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
Strong & flexible

Low productivity & difficult to control

SIPN (Semi-Interpenetrating Polymer Network)

Monomer / Initiator

Suspension reactor
Aqueous media
Seed particle
Monomer droplet
## Project Review (2)

<table>
<thead>
<tr>
<th>Process Stages</th>
<th>Features</th>
<th>Modeling</th>
<th>Control variables</th>
<th>Optimization Approach</th>
<th>Surrogate Model</th>
</tr>
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</table>
|               | *Complex diffusion; single component reaction* | **Particle Growth model** | • Monomer feeding rate  
  • Initiator feeding rate | **Dynamic Optimization** | **Semi-IPN kinetic model**  
  • Initial polymer  
  • Monomer concentration  
  • Initiator concentration  
  • Holding temperature  
  • Holding duration |
Project Review (2)

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**Features**

- Swelling
- Polymerization
- Crosslinking

**Stage I**

**Modeling**

- Semi-IPN kinetic model

**Control variables**

- Initial polymer
- Monomer concentration
- Initiator concentration
- Holding temperature
- Holding duration

**Surrogate Model**
Project Review (2)

Process Stages

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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

\[
\min_{\theta} \sum_{i=1}^{NS} (y_i - y_i^m)^T \Sigma_i (y_i - y_i^m)
\]

\[
s.t. \quad y_i = f_i(x_i, \theta) \\
\quad h_i(x_i, \theta) = 0
\]

- Dynamic optimization under uncertainty

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

\[
\text{S.t.} \quad J_0(\dot{x}(0), x(0), y, u(0), \nu, \tau; \theta) = 0 \\
\quad h((x), x, y, u, \nu, t; \theta) = 0, \\
\quad g((x), x, y, u, v, t; \theta) \leq 0,
\]
Current Researches (1)

• Sequential approaches

( Faver 2003 ):

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

Computationally expensive for derivative evaluation

[Diagram]

- Upper Stage
- Middle Stage
- Lower Stage

- NLP
- Sub-NLP 1
- Simulation 1
- Sub-NLP n
- Simulation n
Current Researches (2)

- Simultaneous approach

(Zavala and Biegler 2007)

\[
\begin{bmatrix}
W_1 & A_1 & \Delta v_1 \\
W_2 & A_2 & \Delta v_2 \\
W_3 & A_3 & \Delta v_3 \\
\vdots & \vdots & \vdots \\
A_1^T & A_2^T & A_3^T & \cdots & W_{NS} & A_{NS} & \Delta v_{NS} & \Delta d
\end{bmatrix}
= 
\begin{bmatrix}
 r_1 \\
r_2 \\
r_3 \\
\vdots \\
r_{NS}
\end{bmatrix}
\]

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

where

\[
r_k^T = -[ (\nabla x_k L_k^l)^T, (c_k^l)^T, (D_k x_k^l - \bar{D}_k d_k^l)^T ] , \quad \Delta v_k^T = [ \Delta x_k^T \Delta \lambda_k^T \Delta \sigma_k^T ] , \quad A_k^T = [ 0 0 - \bar{D}_k^T ] ,
\]

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 Biegler 1991, 1992]
[Gondzio and Gothrey 2005, Gondzio and Sarkissian 2003]
A Two-Stage Algorithm

\[ \min_{\theta^L} \mu S_1 f_1(\mu S_1, \mu L(k)) \text{ s.t. } M_1 \]

\[ \min_{\theta^L} \mu S_2 f_2(\mu S_2, \mu L(k)) \text{ s.t. } M_2 \]

\[ \min_{\theta^L} \mu S_n f_n(\mu S_n, \mu L(k)) \text{ s.t. } M_n \]

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

- Efficient algorithm for better behaved large inner problem
- Robust solver for well-conditioned small outer 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
\[
\mathcal{R}\{f(x)\} = \left. \frac{\partial f(x + \epsilon v)}{\partial \epsilon} \right|_{\epsilon=0}
\]
\[
\mathcal{R}\{f'(x)\} = Hv, \quad \mathcal{R}\{x\} = v \quad \text{Apply } \mathcal{R}\{\} \text{ to Gradient equation}
\]
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 \( k_2 \) is a Linking parameter, \( k_1 \) 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 !