A Brief GAMS Tutorial for Dynamic Optimization

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Dynamic Optimization Problem

$$\min_{\psi} \left( z(t), y(t), u(t), p, t_f \right)$$

s.t. \[ \frac{dz(t)}{dt} = F(z(t), y(t), u(t), t, p) \]
\[ G(z(t), y(t), u(t), t, p) = 0 \]
\[ z^0 = z(0) \]
\[ z^l \leq z(t) \leq z^u \]
\[ y^l \leq y(t) \leq y^u \]
\[ u^l \leq u(t) \leq u^u \]
\[ p^l \leq p \leq p^u \]

\( t, \) time
\( z, \) differential variables
\( y, \) algebraic variables
\( t_f, \) final time
\( u, \) control variables
\( p, \) time independent parameters
DAE Models in Engineering

Differential Equations
• Conservation Laws (Mass, Energy, Momentum)

Algebraic Equations
• Constitutive Equations, Equilibrium (physical properties, hydraulics, rate laws)

Characteristics
• Large-scale models – not easily scaled
• Sparse but no regular structure
• Direct solvers widely used
• Coarse-grained decomposition of linear algebra
Nonlinear Programming Formulation

Nonlinear Dynamic Optimization Problem

Collocation on finite Elements

Continuous variables

Discretized variables

Nonlinear Programming Problem (NLP)
Collocation on Finite Elements

True solution

Polynomials

Collocation points

Mesh points

$t_0, t_1, \ldots, t_f$

Finite element, $i$

Element $i$

$z(t) = \sum_{j=0}^{NCOL} \ell_j(t) z_{ij}$

$\ell_j(t) = \prod_{l=0, l \neq j}^{NCOL} \frac{T - T_j}{T_l - T_j}$

$y(t) = \sum_{j=1}^{NCOL} \bar{\ell}_j(t) y_{ij}$

$u(t) = \sum_{j=1}^{NCOL} \bar{\ell}_j(t) u_{ij}$

Differential variables
Continuous

Algebraic and Control variables
Discontinuous

$t_{ij} = \sum_{i'=1}^{i-1} \alpha_{i'} + \alpha_{i} t_{j}, t \in [0,1]$
Nonlinear Programming Problem

\[
\min \psi(z_{i,j}, y_{i,j}, u_{i,j}, p, t_f)
\]

s.t. \[\sum_{k=0}^{NCOL} \ell_k (r_j) z_{ik} = \alpha_i F(z_{ij}, y_{ij}, u_{ij}, p)\]

\[G(z_{i,j}, y_{i,j}, u_{i,j}, p) = 0\]

\[z_{i+1,0} = \sum_{j=0}^{NCOL} \ell_j (1) z_{ij}\]

\[z^o_1 = z(0), z_f = z^0_{i+1}\]

\[z_i^l \leq z_{i,j} \leq z_i^u\]

\[y_{i,j}^l \leq y_{i,j} \leq y_{i,j}^u\]

\[u_{i,j}^l \leq u_{i,j} \leq u_{i,j}^u\]

\[p^l \leq p \leq p^u\]

\[i = 1, \ldots NFE; \; j = 1, \ldots NCOL\]

\[
\min f(x) \\
\quad \text{s.t.} \quad c(x) = 0
\]

\[x^L \leq x \leq x^u\]
Dynamic Optimization: Methods of Solution

- **GAMS** – requires complex set notation and conditional statements, general formulation with all collocation equations
- **AMPL** – similar to GAMS, more elegant set notation and conditional statements, general formulation with all collocation equations
- **DynoPC** – requires only statement of model, data-driven program in Windows, uses IPOPT and ADOL-C
Example: Hicks Reactor Problem

Consider the liquid-phase stirred tank reactor shown in Figure 1. We assume constant liquid volume ($V$), flow ($F$), density ($\rho$), heat capacity ($C_p$), coolant temperature ($T_c$), coolant flow ($F_c$) and heat of reaction ($\Delta H$), as well as a first order Arrhenius rate law. Following the notation in the figure, the mass and energy balance for the reactor are given by:
Example: Hicks Reactor Problem

\[
\frac{dc}{dt} = F \left( c_f - c(t) \right) - V k_{10} \exp \left( -E/RT \right) c(t), \quad c(0) = c_{\text{init}} \quad (1)
\]

\[
\rho C_p \frac{dT}{dt} = F \rho C_p (T_f - T(t)) + \Delta H \nu k_{10} \exp \left( -E/RT \right) c(t) + U (F_c) A_c (T_c - T), \quad T(0) = T_{\text{init}} \quad (2)
\]

We define aggregated parameters \( \theta = V / F \), \( \alpha = UA_c / (\rho C_p V) \), \( \nu_f = \rho C_p T_f / \Delta H \), \( n = E \rho C_p / (R \Delta H) \), \( \gamma_c = \rho C_p T_c / \Delta H \), and redefine the states: \( c \leftarrow c / c_f \), \( T \leftarrow \rho C_p T / \Delta H \) in order to obtain:

\[
\frac{dc}{dt} = (1 - c(t)) / \theta - k_{10} \exp \left( -n / T \right) c(t), \quad c(0) = c_{\text{init}} \quad (3)
\]

\[
\frac{dT}{dt} = (\nu_f - T(t)) / \theta - k_{10} \exp \left( -n / T \right) c(t) + \alpha u (\gamma_c - T), \quad T(0) = T_{\text{init}} \quad (4)
\]

The parameters are given values in the GAMS file below and the optimal control problem is given by:

\[
\text{Min} \quad \int_0^{t_f} \alpha_1 (\bar{c} - c(t))^2 + \alpha_2 (\bar{T} - T(t))^2 + \alpha_3 (\bar{u} - u(t))^2 \, dt \quad (5)
\]

\[
\text{s.t.} \quad (3) - (4) \quad (6)
\]

where \( \bar{c}, \bar{T}, \bar{u} \) are the desired values of the states and input and \( \alpha_j \) are the desired weights.
Introduction and define Sets

* Title Dynamic Optimization of a Non-Isothermal CSTR

* OFFUPPER
* OFFSYMREF OFFSYMLIST

* option sysout = off;
* OPTION SOLPRINT = OFF;

* This file implements the dynamic optimization of non-isothermal
  CSTR as proposed by Hicks and Ray and later modified to feature
  multiple steady-state behaviour. Full discretization of the model
  and input, output variables renders the problem as a NLP.

* More detail on the model can be found in

* Flores Tlacuahuac, A., S. Terrazas Moreno, and L. T. Biegler,
  *‘On Global Optimization of Highly Nonlinear Dynamic Systems,’*
  *Industrial and Engineering Chemistry Research, 47, 8, pp 2643 – 2655*
  *(2008)*

Sets

i number of finite elements /1*100/

j number of internal collocation points /1*3/;
Alias (j,k);

Scalar cinit initial concentration /0.1367/
tinit initial temperature /0.7293/
tunit initial cooling water /390/
ctdes initial concentration /0.0944/
tedes final temperature /0.7766/
udes final cooling water flowrate /340/
alpha dimensionless parameter /1.95e-04/
alpha1 dimensionless parameter /1e+06/
alpha2 dimensionless parameter /2e+03/
alpha3 dimensionless parameter /1e-03/
k10 rate constant /300/
n /5/
cf /7.6/
tf /300/
tc /290/
theta /20/
yf /0.3947/
cy /0.3816/
time /10/
point /0/
nfe /100/
cp /3/
slopec
slopet
slopecu,
ii,
jj,
point;
Define parameters for collocation

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<th>1</th>
<th>2</th>
<th>3</th>
</tr>
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<td>0.39442431473909</td>
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<tr>
<td>2</td>
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<td>3</td>
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<td>-0.04154875212600</td>
<td>0.1111111111111111</td>
</tr>
</tbody>
</table>

Parameter

\[
\begin{align*}
\text{cguess}(i,j) \\
\text{tguess}(i,j) \\
\text{ttguess}(i,j) \\
\text{uguess}(i,j) \\
h(i)
\end{align*}
\]

* Initial guess of the decision variables

\[
\text{point} = 0; \\
\text{slopec} = (\text{cdes-cinit})/(\text{nfe*ncp}); \\
\text{slopet} = (\text{tdes-tinit})/(\text{nfe*ncp}); \\
\text{slopeu} = (\text{udes-uinit})/(\text{nfe*ncp});
\]

for (ii = 1 to nfe,
     for (jj = 1 to ncp,
     \hspace{-1cm} \text{point} = \text{point}+1;
     \hspace{-1cm} \text{cguess}(i,j) = \text{slopec*point+cinit} ;
     \hspace{-1cm} \text{tguess}(i,j) = \text{slopet*point+tinit} ;
     \hspace{-1cm} \text{ttguess}(i,j) = \text{time*point} ;
     \hspace{-1cm} \text{uguess}(i,j) = \text{slopeu*point+uinit} ;
     \hspace{-1cm});
\hspace{-1cm})
\hspace{-1cm});
\hspace{-1cm}h(i) = 1/\text{nfe} ;
Define Variables and Equations

Variables

\[ c(i,j) \] concentration
\[ t(i,j) \] temperature
\[ tt(i,j) \] time
\[ u(i,j) \] cooling water flowrate
\[ cdot(i,j) \]
\[ tdot(i,j) \]
\[ c0(i) \]
\[ t0(i) \]
\[ tt0(i) \]
\[ u0(i) \]
\[ \phi i \] objective function

Equations

foj

criterion definition

IT, IC, ITT
FECOLc(i,j)
FECOLT(i,j)
FECOLtt(i,j)
CONc(i)
CONt(i)
CONtt(i)
ODEc(i,j)
ODEt(i,j);
Collocation Model

\[ \text{fobj..} \]
\[ \phi = e = \text{sum}((i,j), \ h(i) \cdot a(j, '3') \cdot (\alpha_1 \cdot (\text{sqr}(\text{cdes} - c(i,j))) + \alpha_2 \cdot \text{sqr}(\text{tdes} - t(i,j))) + \alpha_3 \cdot \text{sqr}(\text{udes} - u(i,j)))) ; \]

\[ \text{FECOLc}(i,j) \text{if}(\text{ord}(i) \leq \text{nfe}).. \ c(i,j) = e = c_0(i) + \text{time} \cdot h(i) \cdot \text{sum}(k,a(k,j) \cdot cdot(i,k)) ; \]

\[ \text{FECOLt}(i,j) \text{if}(\text{ord}(i) \leq \text{nfe}).. \ t(i,j) = e = t_0(i) + \text{time} \cdot h(i) \cdot \text{sum}(k,a(k,j) \cdot tdot(i,k)) ; \]

\[ \text{FECOLtt}(i,j) \text{if}(\text{ord}(i) \leq \text{nfe}).. \ tt(i,j) = e = tt_0(i) + \text{time} \cdot h(i) \cdot \text{sum}(k,a(k,j)) ; \]

\[ \text{CONc}(i) \text{if}(\text{ord}(i) > 1 \text{ and ord}(i) \leq \text{nfe}).. \ c_0(i) = e = c_0(i-1) + \text{time} \cdot h(i-1) \cdot \text{sum}(j, \ cdot(i-1,j) \cdot a(j, '3')) ; \]

\[ \text{CONT}(i) \text{if}(\text{ord}(i) > 1 \text{ and ord}(i) \leq \text{nfe}).. \ t_0(i) = e = t_0(i-1) + \text{time} \cdot h(i-1) \cdot \text{sum}(j, \ tdot(i-1,j) \cdot a(j, '3')) ; \]

\[ \text{CONtt}(i) \text{if}(\text{ord}(i) > 1 \text{ and ord}(i) \leq \text{nfe}).. \ tt_0(i) = e = tt_0(i-1) + \text{time} \cdot h(i-1) \cdot \text{sum}(j, \ a(j, '3')) ; \]

\[ \text{ODEc}(i,j) \text{if}(\text{ord}(i) \leq \text{nfe}).. \ cdot(i,j) = e = (1-c(i,j)) / \text{theta} - k_{10} \cdot \text{exp}(-n / t(i,j)) \cdot c(i,j) ; \]

\[ \text{ODEt}(i,j) \text{if}(\text{ord}(i) \leq \text{nfe}).. \ tdot(i,j) = e = (y - t(i,j)) / \text{theta} + k_{10} \cdot \text{exp}(-n / t(i,j)) \cdot c(i,j) - \alpha_1 \cdot u(i,j) \cdot (t(i,j) - y_c) ; \]

IC.. c(0, '1') = e = \text{cinit}.
IT.. t0('1') = e = \text{tinit};
ITT.. tt0('1') = e = 0;
Initialization and Solution

Model hicks /all/;

c.lo(i,j) = 0; c.up(i,j) = 1;
t.lo(i,j) = 0.1; t.up(i,j) = 1;
u.lo(i,j) = 0; u.up(i,j) = 500;
c0.lo(i) = 0; c0.up(i) = cinit;
t0.lo(i) = 0.1; t0.up(i) = 1;
c.l(i,j) = cguess(i,j);
t.l(i,j) = tguess(i,j);
tt.l(i,j) = ttguess(i,j);
u.l(i,j) = uguess(i,j);
c0.l(i) = cinit;
t0.l(i) = tinit;
u0.l(i) = uinit;
cdot.l(i,j) = 1;
tdot.l(i,j) = 1;

option nlp = coinipopt;
* option nlp = baron;
* option nlp = conopt;
* option nlp = minos;
*hicks.optfile = 1;

Solve hicks minimizing phi using nlp;

display tt0.l, c0.l, t0.l;
* option nlp = conopt;
* Solve hicks minimizing phi using nlp;