The Application of PMP for End-Point Optimization

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Outline

Batch Process Applications

The batch mode is used when:

- Production volumes are low
- Isolation is required
- Materials are hard to handle
- Flexible plants are desired near markets of consumption

This mode of operation is popular in the pharmaceutical and specialty chemicals industry.

Batch Operation

Batch Process Characteristics

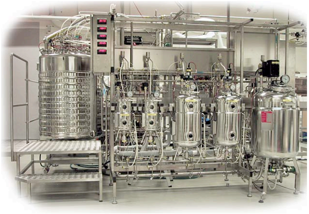
- Inherently dynamic in nature
- Nonlinear dynamics
- Several batches run in the same equipment
- Batch to batch variation in operating conditions
- Optimization objective is product quality and quantity at the batch end-point

Current Industrial Practice

- Development of batch recipe (based on chemistry)
- Open-loop implementation of recipe
- One end-point measurement for quality

Potential for Improvement

- Increased computational power at the factory shopfloor
- Real-time measurements
- Competition from the market



Traditional Optimization Approach

Procedure

- Develop accurate mathematical model
- Solve optimization problem off-line
- Implement solution in "open-loop"

Drawbacks

- Accurate models take too long to develop
- Uncertainties due to differences in lab and industrial equipment
- Model parameters not known accurately
- Open-loop solution not optimal in the presence of uncertainties

Real-Time Optimization Framework

- Utilize an approximate model
- Compute the optimal operating strategy
- Take real-time measurements
- Make periodic corrections to the optimal solution during batch operation to account for uncertainty
- Solution strategy should be simple enough that a plant operator can implement it

Process Plant Reality

I do not need your fancy-shmancy algorithm. I can control anything using my "PLD" knob.

Anonymous plant operator

Mathematical Formulation

$$\min_{u(t),t_f} \; J = \phi(x(t_f)) \qquad \textit{Objective function} \tag{1}$$

subject to

$$\dot{x} = F(x,u) \qquad \textit{System Dynamics} \tag{2}$$

$$x(0) = x_0 \qquad \textit{Initial Conditions} \tag{3}$$

$$S(x,u) \le 0 \qquad \textit{Path Constraints} \tag{4}$$

$$T(x(t_f)) \le 0 \qquad \textit{End-point Constraints} \tag{5}$$

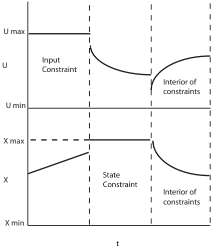
Solution Strategies

- Sequential Approach
  - Parameterize the input vector using a finite number of decision variables
  - Choose an initial guess for the decision variables
  - Integrate the system equations to the final time and compute the performance index J and the constraints S and T
  - Use an optimization algorithm to update the values of the decision variables
  - Repeat the last two steps until the objective function is minimized

- Simultaneous Approach
  - Parameterize both the input vector as well as the state vector using a finite number of decision variables
  - Discretize the dynamic equations. This results in a standard nonlinear program (NLP)
  - Choose an initial guess for the decision variables
  - Iteratively solve for the optimal set of decision variables using an NLP solver

Direct Optimization Methods

- Advantages
  - Simple to setup and code
- Disadvantages
  - Quality of solution depends strongly on the parameterization of the control profile
  - Abrupt changes in the input profile are not easily handled
  - May be slow to converge



PMP Formulation

Equivalent optimization problem:

$$\min_{u(t),t_f} H = \lambda^T F(X,u) + \mu^T S(x,u) \tag{6}$$

subject to

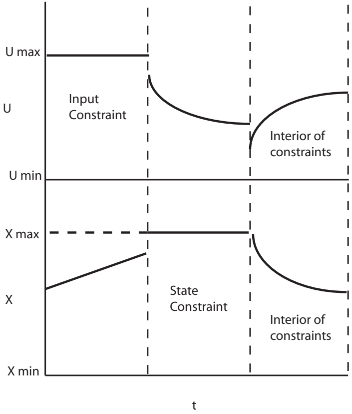
$$\begin{aligned} &\dot{x} = F(x,u) && x(0) = x_0 \\ &\dot{\lambda}^T = -\frac{\partial H}{\partial x} && \lambda^T(t_f) = \frac{\partial \phi}{\partial x}|_{t_f} + \nu^T \frac{\partial T}{\partial x}|_{t_f} \\ &\mu^T S = 0 \\ &\nu^T T = 0 \end{aligned} \tag{7}$$

PMP formulation results in a two point boundary value problem that is computationally difficult to solve

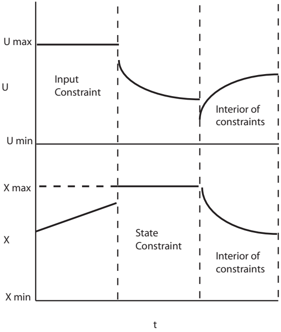
Analytical Solution Method

The solution of the dynamic optimization problem consists of several intervals:

- Solution in an input constraint
- Solution on a state constraint
- Solution in the interior of constraints



- The time instants at which inputs switch from one interval to another are called switching times
- Within each interval, the inputs are continuous and differentiable
- Analytical expressions for the optimal inputs can be computed in each interval



PMP Formulation Revisited

$$\min_{u(t),t_f} \; H(t) = \lambda^T F(x,u) + \mu^T S(x,u) \tag{8}$$

$$H_{u_i} = \lambda^T F_{u_i} + \mu^T S_{u_i} = 0 \tag{9}$$

$$\frac{d^l H_{u_i}}{dt^l} = \lambda^T \Delta^l F_{u_i} - \mu^T \frac{\partial S}{\partial x} \Delta^{l-1} F_{u_i} = 0 \tag{10}$$

where Δ is the Lie Bracket operator
Since the inputs can be (and typically are) affine, H_{u_i} and several of its time derivates are independent of u_i.

Active Path Constraint

- Let ζ_i be the first value of l for which $\lambda^T \Delta^l F_{u_i} \neq 0$
- A non-zero μ is required to satisfy:

$$\frac{d^l H_{u_i}}{dt^l} = \lambda^T \Delta^l F_{u_i} - \mu^T \frac{\partial S}{\partial x} \Delta^{l-1} F_{u_i} = 0 \tag{11}$$

- This implies that at least one of the path constraints is active
- Constraint tracking $\Longrightarrow$ regulation problem of relative degree $r_{ij} = \zeta_i$

Solution Inside the Feasible Region

- Let the order of singularity, σ_i, be the first value of l for which the input u_i appears explicitly and independently in $\lambda^T \Delta^l F_{u_i}$
- Let ρ_i be the dimension of the state space that can be reached by manipulating u_i
- The optimal input depends on $\rho_i - \sigma_i - 1 = \xi_i$ adjoint variables
- An adjoint-free expression in the feasible region can be obtained from:

$$M_i = \left[F_{u_i} \vdots \Delta^1 F_{u_i} \vdots \Delta^2 F_{u_i} \vdots \ldots \vdots \Delta^{\rho_i - 1} F_{u_i} \vdots \ldots \right] \tag{12}$$

where successive Lie brackets are found until the structural rank of M_i is ρ_i

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  - $\xi_i > 0 \Longrightarrow$ Dynamic State Feedback
  - $\xi_i = 0 \Longrightarrow$ Static State Feedback
  - $-\infty < \xi_i < 0 \Longrightarrow$ System is constrained to a surface

Parsimonious Parameterization Approach

- Choose an initial sequence of intervals
- Use analytical expressions for the inputs in each interval
- Determine numerically the optimal switching instants
- Check the necessary conditions of optimality
- If optimality conditions are not satisfied, change the sequence of intervals and go to step 2

Illustrative Example 1

$$min\ J = -XV|_{t_f} \tag{13}$$

$$\begin{aligned} \frac{d(XV)}{dt} &= \mu(S)XV \\ \frac{d(SV)}{dt} &= -\frac{\mu(S)XV}{Y} + s_F u \\ \frac{dV}{dt} &= u \end{aligned} \tag{14}$$

where

$$\mu(S) = \frac{\mu_m S}{K_1 + S} \frac{K_2}{K_2 + S}$$

and

$$V - V_{max} \leq 0 \tag{15}$$

- It can be shown that $\xi_1 = -1$ and so in the feasible region, the system is constrained to the following surface:

$$S - \sqrt{K_1 K_2} = 0 \tag{16}$$

- Start in batch mode ($u = 0$, input at the lower bound) if $S(0) > \sqrt{K_1 K_2}$
- When $S = \sqrt{K_1 K_2}$ regulate system to this surface by manipulating u till the volume is full or final time is reached

Illustrative Example 2

- **Reaction**: $A + B \rightarrow C \rightarrow D$
- **Conditions**: Non-isothermal semi-batch reactor
- **Objective**: Maximize production of C
- **Manipulated inputs**: Feed rate of B and reactor temperature
- **Constraints**: Bounds on feed rate and reactor temperature, constraint on the maximum heat that can be removed by the cooling system, constraint on the maximum volume

Solution Characteristics

- There is a compromise for the temperature between the production and consumption of C
- The feed rate of B is determined first by the heat removal constraint and then by the volume constraint
- Without any constraints, the optimal operation would consist of adding all the available B at the initial time and follow the temperature profile that expresses the compromise between the production and consumption of C.

Optimal Solution

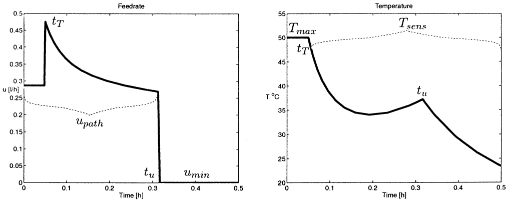


Fig. 4. Optimal feed rate and temperature profiles for Example 4.

- The optimal inputs consist of two arcs, u_{path} and u_{min} for the feed rate and T_{max} and T_{sens} for temperature
- The arc u_{path} is obtained by differentiating the path constraint regarding the heat production rate
- The arc T_{sens} is a dynamic state feedback law
- When the temperature goes inside the feasible region, there is a discontinuity in the feed rate due to the coupling between the two inputs

Presence of Uncertainty

- Model Mismatch
  - Available models often do not correspond to industrial reality
    - Neglected effects, non-ideal behavior
    - Inaccurate parameter values
- Disturbances
  - Run-to-run variations in initial conditions
  - Run-to-run variations in process environment

Reference Tracking

- Determine structure of optimal solution from nominal model
- Batch-to-batch update of switching times
- Within the batch regulation of active constraints
- Tracking sensitivities to nominal trajectories

Real-time optimization problem is reduced to a control problem

Illustrative Example 3

- **Reaction**:

$$A + B \rightarrow C \qquad \textit{rate constant } k_1$$
$$2B \rightarrow D \qquad \textit{rate constant } k_2$$

  Conditions: Semi-batch reactor (feed B), isothermal reactor
- **Objective**: Maximize production of C
- **Manipulated inputs**: Feed rate of B and jacket temperature T_c
- **Path Constraint**: Heat removal limitation ($T_c \geq T_{c,min}$)
- **Terminal Constraint**: Number of moles of D at t_f ($n_{Df} \leq n_{Df,max}$)

Uncertainty in k_1

Effect of Uncertainty

- The real value of $k_1 = 0.75$ but this is not known to the optimizer. The model can assume values of k_1 between 0.4 and 1.2
- Solution consists of the flow rate on the upper constraint, switch to a flow rate in the interior of the constraints, and then a switch to the lower constraint
- The uncertainty in k_1 modifies the values of the switching times, and the flow rate of B but not the sequence of intervals
- Case I: No measurements are used and an open-loop solution is implemented
- Case II: A measurement of D is made at the end of the batch and the switching time t_2 is adjusted in the subsequent batches
- Case III: The temperature, T_c, is measured and the switching time t_1 and the flow rate of B is adjusted to satisfy the path constraint

Results

k_1 unknown, 5% measurement noise

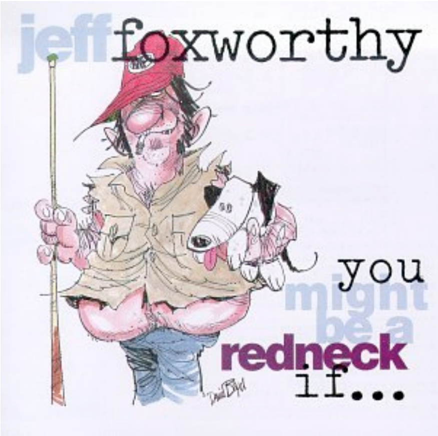
Optimization Scenario	Terminal Constraint $n_D(t_f) < 5$	Path Constraint $T_c(t) > 10$	Cost (mol of C)	Loss (%)
Case I	2.71	12.87	498.8	20
Case II	4.75	11.62	582.6	3
Case III	4.75	11.25	590.9	1.5

Conclusions

- The nominal solution to the dynamic optimization problem can be parameterized efficiently using a PMP formulation
- This solution can be utilized in a real-time optimization framework to account for uncertainty

Future Work

- Model structures for which optimal solution is always on path constraints (e.g. linear systems, feedback linearizable systems, flat systems)
- Parameter estimation for batch-to-batch update
- Stability results for finite-time processes



..... you control your process using the PLD knob.