TECHNICAL REPORT

DOTcvpSB: application to other benchmarks

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October 28, 2009

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CHAPTER 1

Other benchmarks

1.1 SIMPLE BATCH REACTOR

DOTcvp: cdop_SimpleBatchReactorA, B.m

The simple batch reactor given in [3] was considered with the following chemical reaction

$$A \rightarrow B \rightarrow C \tag{1.1}$$

The parameters of the reactor are: $e_1 = 18000\,\text{cal mol}^{-1}$, $e_2 = 30000\,\text{cal mol}^{-1}$, $k_{10} = 0.535\text{x}10^{11}\,\text{min}^{-1}$, $k_{20} = 0.461\text{x}10^{18}\,\text{min}^{-1}$, $r = 2\,\text{cal mol}^{-1}\,\text{K}^{-1}$, $\beta_1 = 0.53\,\text{mol l}^{-1}$, $\beta_2 = 0.43\,\text{mol l}^{-1}$, $\alpha = \frac{e_2}{e_1}$, $c = \frac{k_{20}}{k_{10}^{\alpha}}$, and final time $t_F = 8.0\,\text{min}$.

The objective of the optimization is to maximize an amount of the product B at the final time

$$\max_{u_i,t_i} J_0 = x_2(t_F) \tag{1.2}$$

subject to

$$\dot{x}_1 = -ux_1 \tag{1.3}$$

$$\dot{x}_2 = ux_1 - cu^{\alpha}x_2 \tag{1.4}$$

with the process: $x(0) = [\beta_1; \beta_2]$ and decision: $u(0) = [0.5]$ initial variables. The decision variables have defined lower and upper bounds as follows: $u \in [0.1; 2.0]$. The additional equality constraint was defined. This constraint holds the total time of simulation at the fixed value

$$\sum_{i=1}^{N} t_i = t_F \tag{1.5}$$

```
Final results [single-optimization; the scenario with the free time and with the piecewise constant control trajectory]:
 ............ Problem name: SimpleBatchReactorA
 ...... NLP or MINLP solver: FMINCON
 . Number of time intervals: 6
 ... IVP relative tolerance: 1.000000e-012
 ... IVP absolute tolerance: 1.000000e-012
 . Sens. absolute tolerance: 1.000000e-012
 ........... NLP tolerance: 1.000000e-010
 ....... Final state values: 1.704654e-001 6.794171e-001
 ...... 1th optimal control: ...
 ..... Final size of the dt: 7.469692e-001 1.247365e+000 1.420018e+000 1.495831e+000 1.534227e+000 1.555590e+000
 ..... Final time [sum(dt)]: 8.000000e+000

 ........... Final CPUtime: ... seconds
 . Cost function [max(J_0)]: 0.67941706
```

```
Final results [single-optimization; the scenario with the fixed time and with the piecewise constant control trajectory]:
 ............ Problem name: SimpleBatchReactorB
```

```
 ...... NLP or MINLP solver: FMINCON
 . Number of time intervals: 6
 ... IVP relative tolerance: 1.000000e-012
 ... IVP absolute tolerance: 1.000000e-012
 . Sens. absolute tolerance: 1.000000e-012
 ........... NLP tolerance: 1.000000e-010
 ....... Final state values: 1.704776e-001 6.794113e-001
 ...... 1th optimal control: ...
______________
 ........... Final CPUtime: ... seconds
 . Cost function [max(J_0)]: 0.67941127

______________
Final results [single-optimization; the scenario with the fixed time and with the piecewise linear control trajectory]:
 ............ Problem name: SimpleBatchReactorB
 ...... NLP or MINLP solver: FMINCON
 . Number of time intervals: 6
 ... IVP relative tolerance: 1.000000e-012
 ... IVP absolute tolerance: 1.000000e-012
 . Sens. absolute tolerance: 1.000000e-012
 ........... NLP tolerance: 1.000000e-010
 ....... Final state values: 1.704362e-001 6.794368e-001
 ...... 1th optimal control: ...
 ...... 2th optimal control: ...
______________
 ........... Final CPUtime: ... seconds
 . Cost function [max(J_0)]: 0.67943676
```

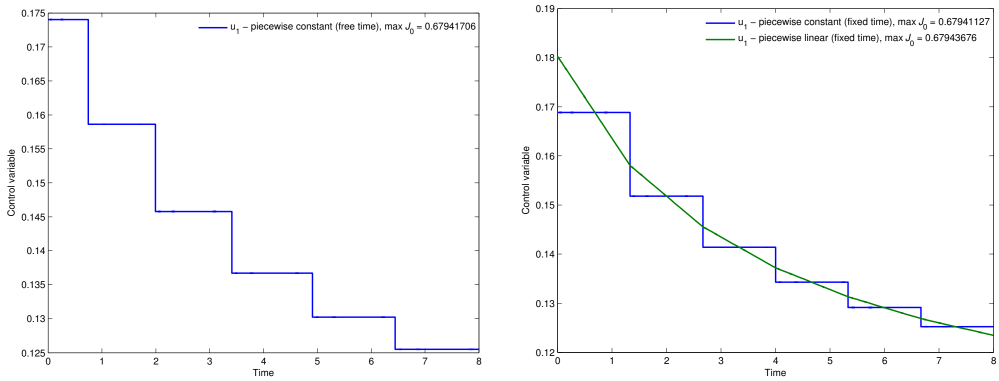

Figure 1.1 – Optimal control profile for the free time scenario (left) and the control profile with the piecewise constant and linear approximation (right) for the simple batch reactor.

1.2 VAN DER POL OSCILLATOR

DOTcvp: cdop_VanDerPolOscillator.m

The van der Pol oscillator problem is taken from [5] and has been solved by many authors [4; 2; 1]. In our case we have expanded this problem with two inequality constraints and one equality constraint. The system with the integral term of the cost function is described with the following set of differential equations with the vector of process initial conditions: $x(0) = [0; 1; 0]$ and with the initial control trajectory: $u(0) = [0.7]$

$$\dot{x}_1 = (1 - x_2^2)x_1 - x_2 + u \tag{1.6}$$

$$\dot{x}_2 = x_1 \tag{1.7}$$

$$\dot{x}_3 = x_1^2 + x_2^2 + u^2 \tag{1.8}$$

The aim of the optimization is to minimize the cost function in the fixed final time ($t_F = 5$)

$$\min_{u_i} J_0 = x_3(t_F) \tag{1.9}$$

subject to the inequality path constraints

$$-0.4 \leq x_1(t) \leq 0.0 \tag{1.10}$$

and equality constraint at the end of the optimization

$$x_2(t_F) = -0.1 \tag{1.11}$$

The control trajectory has the boundaries defined as follows: $u \in [-0.3; 1]$

```
Final results [single-optimization]:
 ............. Problem name: VanDerPolOscillator
 ...... NLP or MINLP solver: FMINCON
 . Number of time intervals: 30
 ... IVP relative tolerance: 1.000000e-007
 ... IVP absolute tolerance: 1.000000e-007
 . Sens. absolute tolerance: 1.000000e-007
 ............ NLP tolerance: 1.000000e-005
 ....... Final state values: 1.009875e-002 -1.000017e-001 2.960991e+000
 ...... 1th optimal control: ...

 ............ Final CPUtime: ... seconds
 . Cost function [min(J_0)]: 2.96099523
```

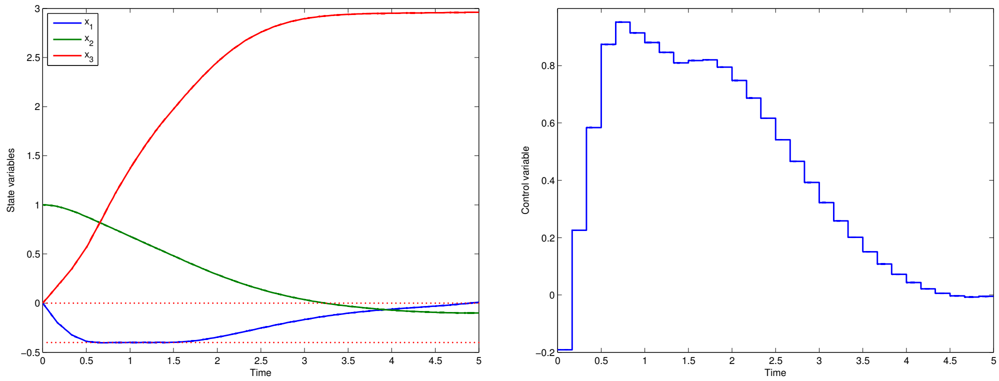

Figure 1.2 – Optimal state trajectories (left) with the upper and lower path constraint for the state variable one (dotted lines) and the control profile (right) for the van der Pol oscillator.

Bibliography

[1] E. Balsa-Canto, J. R. Banga, A. A. Alonso, and V. S. Vassiliadis. Restricted second order information for the solution of optimal control problems using control vector parameterization. *Journal of Process Control*, 12(2):243–255, 2 2002.

[2] J. R. Banga, R. Irizarry-Rivera, and W. D. Seider. Stochastic optimization for optimal and model-predictive control. *Computers and Chemical Engineering*, 22:603–612(10), 1998.

[3] S. Crescitelli and S. Nicoletti. Near optimal control of batch reactors. *Chemical Engineering Science*, 28:463–471, 1973.

[4] P. Tanartkit and L. T. Biegler. Stable decomposition for dynamic optimization. *Industrial and Engineering Chemistry Research*, 34:1253–1266, 1995.

[5] V. S. Vassiliadis. *Computational Solution of Dynamic Optimization Problems with General Differential-Algebraic Constraints*. PhD thesis, University of London, London, UK, 1993.