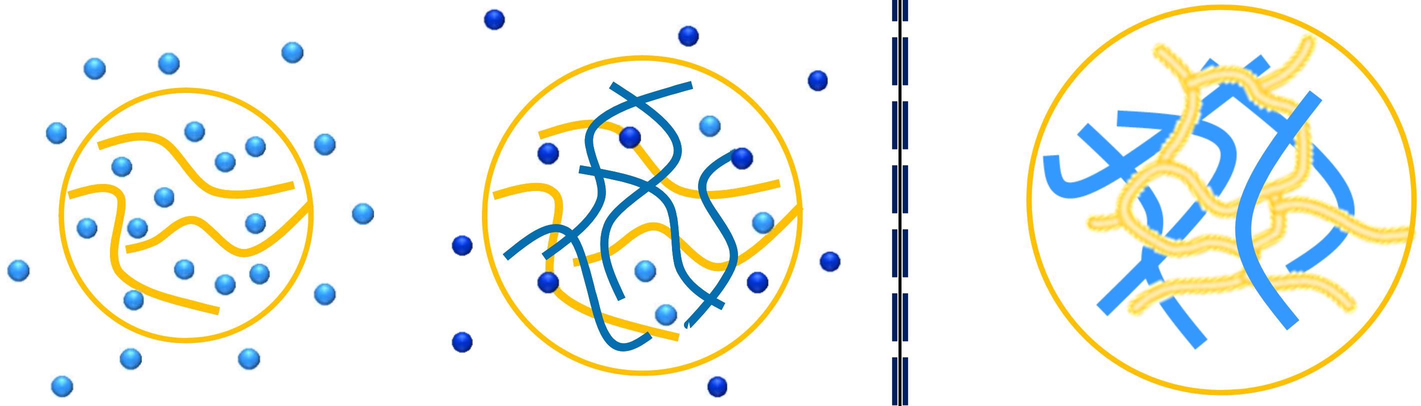
Project Review (2)

Process Stages	 Swelling  Polymerization	 Crosslinking
Features	*Complex diffusion; single component reaction*	*Complex composite networking reaction*
Modeling	**Particle Growth model**	**Semi-IPN kinetic model**
Control variables	• Monomer feeding rate • Initiator feeding rate	• Initial polymer • Monomer concentration • Initiator concentration • Holding temperature • Holding duration
Optimization Approach	**Dynamic Optimization**	**Surrogate Model**

Project Review (2)

Process Stages	 Swelling  Polymerization	 Crosslinking
Features	Stage I	*Complex composite networking reaction*
Modeling		**Semi-IPN kinetic model**
Control variables		• Initial polymer • Monomer concentration • Initiator concentration • Holding temperature • Holding duration
Optimization Approach		**Surrogate Model**

Project Review (2)

Process Stages	 Swelling	Polymerization	Crosslinking
Features	Stage I		Stage II
Modeling			
Control variables			
Optimization Approach			

Project Review (2)

Process Stages	Integrated Model-based Optimization	
Features	Stage I	Stage II
Modeling		
Control variables		
Optimization Approach		

New Challenges

- Continuous effect for process improvement
- Improve model reliability

  Additional information acquisition

  – Update model / parameters
- Improve solution robustness

  Uncertainty consideration

  – Optimization under uncertainty

Multi-scenario Dynamic Optimization

- Parameter estimation from multiple data sets

$$
\begin{aligned}
\min_{\theta} \quad & \sum_{i=1}^{NS} (y_i - y_i^m)^T \Sigma_i (y_i - y_i^m) \\
s.t. \quad & y_i = f_i(x_i, \theta) \\
& h_i(x_i, \theta) = 0
\end{aligned}
$$

- Dynamic optimization under uncertainty

$$
\max_{u,v,\tau} E_\theta\{\Phi(\dot{x}, x, y, u, \nu, \tau; \theta)\} = \max_{u,v,\tau} \int_{\theta \in \Theta} \Psi(\theta)\Phi(\dot{x}, x, y, u, \nu, \tau; \theta) d\theta
$$

S.t.

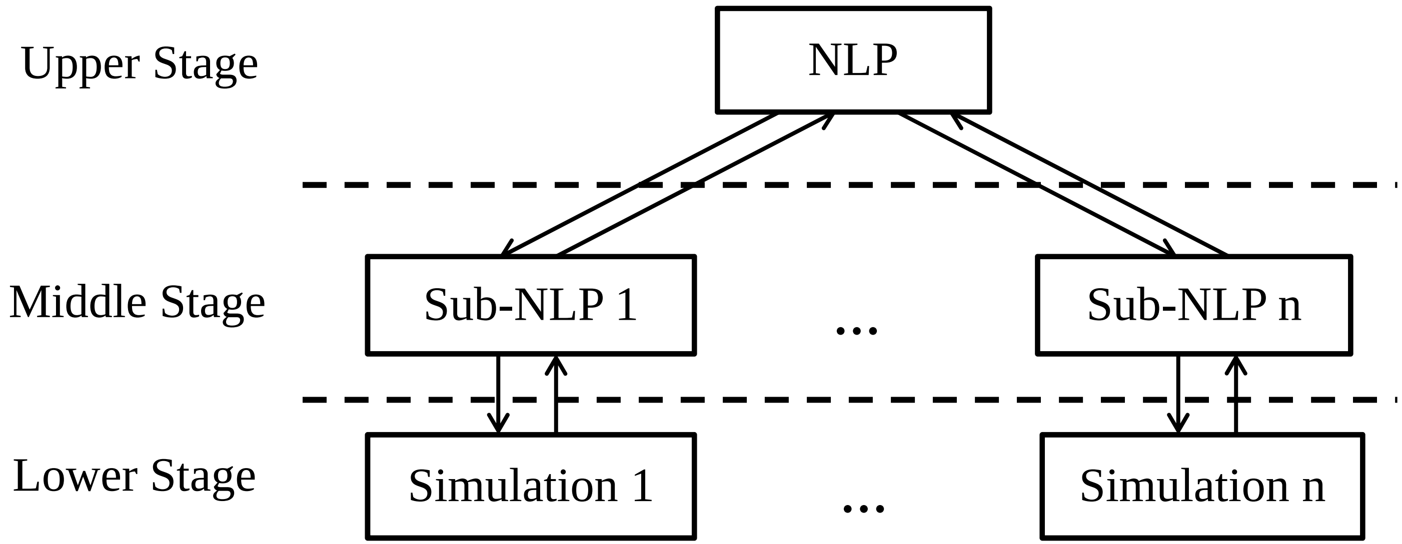
$$
\begin{aligned}
& J_0(\dot{x}(0), x(0), y, u(0), \nu, \tau; \theta) = 0 \\
& h(\dot{(x)}, x, y, u, v, t; \theta) = 0, \\
& g(\dot{(x)}, x, y, u, v, t; \theta) \leq 0,
\end{aligned}
$$

Current Researches (1)

- Sequential approaches

  (Faver 2003):

Computationally expensive for derivative evaluation



- [Anderson 1978], [Rod 1980], [Reilly 1981], [Dovi 1989], [Kim 1990],

Current Researches (2)

- Simultaneous approach

(Zavala and Biegler 2007)

Difficult for highly nonlinear, ill-condition problem

$$\begin{bmatrix} W_1 & & & & & A_1 \\ & W_2 & & & & A_2 \\ & & W_3 & & & A_3 \\ & & & \ddots & & \cdots \\ & & & & W_{NS} & A_{NS} \\ A_1^T & A_2^T & A_3^T & \cdots & A_{NS}^T & \delta_1 I \end{bmatrix} \cdot \begin{bmatrix} \Delta v_1 \\ \Delta v_2 \\ \Delta v_3 \\ \vdots \\ \Delta v_{NS} \\ \Delta d \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \\ r_{NS} \\ r_d \end{bmatrix}$$

$$W_k = \begin{bmatrix} H_k^l + \delta_1 I & \nabla_{x_k} c_k^l & D_k^T \\ (\nabla_{x_k} c_k^l)^T & -\delta_2 I & 0 \\ D_k & 0 & -\delta_2 I \end{bmatrix}$$

where

$$r_k^T = -[(\nabla_{x_k}\mathcal{L}_k^l)^T, (c_k^l)^T, (D_k x_k^l - \bar{D}_k d^l)^T],\ \Delta v_k^T = [\Delta x_k^T\ \Delta\lambda_k^T\ \Delta\sigma_k^T],\ A_k^T = [0\ 0\ -\bar{D}_k^T],$$

Schur complement

$$[\delta_1 I - \sum_{k=1}^{NS} A_k^T (W_k)^{-1} A_k]\Delta d = r_d - \sum_{k=1}^{NS} A_k^T (W_k)^{-1} r_k$$

[Tjoa and Biegler1991,1992]
[Gondzio and Gothrey 2005, Gondzio and Sarkissian 2003]

A Two-Stage Algorithm

$$\min_{\theta^L} F(\theta^L) = \sum_{j=1}^{NS} f_j(\theta^L)$$

$$\theta^L_{(k)} \qquad \frac{df_j}{d\theta^L_{(k)}}, \frac{d^2 f_j}{d^2\theta^L_{(k)}}$$

$$\min_{\theta^{S_1}} \; f_1(\theta^{S_1}, \theta^L_{(k)}) \qquad s.t. \quad \mathcal{M}_1$$

$$\min_{\theta^{S_2}} \; f_2(\theta^{S_2}, \theta^L_{(k)}) \qquad s.t. \quad \mathcal{M}_2$$

…

$$\min_{\theta^{S_n}} \; f_n(\theta^{S_n}, \theta^L_{(k)}) \qquad s.t. \quad \mathcal{M}_n$$

- Efficient algorithm for better behaved large inner problem
- Robust solver for well-conditioned small outer problem

Sensitivity from Inner Optimization Problem

- **“As-NMPC”**

  Features: NLP sensitivity evaluation

  - At the solution point, the primal-dual system satisfies

$$\phi(s_*(\eta), \eta) = 0$$

  - Applying the implicit function theorem

$$\bar{K}_*(\eta_0)\frac{\partial s_*}{\partial \eta} = -\frac{\partial \phi(s_*(\eta_0), \eta_0)}{\partial \eta}$$

Substitute the right hand size with “I” at the desired parameter constraints

Exact gradient information is conveniently available at the optimal point

Sensitivity from Inner Optimization Problem

- **Hessian evaluation**
  - When Hessian information is required, Hessian-vector product is computed
    - Forward difference

$$H(x) \cdot v \approx \frac{G(x+\epsilon v) - G(x)}{\epsilon}$$

    - Central difference

$$H(x) \cdot v \approx \frac{G(x+\epsilon v) - G(x-\epsilon v)}{2\epsilon}$$

Exact Hessian-vector product (Pearlmutter, 1994)

Operator $\mathcal{R}\{f(x)\} = \frac{\partial f(x+\epsilon v)}{\partial \epsilon}\Big|_{\epsilon=0}$

$\mathcal{R}\{f'(x)\} = Hv, \ \ \mathcal{R}\{x\} = v$ Apply R{} to Gradient equation

Outer Optimization Problem

- Solvers:
  - Bound constrained optimization algorithms
    - L-BFGS-B

      A limited-memory quasi-Newton code for bound-constrained optimization
    - TRON

      Trust region Newton method for the solution of bound-constrained optimization problems.
    - ACO

      Adaptive cubic overestimation
    - …

An Illustrative Example

- Parameter Estimation from Multiple data sets

First-order Irreversible Chain reaction

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$$\frac{dy_A}{dt} = -k_1 y_A$$

$$\frac{dy_B}{dt} = k_1 y_A - k_2 y_B$$

Assume k2 is a Linking parameter, k1 is a separate parameter.
20 data sets were generated from model simulation.

Outer problem solved in TRON, converged in 3 iterations.
Inner problem solved in As-NMPC converged in 6 iterations in average.

The same optimal solution is found at the optimal.

Current Direction

- Reduce kinetic parameter uncertainty by multi-scenario parameter estimation
- Optimization of operation condition under uncertainty
- Investigation of efficient algorithm for outer optimization problem
- Pilot plant study for optimal solution
- Extension of model application for broader products

Summary

- Multi-scenario optimization for dynamic system is often desired but challenging.
- Current sequential and simultaneous algorithms have limitations in terms of efficiency and robustness.
- A two-stage algorithm is proposed which takes advantage of efficient interior-point method and robust bound constraint algorithm.
- Small test problems are studied. Application to the process model is planned.

Thank You !