1. Consider the reactor optimization problem given by:

\[
\begin{align*}
\text{min} & \quad L - 500 \int_0^L (T(t) - T_S) dt \\
\text{s.t.} & \quad \frac{dq}{dt} = 0.3(1 - q(t)) \exp(20(1 - 1/T(t))), \quad q(0) = 0 \\
& \quad \frac{dT}{dt} = -1.5(T(t) - T_S) + 2/3 \frac{dq}{dt}, \quad T(0) = 1
\end{align*}
\]

where \( q(t) \) and \( T(t) \) are the normalized reactor conversion and temperature, respectively, and the decision variables are \( T_S \in [0.5, 1] \) and \( L \in [0.5, 1.25] \).

(a) Derive the direct sensitivity equations for the DAEs in this problem.

(b) Using MATLAB or a similar package, apply the sequential approach to find the optimum values for the decision variables.

(c) How would you reformulate the problem so that the path constraint \( T(t) \leq 1.45 \) can be enforced?

2. Consider the system of differential equations:

\[
\begin{align*}
\frac{dz_1}{dt} &= z_2 \\
\frac{dz_2}{dt} &= 1600 z_1 - (\pi^2 + 1600) \sin(\pi t)
\end{align*}
\]

(a) Show that the analytic solution of these differential equations are the same for the initial conditions \( z_1(0) = 0, z_2(0) = \pi \) and the boundary conditions \( z_1(0) = z_1(1) = 0 \).

(b) Find the analytic solution for the initial and boundary value problems. Comment on the dichotomy of each system.

3. Consider the following reactor optimization problem.

\[
\begin{align*}
\text{max} & \quad c_2(1) \\
\text{s.t.} & \quad \frac{dc_1}{dt} = -k_1(T)c_1^2, \quad c_1(0) = 1 \\
& \quad \frac{dc_2}{dt} = k_2(T)c_1^2 - k_3(T)c_2, \quad c_2(0) = 0
\end{align*}
\]

where \( k_1 = 4000 \exp(-2500/T), k_2 = 62000 \exp(-5000/T) \) and \( T \in [298, 398] \). Discretize the temperature profile as piecewise constants over \( N_T \) periods and perform the following.

(a) Derive the direct sensitivity equations for the DAEs in this problem.

(b) Derive the adjoint sensitivity equations for the DAEs in this problem.

(c) Solve using the sequential strategy with MATLAB or a similar package.

(d) Solve using the multiple shooting strategy with MATLAB or a similar package.
\[ \text{Solution: HW 9} \]

1. \[ \text{Min } \int \left[ L - 500 \left( T - T_s \right) \right] dt \]

s.t. \[ \begin{align*}
\dot{q}(t) &= 0.3 \left( 1 - q \right) \exp \left( 20(1 - \frac{t}{T}) \right) \\
q(0) &= 0 \\
\dot{T}(t) &= -1.5 \left( T(t) - T_s \right) + \frac{q(t)}{3T} \\
T(0) &= 1 \\
0 &\leq \left[ \begin{array}{c} 0.5 \\ 1.25 \end{array} \right], \quad T_s \leq 0.5, 1 \end{align*} \]

2. Sensitivity eqns.
   - Note that \( t \in [0, L] \) as we need to normalize length: \( t = \frac{\xi}{L}, \quad T \leq 0, 1 \)
   - This leads to:
     \[ \text{Min } \int \left[ L - 500 \cdot \tilde{q}(t) \right] dt \]
     \[ \frac{dq}{dt} = 0.3 L \left( 1 - \tilde{q} \right) \exp \left( 20 \left( 1 - \frac{t}{T} \right) \right), \quad q(0) = 0 \]
     \[ \frac{dT}{dt} = -1.5 L \left( T - T_s \right) \]
     \[ + 0.2 L \left( 1 - \tilde{q} \right) \exp \left( 20 \left( 1 - \frac{t}{T} \right) \right), \quad T(0) = 1 \]
     \[ \frac{d\tilde{q}}{dt} = L \left( T - T_s \right), \quad \tilde{q}(0) = 0 \]

Sensitivity w.r.t. \( T_s + L \)

\[ \frac{\delta T}{\delta T_s} = \left. -0.3 L \exp \left( 20 \left( 1 - \frac{t}{T} \right) \right) \right|_{T_s, L} \]
\[ + 0.3 \left( 1 - \tilde{q} \right) \exp \left( 20 \left( 1 - \frac{t}{T} \right) \right) \cdot \frac{\delta T}{\delta L} \\
+ \frac{\delta L}{\delta T} \left[ \frac{\delta T}{\delta T_s} \right] \exp \left( 20 \left( 1 - \frac{t}{T} \right) \right) \cdot \frac{\delta T}{\delta L} \]
\[ \dot{S}_{T S} = -0.3 \frac{2T_S}{\lambda_T} \exp \left( 20 \left( 1 - \frac{1}{T} \right) \right) S_{T S} + 0.2 \left( 1 - q \right) \exp \left( 20 \left( 1 - \frac{1}{T} \right) \right) S_{T S} + 0.2 \left( 1 - q \right) S_{T S} \]

\[ S_{T S} = -1.5 \left( T - T_S \right) - 1.5 \frac{S_{T S}}{T_S} \]

\[ \frac{\dot{S}_{T E}}{T_E} = -1.5 \frac{S_{T S}}{T_S} + 1.5 \left[ 0.2 \frac{S_{T E}}{T_E} \exp \left( 20 \left( 1 - \frac{1}{T} \right) \right) \right] \frac{20 \left( 1 - q \right) S_{T E}}{T_E} - \frac{q d S_{T E}}{T_E} \]

\[ S_{T E} = (T - T_S) \quad S_{T E}^{(0)} = 0. \]

b) Solution of integral problem

(closed of AMPC as a test form with profiles below.)

c) An sequential approach, it is difficult to guess brains on states. One trick is to define

\[ \dot{z} = \text{max} \left( 0, T - 1.45 \right)^2, \quad z(0) = 0 \]

and to impose \( z(1) \leq 8 \) as a final time constraint. This realistic L1/0 but is unsmooth.

Profiles for \( T(t) \leq 1.45 \) are given on next page.
# Dynamic Optimization of Hot Spot Reactor - Problem 1 in HW 9

# This file implements the dynamic optimization of a hot spot reactor.
# It uses the simultaneous approach but is meant to provide a solution
# requested for the sequential approach.

# Written by L. T. Biegler/ CMU, 4-17-2011

param nfe;
let nfe:= 100;
set I:= 1..nfe;
set J:= 1..3;

param qinit := 0.;
param tinit := 1;
param zinit := 0;

param omega(I,J);

let omega(1,1) := 0.19681547722366;
let omega(1,2) := 0.39442431473909;
let omega(1,3) := 0.37640306270047;
let omega(2,1) := -0.06553542585020;
let omega(2,2) := 0.29207341166523;
let omega(2,3) := 0.51248582618842;
let omega(3,1) := 0.02377097434822;
let omega(3,2) := -0.04154875212600;
let omega(3,3) := 0.11111111111111;

param h(i in I) := 1/nfe;

# Initial guess of the decision variables

var q(i in I, j in J) >= 0., <= 1., := 0.5;
var t(i in I, j in J) >= 0., <= 10., := 10;
var z(i in I, j in J) >= 0., <= 10., := 1;
var tt(i in I, j in J) >= 0., <= 1., := tinit;
var qdot(i, j);
var tdot(i, j);
var zdot(i, j);
var ts >= 0.05, <= 1. := 0.7;
var ll >= 0.5, <= 1.25 := 0.8;
# var ll := 0.5, <= 1.25 := 0.8;
var q0(i in I) >= 0, <= 1, := qinit;
var t0(i in I) >= 0, <= 10, := tinit;

minimize phi: 11 - 500*zf;

FECOLc(i in I, j in J):
q[i,j] = (q0[i]+h[i]*sum{k in J}
(omega[k,j]*qdot[i,k]));

FECOLt(i in I, j in J):
t[i,j] = (t0[i]+h[i]*sum{k in J}
(omega[k,j]*tdot[i,k]));

FECOLz(i in I, j in J):
z[i,j] = (z0[i]+h[i]*sum{k in J}
(omega[k,j]*zdot[i,k]));

FECOLtt(i in I, j in J):
tt[i,j] = tt0[i]+h[i]*sum{k in J}
(omega[k,j]*ll);

CONQ{i in I} diff {1}:
q0[i] = (q0[i-1] + h[i-1]*sum{j in J}
(qdot[i-1,j]*omega[j,3]));

CONt{i in I} diff {1}:
t0[i] = (t0[i-1] + h[i-1]*sum{j in J}
(tdot[i-1,j]*omega[j,3]));

CONz{i in I} diff {1}:
z0[i] = (z0[i-1] + h[i-1]*sum{j in J}
(zdot[i-1,j]*omega[j,3]));

CONTt{i in I} diff {1}:
tt0[i] = tt0[i-1] + h[i-1]*sum{j in J}
(ll*omega[j,3]);

ODEq{i in I, j in J}:
qdot[i,j] = ll*(0.3*(1-
q[i,j])/exp(20*(1-1/t[i,j])));

ODEt{i in I, j in J}:
tdot[i,j] = ll*(-1.5*(t[i,j]-ts) +
2/3*qdot[i,j]);

ODEz{i in I, j in J}:
zdot[i,j] = ll*(t[i,j]-ts);

FINq: qf = q[nfe, 3];
FINt: tf = t[nfe, 3];
FINz: zf = z[nfe, 3];
FINnt: ttf = tt[nfe, 3];

IT: t0[1] = tinit;
IZ: z0[1] = zinit;

IT: tt0[1] = 0;

add constraint

tc{i in I, j in J}: t[i, j] <= 1.45;
solve;
2. Böck problem

\[
\begin{align*}
\dot{z}_1 &= \dot{z}_2 \\
\dot{z}_2 &= 1600 z_1 - (\pi^2 + 1/600) \sin \pi t
\end{align*}
\]

a) \[z_1(0) = 0 \quad \text{has solution} \quad z_1 = \sin \pi t \]
\[z_2(0) = \pi \quad z_2 = \pi \cos \pi t \]

This is some solution on:

\[z_1(0) = 0 \]
\[z_1(1) = 0 \]

b) For initial value problem, the unstable mode is not "pinned down" and there is no dichotomy.

For boundary value problem, both stable and unstable modes are "pinned down."
3. \[ \begin{align*}
\text{min } & = x_2(1.0) \\
\text{s.t. } & \quad \begin{align*}
\dot{x}_1 & = -k_1(T)(T)x_1^2, \quad x_1(0) = 1 \\
\dot{x}_2 & = k_1(T)x_1^2 - k_2(T)x_2, \quad x_2(0) = 0 \\
k_1 & = 4000 \exp(-2500/T) \\
k_2 & = 62000 \exp(-5000/T) \\
T & \in [298, 398]
\end{align*}
\end{align*} \]

a) Sensitivity analysis wrt \( T_j \)

(1) \[ \begin{align*}
\dot{S}_{ij} & = -2k_1(T_j)x_i S_{ij}, \quad S_{ij}(0) = 0
\end{align*} \]

(2) \[ \begin{align*}
\dot{S}_{ij} & = 2k_1(T_j)x_i S_{ij} - k_2(T_j)x_i S_{ij}, \quad S_{ij}(0) = 0 \\
& \quad \text{for } t \notin [T_j-1, T_j]
\end{align*} \]

(3) \[ \begin{align*}
\dot{S}_{ij} & = -2k_1(T_j)x_i S_{ij} - \frac{\partial k_1}{\partial T_j}x_i^2, \quad S_{ij}(0) = 0
\end{align*} \]

(4) \[ \begin{align*}
\dot{S}_{ij} & = 2k_1(T_j)x_i S_{ij} - k_2(T_j)x_i S_{ij} + 2 \frac{\partial k_1}{\partial T_j}x_i^2 - \frac{\partial k_2}{\partial T_j}x_i \\
\frac{\partial k_1}{\partial T_j} & = 1.6 \exp(-2500/T) \\
\frac{\partial k_2}{\partial T_j} & = 12.4 \exp(-5000/T)
\end{align*} \]

\[ \frac{dT_i}{dT_j} = -S_{2ij}(1) \]
b) Adjoint sensitivity

\[ J^T = \lambda_1 (-k_1(T)c_1^2) + \lambda_2 (k_2(T)c_1^2 - k_2(T)c_2^2) \]

\[ \dot{\lambda}_1 = 2k_1(T)c_1(\lambda_1 - \lambda_2), \quad \lambda_1(1) = 0 \]

\[ \dot{\lambda}_2 = k_2(T), \quad \lambda_2(1) = -1 \]

\[ \frac{dC_2}{dT} = \int_{T_i}^{T_{i+1}} \left( \frac{\partial^2 C_2}{\partial T^2} - \frac{\partial C_2}{\partial T} \right) \frac{dk_1}{\partial T} \frac{dC_1}{\partial T} dt \]

\[ \frac{dC_1}{dT} = \frac{1}{T_c} \left[ \frac{\partial C_1}{\partial t} \right] \]

\[ c) \text{ Solution w/ sequential approach.} \]

Solve \( \text{Min} = C_2(1) \)

s.t. \( 298 \leq T_j \leq 398 \)

with \( c_1(T), c_2(T) \) and \( \frac{\partial C_2}{\partial T} \)

evaluated from part a) or b).

The solution is on next page.

d) Solution with multiple shooting

Solve \( \text{Min} = C_2(1) \)

s.t. \( 298 \leq T_j \leq 398 \)

\[ c_{ij}(t_j) = \frac{1}{T_c} \left[ \frac{\partial C_1}{\partial t} \right] = 0 \]

\[ C_{2j}(t_j) = C_{2j+1} = 0 \]

\[ j = 1, \ldots, NT-1 \]

where \( C_{2j} \) are also initial conditions for each segment of
Solution Profiles: Nonisothermal Batch Reactor (Max c2(1))

Optimal Temperature Profile

Optimal Concentration Profiles

# Dynamic Optimization of Hot Spot Reactor - Problem 1 in HW 9

# This file implements the dynamic optimization of a nonisothermal

# batch reactor. It uses the simultaneous approach but is meant to
# provide a solution requested for the sequential or multiple shooting
# approach.
param nfe;
let nfe:= 20;
set I:= 1..nfe;
set J:= 1..3;

param c1init := 1.
param c2init := 0.

param omega{J,J};

let omega[1,1] := 0.19681547722366;
let omega[1,2] := 0.39442431473909;
let omega[1,3] := 0.37640306270047;
let omega[2,1] := -0.06553542585020;
let omega[2,2] := 0.29207341166523;
let omega[2,3] := 0.51248582618842;
let omega[3,1] := 0.02377097434822;
let omega[3,2] := -0.04154875212600;
let omega[3,3] := 0.11111111111111;

param h{i in I} := 1/nfe;

# Initial guess of the decision variables
var c1{i in I, j in J} >= 0., <= 1., := 0.5;
var c2{i in I, j in J} >= 0., <= 1., := 0.5;
var t{i in I, j in J} >= 298., <= 398., := 350;
var tt{i in I, j in J} >= 0.;
var c1dot{I,J};
var c2dot{I,J};

var c10{i in I} >= 0., <= 1., := 0.5;
var c20{i in I} >= 0., <= 1., := 0.5;
var tt0{i in I} >= 0;
var clf := 0., <= 1., := 0.5;
var c2f := 0., <= 1., := 0.5;
var ttf := 0;

minimize phi: -c2f;

FECOL1{i in I, j in J}:
c1[i,j] = (c10[i]+h[i]*sum{k in J}(omega[k,j]*c1dot[i,k]));

FECOL2{i in I, j in J}:
c2[i,j] = (c20[i]+h[i]*sum{k in J}(omega[k,j]*c2dot[i,k]));

FECOLtt{i in I, j in J}:
tt[i,j] = tt0[i]+h[i]*sum{k in J}(omega[k,j]);

CONC1{i in I} diff {1}:
c10[i] = (c10[i-1]+h[i-1]*sum{j in J}(c1dot[i-1,j] * omega[j,3]));

CONC2{i in I} diff {1}:
c20[i] = (c20[i-1]+h[i-1]*sum{j in J}(c2dot[i-1,j]*omega[j,3]));

CONtt{i in I} diff {1}:
tt0[i] = tt0[i-1]+h[i-1]*sum{j in J}(omega[j,3]);

ODE1{i in I, j in J}:
c1dot[i,j] = -4000*exp(-2500/t[i,j])*c1[i,j]*c1[i,j];

ODE2{i in I, j in J}:
c2dot[i,j] = 4000*exp(-2500/t[i,j])*c1[i,j]*c1[i,j] - 62000*exp(-5000/t[i,j])*c2[i,j];

FINc1: clf = c1[nfe, 3];
FINc2: c2f = c2[nfe, 3];
FINtt: ttf = tt[nfe, 3];

IC1: c10[1] = c1init;
IC2: c20[1] = c2init;
ITT: tt0[1] = 0;

option solver Ipopt;
solve;
the state equations:

\[ \dot{c}_{\bar{j}} = -k_1(T_j) c_{\bar{j}}^2, \quad c_{\bar{j}}(t_{j-1}) = c_{\bar{j}} \]

\[ \dot{c}_{\bar{2}j} = k_2(T_j) c_{\bar{2}j}^2 - k_1(T_j) c_{\bar{j}} \quad c_{\bar{2}j}(t_j) = \bar{c}_{\bar{2}j} \]

Sensitivity equations for each segment are:
the same as (3)-(4) for \( T_j \), but not (1)-(2). The initial condition sensitivities are given by:

\[ \bar{S}_{\bar{j}} = -2k_1(T_j) \bar{S}_{\bar{j}} \quad \bar{S}_{\bar{j}}(t_{j-1}) = 1 \]

\[ \bar{S}_{\bar{2}j} = 2k_1(T_j) \bar{S}_{\bar{j}} - k_2(T_j) \bar{S}_{\bar{2}j} \quad \bar{S}_{\bar{2}j}(t_j) = \bar{S}_{\bar{2}j} \]

for \( t \in [t_{j-1}, t_j] \), \( j = 2, \ldots, N \)

The solution profiles are on the next page.