Mid-Term Exam

Dynamic Optimization

Instructor: John D. Hedengren

330L EB

801-422-2590 (office)

801-477-7341 (cell)

john_hedengren@byu.edu

Open Book, Notes, Homework, Internet

Time Limit: 8 hours (not necessarily consecutive)

Time(s) started: ____________________________________

Time(s) stopped: ___________________________________

Cumulative time:___________________________________

Name___________________________________

1. (35 pts) Orthogonal Collocation on Finite Elements

Objective: Optimize an objective function subject to two differential equations. Use orthogonal collocation on finite elements to discretize the differential equations and the condition of optimality $(x_2(t_f) = 5)$ to minimize the objective function.

Solve the following coupled differential equation from time starting at 0 until a final time of $t_f = 1$. Solve the system of equations with orthogonal collocation on finite elements with 3 nodes (time points) at $t = [0 \quad 0.5 \quad 1.0]$ for discretization points. Only one value of u can be selected for the entire time period.

$$\min_u \left(x_2(t_f) - 5\right)^2$$

$$5\frac{dx_1}{dt} = -x_1 + 2\,u^2$$

$$3\frac{dx_2}{dt} = -x_2 + x_1^2$$

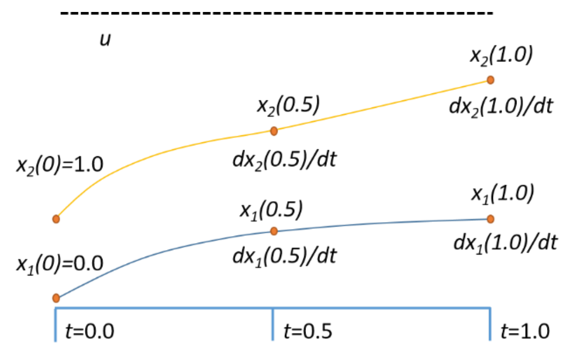

Figure 1. Collocation interval.

The initial conditions are $x_1(0) = 0.0$ and $x_2(0) = 1.0$. The following is available for approximation of the derivative values of x, where $x(t)$ is a collocation point at $t = 0, 0.5, 1.0$ (see article for additional details on orthogonal collocation):

$$\begin{bmatrix} 0.75 & -0.25 \\ 1.00 & 0.00 \end{bmatrix} \begin{bmatrix} \frac{dx(0.5)}{dt} \\ \frac{dx(1.0)}{dt} \end{bmatrix} = \begin{bmatrix} x(0.5) \\ x(1.0) \end{bmatrix} - \begin{bmatrix} x(0) \\ x(0) \end{bmatrix}$$

Differentiating the objective function with respect to $x_2(t_f)$ and setting the expression equal to zero gives the final equation $(x_2(t_f) = 5)$ necessary to satisfy the optimality conditions (Karush-Kuhn-Tucker conditions). Report the solution of u, x_1, and x_2 and derivative values ($\dot{x}_1$ and $\dot{x}_2$) at $t_1 = 0.5$ and $t_2 = 1.0$. Show the solution to the system of 9 variables and 9 equations.

$$\left(u, x_1(0.5), x_1(1.0), x_2(0.5), x_2(1.0), \frac{dx_1(0.5)}{dt}, \frac{dx_1(1.0)}{dt}, \frac{dx_2(0.5)}{dt}, \frac{dx_2(1.0)}{dt}\right)$$

Do not use GEKKO/APMonitor's built-in collocation to set up and solve the equations for this problem. It should be a set of 9 variables (unknowns) and 9 algebraic equations that can be solved with software such as fsolve (see Python or MATLAB examples) or any equation-solving tool (such as GEKKO with IMODE=1 or IMODE=3). Collocation is the process of transforming a differential equation into a set of algebraic equations. The purpose of this problem is to demonstrate your ability to set up and solve these equations independently of software that may automate the process (such as APMonitor or GEKKO with IMODE≥4).

2. (30 pts) Dynamic Optimization

Objective: Solve the following dynamic optimization problem.

Adjust the parameter *u* (acceleration) over the time horizon from a starting time of zero to a final time of one to minimize the objective function subject to the constraints. The variable *x* is the position and *v* is the velocity. The notation *x(t)* indicates the value of *x* at time *t*. The initial and final position are zero while the initial velocity is 1.0 and the final velocity is -1.0.

$$\min_{u} \quad J = \frac{1}{2}\int_0^1 u^2(t)dt$$

$$s.t. \quad \frac{dx(t)}{dt} = v(t)$$

$$\frac{dv(t)}{dt} = u(t)$$

$$x(0) = x(1) = 0$$

$$v(0) = 1$$

$$v(1) = -1$$

$$x(t) < \frac{1}{9}$$

Report the optimal objective value, display a plot of relevant variables (x, v, u), and discuss whether the constraints are satisfied. Note that this problem has both initial conditions as well as final conditions that must be satisfied. It is the integral of the objective, not just the final value of u that must be minimized by adjusting the value of u throughout the time period. Show that the solution has sufficient grid points to accurately represent the system dynamics and objective.

3. (35 pts) Parameter Regression / Machine Learning

Objective: Determine the kinetic constants ($0 \leq K_f \leq 0.01$ and $0 \leq K_b \leq 0.01$) of a reversible reaction ($A + 2B <=> C + D$) in a batch reactor. The rate equation that describes the concentration of C (C_C) is:

$$\frac{dC_C}{dt} = K_f C_A C_B^2 - K_b C_C C_D$$

Laboratory technicians have collected data for the concentrations as shown below.

Time (min): [0, 5, 10, 20, 30, 40, 50, 60, 90, 120, 150, 180, 240, 300, 360, 480, 600, 720]

C_C (mol/L) : [0.00, 0.57, 0.78, 0.92, 1.04, 1.19, 1.29, 1.36, 1.59, 1.68, 1.84, 1.96, 2.01, 2.13, 2.21, ***5.32***, 2.38, 2.44]

Although there is one outlier (5.32), do not remove or change this value. The initial concentrations of the reactants are $C_A = 4.84$ and $C_B = 9.67$. There is no C or D at the start but they start to form when the reactants are mixed together. Differential equations describe the dynamics of species concentrations for A, B, and D as shown below.

$$\frac{dC_A}{dt} = -\frac{dC_C}{dt} \qquad \frac{dC_B}{dt} = -2\frac{dC_C}{dt} \qquad \frac{dC_D}{dt} = \frac{dC_C}{dt}$$

In addition to reporting the best kinetic constants, show plots of each species concentration. Explain the objective function used to perform the parameter estimation such as whether an ℓ_1-norm or squared error objective is preferable for this problem. The default number of nodes (APM.NODES=3 in APM MATLAB or m.options.NODES=2 in GEKKO) per time step with orthogonal collocation on finite elements may need to be increased.