Optimal trajectory approximation by cubic splines on fed-batch control problems

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Outline

1. Motivation for optimal control
2. Optimal control
3. Used approaches
4. Some numerical results
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A great number of valuable products are produced using fermentation processes and thus optimizing such processes is of great economic importance.

Fermentation modeling process involves, in general, highly nonlinear and complex differential equations.

Often optimizing these processes results in control optimization problems for which an analytical solution is not possible.
Motivation

- A great number of valuable products are produced using fermentation processes and thus optimizing such processes is of great economic importance.
- Fermentation modeling process involves, in general, highly nonlinear and complex differential equations.
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The optimal control problem is described by a set of differential equations \( \dot{x} = h(x, u, t) \), \( x(t^0) = x^0 \), \( t^0 \leq t \leq t^f \), where \( x \) represent the state variables and \( u \) the control variables.

The performance index \( J \) can be generally stated as

\[
J(t^f) = \varphi(x(t^f), t^f) + \int_{t^0}^{t^f} \phi(x, u, t) dt,
\]

where \( \varphi \) is the performance index of the state variables at final time \( t^f \) and \( \phi \) is the integrated performance index during the operation.

Additional constraints that often reflect some physical limitation of the system can be imposed.
The control problem

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The general maximization problem \((P)\) can be posed as

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\begin{align*}
\text{max} & \quad J(t^f) \\
\text{s.t.} & \quad \dot{x} = h(x, u, t) \\
& \quad x \leq x(t) \leq \bar{x}, \quad (3) \\
& \quad u \leq u(t) \leq \bar{u}, \quad (4) \\
& \quad \forall t \in [t^0, t^f] \quad (5)
\end{align*}
\]

Where the state constraints \((3)\) and control constraints \((4)\) are to be understood as componentwise inequalities.
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The general maximization problem \((P)\) can be posed as

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\begin{align*}
\text{max} & \quad J(t_f) \\
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(1) 

(2) 

(3) 

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How we addressed problem \((P)\)?
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Used approaches

**Approaches** - Fed trajectory $u(t)$ approximated by a Linear spline $w(t)$.

- Penalty function for state constraints
- Find potential active constraints is easy to solve

**Objective function**

$$\hat{J}(t^f) = \begin{cases} 
J(t^f) & \text{if } \underline{x} \leq x(t) \leq \overline{x}, \\
\forall t \in [t^0, t^f] & \\
-\infty & \text{otherwise}
\end{cases}$$

**State constraints**

$$u \leq w(t^i) \leq \bar{u}, \quad i = 1, \ldots, n$$

Where $t^i$ are the spline knots.

The maximization NLP problem is

$$\max_{w(t^i)} \hat{J}(t^f), \quad s.t. \ u \leq w(t^i) \leq \bar{u}, \quad i = 1, \ldots, n$$
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- A new penalty function defined for control constraints

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**New objective function**

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Implementation details

- The AMPL modeling language:
  - was used to model five optimal control problems
  - dynamic external library facility was used to solve the ordinary differentiable equations

AMPL - A Modeling Programming Language
www.ampl.com

- The ordinary differentiable equations were solved using the CVODE software package.
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- A stochastic algorithm based on particle swarm was used to solve the non-differentiable optimization problem.
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The problems set

- We obtained numerical results for five case studies.

- Problem
  - Penicillin refers to a problem of fed-batch fermentation process
    where the optimal feed trajectory is to be computed while the penicillin
    production is to be maximized.
  - Ethanol refers to a similar optimal control problem where the ethanol
    production is to be maximized.
  - Chemotherapy is the only optimal control problem that does not refer
    to a fed-batch fermentation process. It is a problem of drug
    administration in chemotherapy. The optimal trajectory to be
    computed is the quantity of drug that must be present in order to
    achieve a specified tumor reduction.
  - Lipoprotein optimal control problem is to compute a unique trajectory
    (substrate to be fed) problem. It process includes also a trajectory for
    an inducer. Both problems refer to a maximization for protein
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**Characteristics and parameters**

- The time displacement ($h_i$) are fixed while the optimal trajectory values are to be approximated.
- Particle swarm is a population based optimization algorithm and a population size of 60 was used with a maximum of 1000 iterations.
- Since a stochastic algorithm was used we performed 10 runs of the solver and the best solution is reported.
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Numerical results

<table>
<thead>
<tr>
<th>Problema</th>
<th>NT</th>
<th>n</th>
<th>(t^f)</th>
<th>Cubic (J(t^f))</th>
<th>Linear (\tilde{J}(t^f))</th>
<th>Literature (\bar{J}(t^f))</th>
</tr>
</thead>
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<tr>
<td>penicillin</td>
<td>1</td>
<td>5</td>
<td>132.00</td>
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<td>ethanol</td>
<td>1</td>
<td>5</td>
<td>61.20</td>
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<td>20839.00</td>
</tr>
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<td>chemotherapy</td>
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<td>84.00</td>
<td>15.75</td>
<td>16.83</td>
<td>14.48</td>
</tr>
<tr>
<td>hprotein</td>
<td>1</td>
<td>5</td>
<td>15.00</td>
<td>38.86</td>
<td>32.73</td>
<td>32.40</td>
</tr>
<tr>
<td>rprotein</td>
<td>2</td>
<td>5</td>
<td>10.00</td>
<td>0.13</td>
<td>0.12</td>
<td>0.16</td>
</tr>
</tbody>
</table>

\[ J(t^f) = \hat{J}(t^f) = \bar{J}(t^f), \text{ for all feasible points - splines} \]

Similar results between approaches. A new solution for the ethanol case.
Some numerical results

Plots - Linear spline approximation - ethanol case

Control profile

State profile

Vaz, Ferreira and Mota (UMinho - PT)
Some numerical results

**Plots - Cubic spline approximation - Similar result**

**Control profile**
- \( u \) - Substrate feed

**State profile**
- \( X_1 \) - Cell mass
- \( X_2 \) - Substrate
- \( X_3 \) - Product
- \( X_4 \) - Volume

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Some numerical results

Plots - Cubic spline approximation - Best result

Control profile

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Some intermediate conclusions and future work

Conclusions

Viability of the cubic spline approach on fed-batch optimal control.
Shown numerical results with particle swarm
Similar numerical results with the two approaches

Future work

Numerical experiments with the E. coli bacteria
Laboratory confirmation of the obtained results (a lab bioreactor will be available)
Laboratory confirmation of the two approaches and we expect the cubic approach to obtain a lower gap between simulated and real performance.
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Universidade do Minho

September 12-15, 2007
Guimarães – Portugal

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