Programming Exercise 3

Applied Numerical Optimization

Wintersemester 2012/13

Dynamic Optimization

Introduction

In this programming exercise, you will solve a dynamic optimization problem, more precisely, an optimal control problem. Optimal control problems are a special case of the dynamic optimization problems. For solving this exercise, we introduce the following class of optimal control problems.

$$\min_{u(t)} \Phi(x(t_2)) \tag{1a}$$

$$\text{s.t. } \frac{dx}{dt}(t) = f(x(t), u(t)), \quad x(t_1) = x_0, \quad t \in [t_1, t_2] \tag{1b}$$

$$lb \leq u(t) \leq ub, \quad \forall t \in [t_1, t_2] \tag{1c}$$

The variables $x(t) \in R^{n_x}$ and $u(t) \in R^{n_u}$ are time-dependent ($n_x, n_u \in N$). The objective function $\Phi : R^{n_x} \to R$ is evaluated only at the final time t_2. The constraints are ordinary differential equations (1b) and simple lower and upper bounds $lb \in R^{n_u}$ and $ub \in R^{n_u}$ on $u(t)$. The right hand side of the ordinary differential equations (1b) is given by the function $f : R^{n_x} \times R^{n_u} \to R^{n_x}$. We distinguish between state $x(t)$ and control variables $u(t)$. The state variables $x(t)$ are uniquely determined by the differential equation, when fixing the control variables $u(t)$. Thus, the control variables $u(t)$ are the real (infinite-dimensional) degrees of freedom.

Early discretization approach

The so-called early discretization approach discretizes state and control variables, the objective function as well as the differential equations. Thus, the original optimal control problem is transformed in an ordinary nonlinear program (NLP). We use the method of orthogonal

collocation to reformulate the ordinary differential equation (1b) into a set of nonlinear equations, in order to solve the differential equations. The procedure to obtain a nonlinear program is now described in detail:

finite elements The first step is to divide the time horizon $[t_1, t_2]$ into $K \in N$ equally distributed intervals, so-called finite elements. By means of this discretization, the state and control variables are discretized with respect to the finite elements. We assume, that the control variables are constant on each finite element (i.e. we do piecewise-constant parametrization). Hence the state variables $x(t)$ are reformulated in the vector $\begin{pmatrix} x_1 \\ \vdots \\ x_K \end{pmatrix} \in R^{K \cdot n_x}$, whereas $x_k = x(t_k) \in R^{n_x}$. Similary, the control variables are reformulated into the vector $\begin{pmatrix} u_1 \\ \vdots \\ u_K \end{pmatrix} \in R^{K \cdot n_u}$. Figure 1 illustrates the discretization. Note that the state variables $x(t)$ are continuous during the overall time interval, but the controls $u(t)$ are not continuous.

solve the differential equation We use the Radau quadrature of order 5 to integrate the differential equations (1b) on each finite element. Therefore each finite element $k \in \{1, ..., K\}$ is further discretized by 3 points $g_{k,1}, g_{k,2}$ and $g_{k,3}$, the so-called collocation points (cp. Figure 1). The state variable x_{k+1} of the $k+1$st finite element is calculated by

$$x_k = x_{k-1} + \frac{t_2 - t_1}{K} \cdot \sum_{j=1}^{3} b_j \cdot f(g_{k,j}, u_k), \quad \forall k \in \{1, ..., K\} \tag{2}$$

The collocation points $g_{k,1}, g_{k,2}$ and $g_{k,3}$ are calculated by solving the following nonlinear equation system

$$g_{k,1} = x_{k-1} + \frac{t_2 - t_1}{K} \cdot \sum_{j=1}^{3} a_{1,j} f(g_{k,j}, u_k), \quad \forall k \in \{1, ..., K\} \tag{3a}$$

$$g_{k,2} = x_{k-1} + \frac{t_2 - t_1}{K} \cdot \sum_{j=1}^{3} a_{2,j} f(g_{k,j}, u_k), \quad \forall k \in \{1, ..., K\} \tag{3b}$$

$$g_{k,3} = x_{k-1} + \frac{t_2 - t_1}{K} \cdot \sum_{j=1}^{3} a_{3,j} f(g_{k,j}, u_k), \quad \forall k \in \{1, ..., K\} \tag{3c}$$

Using the Radeau quadrature, we set $a = \begin{pmatrix} \frac{88-7\sqrt{6}}{360} & \frac{296-169(\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{255} \\ \frac{296+169(\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{255} \\ \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \end{pmatrix}$ and

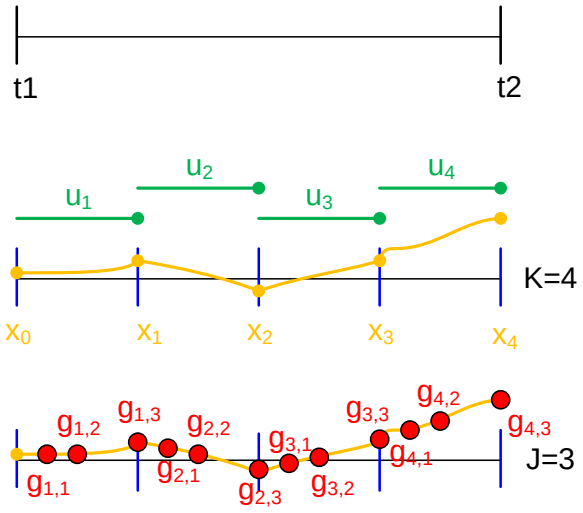

Figure 1: Discretization of the time axes into $K = 4$ finite elements.

$$b = \begin{pmatrix} \frac{16-\sqrt{6}}{36} \\ \frac{16+\sqrt{6}}{36} \\ \frac{1}{9} \end{pmatrix}.$$

nonlinear program Now, we can state the nonlinear program resulting from (1) after applying the described collocation method on finite elements.

$$\min_{u_1,\ldots,u_K,x_1,\ldots,x_K,g_{1,1},\ldots,g_{K,3}} \Phi(x_K) \tag{4a}$$

$$\text{s.t. Eqs. (2),(3)} \tag{4b}$$

$$x_0 \text{ given} \tag{4c}$$

$$lb \leq u_k \leq ub \quad \forall k \in K \tag{4d}$$

Illustrative example

Let's consider the following dynamic optimization problem:

$$\min_{u(t)} x(5)^2 \tag{5a}$$

$$\text{s.t. } \frac{dx}{dt}(t) = x(t) + u(t), \quad x(0) = 3, \quad t \in [0,5] \tag{5b}$$

$$1 \leq u(t) \leq 2, \quad \forall t \in [0,5] \tag{5c}$$

We assume $K = 2$ finite elements. The resulting NLP is

$$\min_{u_1,u_2,x_1,x_2,g_{1,1},\ldots,g_{2,3}} x_2^2 \tag{6a}$$

$$x_k = x_{k-1} + \frac{5}{2} \cdot \sum_{j=1}^{3} b_j \cdot (g_{k,j} + u_k), \quad k = 1,2 \tag{6b}$$

$$g_{k,1} = x_{k-1} + \frac{5}{2} \cdot \sum_{j=1}^{3} a_{1,j} \cdot (g_{k,j} + u_k), \quad k = 1,2 \tag{6c}$$

$$g_{k,2} = x_{k-1} + \frac{5}{2} \cdot \sum_{j=1}^{3} a_{2,j} \cdot (g_{k,j} + u_k), \quad k = 1,2 \tag{6d}$$

$$g_{k,3} = x_{k-1} + \frac{5}{2} \cdot \sum_{j=1}^{3} a_{3,j} \cdot (g_{k,j} + u_k), \quad k = 1,2 \tag{6e}$$

$$x_0 = 3 \tag{6f}$$

$$1 \leq u_k \leq 2 \qquad k = 1,2 \tag{6g}$$

The model

The model describes a catalytic reaction $A \to B \to C$. The mole fraction of species $i \in \{A, B, C\}$ with respect to time t is denoted by $x_i(t)$. The differential equations describing the system are

$$\frac{dx_A}{dt}(t) = u(t)(10x_B(t) - x_A(t)), \quad x_A(0) = 1 \tag{7a}$$

$$\frac{dx_B}{dt}(t) = -u(t)(10x_B(t) - x_A(t)) - (1 - u(t))x_B(t), \quad x_B(0) = 0 \tag{7b}$$

The goal is to maximize the mole fraction of product C, namely $x_C(1) = 1 - x_A(1) - x_B(1)$ at the final time ($t_2 = 1$).

Your task

1. Set up the nonlinear problem resulting from applying the collocation method with different $K \in \{1, ..., 5\}$ finite elements for the catalytic reaction model.

2. Solve the nonlinear optimization problem by applying the built-in function "fmincon" in Matlab. The code should be flexible with respect to the number of finite elements K. You can hard-code the model specific equations. Use the value 0.5 as initial guess for u_k and 1 for all other variables. Moreover, please apply the interior-point method (available within fmincon).

For task 2, we want to give you some **hints**:

- the optimal value of $g_{k,3}$ is equal to the optimal value of x_k. This has to do with the construction of the matrix a and vector b. (Compare vector b with the last row of matrix a). This also means, that if you set all variables to the same value, then the value of $g_{k,3}$ and x_k for $k \neq 1$ also has to be the same (maybe helpful for debugging).

- you should generate the derivatives of the equations and give these information to fmincon. (In general, this is not necessary. But in our solution it did not work without these information).

- the optimal mole fraction $x_C^* = 0.04805$. This solution was optained by a different approach, namely the so-called "late discretization approach". In our solution (early discretization approach), we obtained a value in the interval of $[0.039, 0.048]$ (i.e. less than x_C^*) depending on the size of K.

Further information

The collocation method used is a special kind of Runge-Kutta methods [1, 2]. Several optimal control problems are solved via this method , for example, in [3, 4, 5]

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