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

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Outline

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1. Motivation for optimal control
2. Optimal control
3. Used approaches
4. Some numerical results

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

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The control problem

- 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 φ is the performance index of the state variables at final time t^f and ϕ is the integrated performance index during the operation.
- Additional constraints that often reflet some physical limitation of the system can be imposed.

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The control problem

The general maximization problem (P) can be posed as

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$$
\begin{aligned}
&\max \quad J(t^f) && (1)\\
&s.t. \quad \dot{x} = h(x,u,t) && (2)\\
&\qquad \underline{x} \le x(t) \le \overline{x}, && (3)\\
&\qquad \underline{u} \le u(t) \le \overline{u}, && (4)\\
&\qquad \forall t \in [t^0, t^f] && (5)
\end{aligned}
$$

Where the state constraints (3) and control constraints (4) are to be understood as componentwise inequalities.

How we addressed problem (P)?

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

- Penalty function for state constraints
- Find potencial 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

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

Where t^i are the spline knots.

The maximization NLP problem is

$$\max_{w(t^i)} \hat{J}(t^f), \quad s.t. \ \underline{u} \leq w(t^i) \leq \overline{u}, \quad i = 1, \ldots, n$$

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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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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 refers to a fed-batch fermentation processe. 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.
  - `hprotein` optimal control problem is to compute a unique trajectory (substrate to be fed) problem `rprotein` includes also a trajectory for an inducer. Both problems refer to a maximization for protein production.

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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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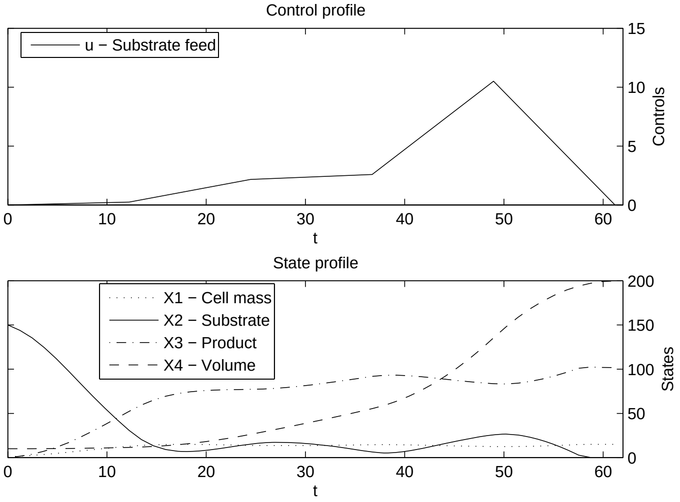
Numerical results

Problema	NT	n	t^f	Cubic $J(t^f)$	Linear $J(t^f)$	Literature $J(t^f)$
penicillin	1	5	132.00	87.70	88.29	87.99
ethanol	1	5	61.20	20550.70	20379.50	20839.00
chemotherapy	1	4	84.00	15.75	16.83	14.48
hprotein	1	5	15.00	38.86	32.73	32.40
rprotein	2	5	10.00	0.13	0.12	0.16

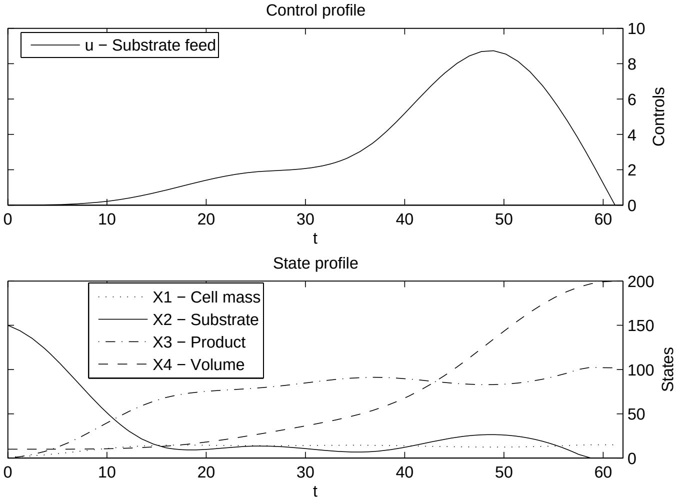
$$J(t^f) = \hat{J}(t^f) = \bar{J}(t^f), \quad \text{for all feasible points - splines}$$

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

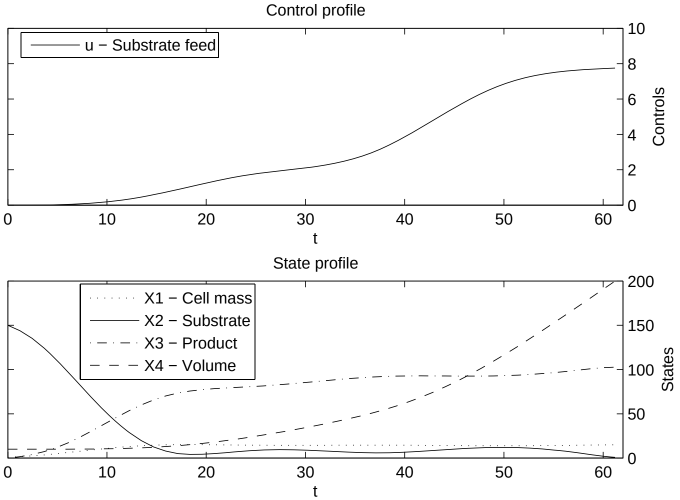
Plots - Linear spline approximation - ethanol case



Plots - Cubic spline approximation - Similar result



Plots - Cubic spline approximation - Best result



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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