Dynamic Optimization and NLP Structure of a CSTR Reactor

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1. NLP Problem Structure.

Consider the NLP problem from the Hicks-Ray reactor dynamic optimization problem,

$$\begin{aligned}
\min \quad & \sum_{i=1}^{n_f}\sum_{j=1}^{n_c}\varphi_{i,j} = \sum_{i=1}^{n_f}\sum_{j=1}^{n_c} h_i W_j \left[w_{z_c}(z_{c_{i,j}} - z_c^{des})^2 + w_{z_t}(z_{t_{i,j}} - z_t^{des})^2 + w_u(u_{i,j} - u^{des})^2 \right] \\
\text{s.t.} &
\end{aligned}$$

$$\begin{aligned}
g_{i,j}^c(\cdot) &= y_{c_{i,j}} + \frac{z_{c_{i,j}} - 1}{\theta} + k \cdot z_{c_{i,j}} \exp\left[\frac{-E_a}{z_{t_{i,j}}}\right] = 0 \\
g_{i,j}^t(\cdot) &= y_{t_{i,j}} + \frac{z_{t_{i,j}} - z_f}{\theta} - k \cdot z_{c_{i,j}} \exp\left[\frac{-E_a}{z_{t_{i,j}}}\right] + \alpha \cdot u_{i,j}(z_{t_{i,j}} - t_{cw}) = 0 \\
f_{i,j}^c(\cdot) &= z_{c_{i,j}} - z_{c_i}^0 - h_i \sum_{k=1}^{n_c} \mathbf{\Omega}_{k,j} y_{c_{i,k}} = 0 \\
f_{i,j}^t(\cdot) &= z_{t_{i,j}} - z_{t_i}^0 - h_i \sum_{k=1}^{n_c} \mathbf{\Omega}_{k,j} y_{t_{i,k}} = 0 \\
c_i^c(\cdot) &= z_{c_i}^0 - z_{c_{i-1,n_c}} = 0 \\
c_i^t(\cdot) &= z_{t_i}^0 - z_{t_{i-1,n_c}} = 0 \\
c_1^c(\cdot) &= z_{c_1}^0 - \hat{z}_c(\ell) = 0 \\
c_1^t(\cdot) &= z_{t_1}^0 - \hat{z}_t(\ell) = 0 \\
u_{i,j} &\geq 0. \qquad (1)
\end{aligned}$$

define the variable vector $x_i = [z_{c_i}^0 \; z_{t_i}^0 \; y_{c_{i,1}} \; \ldots \; y_{c_{i,n_c}} \; y_{t_{i,1}} \; \ldots \; y_{t_{i,n_c}} \; u_{i,1} \; z_{c_{i,1}} \; z_{t_{i,1}} \ldots \; u_{i,n_c} \; z_{c_{i,n_c}} \; z_{t_{i,n_c}}]$ and the multipliers, $\lambda_i = [\lambda_{c_i}^c \; \lambda_{t_i}^c \; \lambda_{c_{i,1}}^g \; \lambda_{t_{i,1}}^g \ldots \lambda_{c_{i,n_c}}^g \; \lambda_{t_{i,n_c}}^g \; \lambda_{c_{i,1}}^f \ldots \lambda_{c_{i,n_c}}^f \; \lambda_{t_{i,1}}^f \ldots \; \lambda_{t_{i,n_c}}^f]$ for every finite element i. Symbols $\hat{z}_c(\ell)$ and $\hat{z}_t(\ell)$ denote the initial conditions.

The associated Lagrange function of this problem is given by,

$$\mathcal{L} = \sum_{i=1}^{n_f}\sum_{j=1}^{n_c}\left[\varphi_{i,j} + \lambda_{c_{i,j}}^g g_{i,j}^c + \lambda_{t_{i,j}}^g g_{i,j}^t + \lambda_{c_{i,j}}^f f_{i,j}^c + \lambda_{t_{i,j}}^f f_{i,j}^t\right] + \sum_{i=1}^{n_f}\left[\lambda_{c_i}^c c_i^c + \lambda_{t_i}^c c_i^t\right] - \sum_{i=1}^{n_f}\sum_{j=1}^{n_c} \nu_{u_{i,j}} u_{i,j} \qquad (2)$$

The constraint Jacobian defined at finite element i for 3-point collocation has the following structure,

$$
\begin{array}{c|ccccccccccccccccccc}
 & z_{c_{i-1,3}} & z_{t_{i-1,3}} & z^0_{c_i} & z^0_{t_i} & y_{c_1} & y_{c_2} & y_{c_3} & y_{t_1} & y_{t_2} & y_{t_3} & u_1 & z_{c_1} & z_{t_1} & u_2 & z_{c_2} & z_{t_2} & u_3 & z_{c_3} & z_{t_3} \\
\hline
c^c_i & -1 & & 1 & & & & & & & & & & & & & & & & \\
c^t_i & & -1 & & 1 & & & & & & & & & & & & & & & \\
g^c_1 & & & & & 1 & & & & & & g^c_{u,1} & g^c_{z,1} & g^c_{t,1} & & & & & & \\
g^t_1 & & & & & & & & 1 & & & g^t_{u,1} & g^t_{z,1} & g^t_{t,1} & & & & & & \\
g^c_2 & & & & & & 1 & & & & & & & & g^c_{u,2} & g^c_{z,2} & g^c_{t,2} & & & \\
g^t_2 & & & & & & & & & 1 & & & & & g^t_{u,2} & g^t_{z,2} & g^t_{t,2} & & & \\
g^c_3 & & & & & & & 1 & & & & & & & & & & g^c_{u,3} & g^c_{z,3} & g^c_{t,3} \\
g^t_3 & & & & & & & & & & 1 & & & & & & & g^t_{u,3} & g^t_{z,3} & g^t_{t,3} \\
f^c_1 & & & -1 & & \Omega_{11} & \Omega_{21} & \Omega_{31} & & & & & 1 & & & & & & & \\
f^c_2 & & & -1 & & \Omega_{12} & \Omega_{22} & \Omega_{32} & & & & & & & & 1 & & & & \\
f^c_3 & & & -1 & & \Omega_{13} & \Omega_{23} & \Omega_{33} & & & & & & & & & & & 1 & \\
f^t_1 & & & & -1 & & & & \Omega_{11} & \Omega_{21} & \Omega_{31} & & & 1 & & & & & & \\
f^t_2 & & & & -1 & & & & \Omega_{12} & \Omega_{22} & \Omega_{32} & & & & & & 1 & & & \\
f^t_3 & & & & -1 & & & & \Omega_{13} & \Omega_{23} & \Omega_{33} & & & & & & & & & 1 \\
\hline
h^c_{i+1} & & & & & & & & & & & & & & & & & & -1 & \\
h^t_{i+1} & & & & & & & & & & & & & & & & & & & -1
\end{array}
\tag{3}
$$

where,

$$
\begin{aligned}
g^c_{c_{i,j}} &= \frac{\partial g^c_{i,j}}{\partial z_{c_{i,j}}} = \theta^{-1} + k \cdot \exp\left[\frac{-E_a}{z_{t_{i,j}}}\right] \\
g^c_{t_{i,j}} &= \frac{\partial g^c_{i,j}}{\partial z_{t_{i,j}}} = -\frac{k \cdot z_{c_{i,j}} E_a}{{z_{t_{i,j}}}^2} \exp\left[\frac{-E_a}{z_{t_{i,j}}}\right] \\
g^c_{u_{i,j}} &= \frac{\partial g^c_{i,j}}{\partial u_{i,j}} = 0 \\
g^t_{c_{i,j}} &= \frac{\partial g^t_{i,j}}{\partial z_{c_{i,j}}} = -k \cdot \exp\left[\frac{-E_a}{z_{t_{i,j}}}\right] \\
g^t_{t_{i,j}} &= \frac{\partial g^t_{i,j}}{\partial z_{t_{i,j}}} = \theta^{-1} + \frac{k \cdot z_{c_{i,j}} E_a}{{z_{t_{i,j}}}^2} \exp\left[\frac{-E_a}{z_{t_{i,j}}}\right] + u_{i,j} \\
g^t_{u_{i,j}} &= \frac{\partial g^t_{i,j}}{\partial u_{i,j}} = z_{t_{i,j}} - t_{cw}
\end{aligned}
\tag{4}
$$

notice that the first two columns in the Jacobian are not defined for $i = 1$.

For a Bolza-type objective function, the Hessian of the Lagrangian is block diagonal. For a given element i,

$$
\begin{array}{c|ccccccccccccccccc}
 & z^0_{c_i} & z^0_{t_i} & y_{c_1} & y_{c_2} & y_{c_3} & y_{t_1} & y_{t_2} & y_{t_3} & u_1 & z_{c_1} & z_{t_1} & u_2 & z_{c_2} & z_{t_2} & u_3 & z_{c_3} & z_{t_3} \\
\hline
z^0_{c_i} & & & & & & & & & & & & & & & & & \\
z^0_{t_i} & & & & & & & & & & & & & & & & & \\
y_{c_1} & & & & & & & & & & & & & & & & & \\
y_{c_2} & & & & & & & & & & & & & & & & & \\
y_{c_3} & & & & & & & & & & & & & & & & & \\
y_{t_1} & & & & & & & & & & & & & & & & & \\
y_{t_2} & & & & & & & & & & & & & & & & & \\
y_{t_3} & & & & & & & & & & & & & & & & & \\
u_1 & & & & & & & & & \mathcal{L}^1_{uu} & \mathcal{L}^1_{uc} & \mathcal{L}^1_{ut} & & & & & & \\
z_{c_1} & & & & & & & & & \mathcal{L}^1_{uc} & \mathcal{L}^1_{cc} & \mathcal{L}^1_{ct} & & & & & & \\
z_{t_1} & & & & & & & & & \mathcal{L}^1_{ut} & \mathcal{L}^1_{ct} & \mathcal{L}^1_{tt} & & & & & & \\
u_2 & & & & & & & & & & & & \mathcal{L}^2_{uu} & \mathcal{L}^2_{uc} & \mathcal{L}^2_{ut} & & & \\
z_{c_2} & & & & & & & & & & & & \mathcal{L}^2_{uc} & \mathcal{L}^2_{cc} & \mathcal{L}^2_{ct} & & & \\
z_{t_2} & & & & & & & & & & & & \mathcal{L}^2_{uc} & \mathcal{L}^2_{ct} & \mathcal{L}^2_{tt} & & & \\
u_3 & & & & & & & & & & & & & & & \mathcal{L}^3_{uu} & \mathcal{L}^3_{uc} & \mathcal{L}^3_{ut} \\
z_{c_3} & & & & & & & & & & & & & & & \mathcal{L}^3_{uc} & \mathcal{L}^3_{cc} & \mathcal{L}^3_{ct} \\
z_{t_3} & & & & & & & & & & & & & & & \mathcal{L}^3_{uc} & \mathcal{L}^3_{ct} & \mathcal{L}^3_{tt}
\end{array}
\tag{5}
$$

where,

$$
\begin{aligned}
\mathcal{L}_{cc}^{i,j} = \frac{\partial^2 \mathcal{L}}{\partial z_{c_{i,j}}^2} &= 2h_i W_j w_{z_c} \\
\mathcal{L}_{tt}^{i,j} = \frac{\partial^2 \mathcal{L}}{\partial z_{t_{i,j}}^2} &= 2h_i W_j w_{z_t} + (\lambda_{c_i}^g - \lambda_{t_i}^g) k \frac{z_{c_{i,j}} E_a}{{z_{t_{i,j}}}^3} \left(\frac{Ea}{z_{t_{i,j}}} - 2 \right) \exp\left[\frac{-Ea}{z_{t_{i,j}}} \right] \\
\mathcal{L}_{ct}^{i,j} = \frac{\partial^2 \mathcal{L}}{\partial z_{c_{i,j}} \partial z_{t_{i,j}}} &= (\lambda_{c_{i,j}}^g - \lambda_{t_{i,j}}^g) \left(k \frac{E_a}{{z_{t_{i,j}}}^2} \exp\left[\frac{-E_a}{z_{t_{i,j}}} \right] \right) \\
\mathcal{L}_{uu}^{i,j} = \frac{\partial^2 \mathcal{L}}{\partial u_{i,j}^2} &= 2h_i W_j w_u \\
\mathcal{L}_{tu}^{i,j} = \frac{\partial^2 \mathcal{L}}{\partial z_{t_{i,j}} \partial u_{i,j}} &= \alpha \lambda_{t_{i,j}}^g
\end{aligned} \tag{6}
$$

The first-order optimality conditions are given by,

$$
\nabla_x \mathcal{L} = \nabla_x \varphi(x) + J_c(x)^T \lambda - \nu_u = 0 \tag{7}
$$

expanding terms,

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial z_{c_i}^0} = 0 &= -\sum_{j=1}^{nc} \lambda_{c_{i,j}}^f + \lambda_{c_i}^c \\
\frac{\partial \mathcal{L}}{\partial z_{t_i}^0} = 0 &= -\sum_{j=1}^{nc} \lambda_{t_{i,j}}^f + \lambda_{t_i}^c \\
\frac{\partial \mathcal{L}}{\partial y_{c_{i,j}}} = 0 &= \lambda_{c_{i,j}}^g - h_i \sum_{k=1}^{n_c} \lambda_{c_{i,k}}^f \mathbf{\Omega}_{j,k} \\
\frac{\partial \mathcal{L}}{\partial y_{t_{i,j}}} = 0 &= \lambda_{t_{i,j}}^g - h_i \sum_{k=1}^{n_c} \lambda_{t_{i,k}}^f \mathbf{\Omega}_{j,k} \\
\frac{\partial \mathcal{L}}{\partial u_{i,j}} = 0 &= \varphi_{u_{i,j}} + \lambda_{c_{i,j}}^g g_{u_{i,j}}^c + \lambda_{t_{i,j}}^g g_{u_{i,j}}^t - \nu_{u_{i,j}} \\
\frac{\partial \mathcal{L}}{\partial z_{c_{i,j}}} = 0 &= \varphi_{c_{i,j}} + \lambda_{c_{i,j}}^g g_{c_{i,j}}^c + \lambda_{t_{i,j}}^g g_{c_{i,j}}^t + \lambda_{c_{i,j}}^f + \delta_{j,3}(-\lambda_{c_{i+1}}^c) \\
\frac{\partial \mathcal{L}}{\partial z_{t_{i,j}}} = 0 &= \varphi_{t_{i,j}} + \lambda_{c_{i,j}}^g g_{t_{i,j}}^c + \lambda_{t_{i,j}}^g g_{t_{i,j}}^t + \lambda_{t_{i,j}}^f + \delta_{j,3}(-\lambda_{t_{i+1}}^c) \\
0 &= g_{i,j}^c(\cdot) \\
0 &= g_{i,j}^t(\cdot) \\
0 &= z_{c_{i,j}} - z_{c_i}^0 - h_i \sum_{k=1}^{n_c} \mathbf{\Omega}_{k,j} y_{c_{i,k}} \\
0 &= z_{t_{i,j}} - z_{t_i}^0 - h_i \sum_{k=1}^{n_c} \mathbf{\Omega}_{k,j} y_{t_{i,k}} \\
0 &= z_{c_i}^0 + (1 - \delta_{i,1}) \left(-z_{c_{i-1,n_c}} \right) + \delta_{i,1} \left(-\hat{z}_c(\ell) \right) \\
0 &= z_{t_i}^0 + (1 - \delta_{i,1}) \left(-z_{t_{i-1,n_c}} \right) + \delta_{i,1} \left(-\hat{z}_t(\ell) \right) \\
0 &= \nu_{u_{i,j}} u_{i,j} - \mu
\end{aligned} \tag{8}
$$

where $\delta_{i,j}$ is the Kronecker delta and,

$$
\begin{aligned}
\varphi_{c_{i,j}} &= 2h_i W_j w_{z_c} (z_{c_{i,j}} - z_c^{des}) \\
\varphi_{t_{i,j}} &= 2h_i W_j w_{z_t} (z_{t_{i,j}} - z_t^{des}) \\
\varphi_{u_{i,j}} &= 2h_i W_j w_u (u_{i,j} - u^{des})
\end{aligned} \tag{9}
$$

Linearizing the above expressions around an arbitrary point (x^k, λ^k, ν^k),

$$\nabla_{xx}\mathcal{L}(x^k, \lambda^k)\Delta x^k + J_c(x^k)^T \Delta\lambda^k - \Delta\nu_u^k = -\nabla_x \mathcal{L}(x^k) \tag{10}$$

expanding terms,

$$\begin{aligned}
-\sum_{j=1}^{nc} \Delta\lambda^f_{c_{i,j}} + \Delta\lambda^c_{c_i} &= \sum_{j=1}^{nc} \lambda^f_{c_{i,j}} - \lambda^c_{c_i} \\
-\sum_{j=1}^{nc} \Delta\lambda^f_{t_{i,j}} + \Delta\lambda^c_{t_i} &= \sum_{j=1}^{nc} \lambda^f_{t_{i,j}} - \lambda^c_{t_i} \\
\Delta\lambda^g_{c_{i,j}} - h_i \sum_{k=1}^{n_c} \Delta\lambda^f_{c_{i,k}} \mathbf{\Omega}_{j,k} &= -\lambda^g_{c_{i,j}} + h_i \sum_{k=1}^{n_c} \lambda^f_{c_{i,k}} \mathbf{\Omega}_{j,k} \\
\Delta\lambda^g_{t_{i,j}} - h_i \sum_{k=1}^{n_c} \Delta\lambda^f_{t_{i,k}} \mathbf{\Omega}_{j,k} &= -\lambda^g_{t_{i,j}} + h_i \sum_{k=1}^{n_c} \lambda^f_{t_{i,k}} \mathbf{\Omega}_{j,k} \\
\mathcal{L}^{i,j}_{uz_c} \Delta z_{c_{i,j}} + \mathcal{L}^{i,j}_{uz_t} \Delta z_{t_{i,j}} + \mathcal{L}^{i,j}_{uu} \Delta u_{i,j} + g^c_{u_{i,j}} \Delta\lambda^g_{c_{i,j}} + g^t_{u_{i,j}} \Delta\lambda^g_{t_{i,j}} - \Delta\nu_{u_{i,j}} &= -\frac{\partial \mathcal{L}}{\partial u_{i,j}} \\
\mathcal{L}^{i,j}_{z_c z_c} \Delta z_{c_{i,j}} + \mathcal{L}^{i,j}_{z_c z_t} \Delta z_{t_{i,j}} + \mathcal{L}^{i,j}_{z_c u} \Delta u_{i,j} + g^c_{c_{i,j}} \Delta\lambda^g_{c_{i,j}} + g^t_{c_{i,j}} \Delta\lambda^g_{t_{i,j}} + \Delta\lambda^f_{c_{i,j}} + \delta_{j,3}(-\Delta\lambda^c_{c_{i+1}}) &= -\frac{\partial \mathcal{L}}{\partial z_{c_{i,j}}} \\
\mathcal{L}^{i,j}_{z_t z_c} \Delta z_{c_{i,j}} + \mathcal{L}^{i,j}_{z_t z_t} \Delta z_{t_{i,j}} + \mathcal{L}^{i,j}_{z_t u} \Delta u_{i,j} + g^c_{t_{i,j}} \Delta\lambda^g_{c_{i,j}} + g^t_{t_{i,j}} \Delta\lambda^g_{t_{i,j}} + \Delta\lambda^f_{t_{i,j}} + \delta_{j,3}(-\Delta\lambda^c_{t_{i+1}}) &= -\frac{\partial \mathcal{L}}{\partial z_{t_{i,j}}} \\
\Delta y_{ci,j} + g^c_{c_{i,j}} \Delta z_{c_{i,j}} + g^c_{t_{i,j}} \Delta z_{t_{i,j}} + g^c_{u_{i,j}} \Delta u_{i,j} &= -g^c_{i,j} \\
\Delta y_{ti,j} + g^t_{c_{i,j}} \Delta z_{c_{i,j}} + g^t_{t_{i,j}} \Delta z_{t_{i,j}} + g^t_{u_{i,j}} \Delta u_{i,j} &= -g^t_{i,j} \\
\Delta z_{c_{i,j}} - \Delta z^0_{c_i} - h_i \sum_{k=1}^{n_c} \mathbf{\Omega}_{k,j} \Delta y_{c_{i,k}} &= -z_{c_{i,j}} + z^0_{c_i} + h_i \sum_{k=1}^{n_c} \mathbf{\Omega}_{k,j} y_{c_{i,k}} \\
\Delta z_{t_{i,j}} - \Delta z^0_{t_i} - h_i \sum_{k=1}^{n_c} \mathbf{\Omega}_{k,j} \Delta y_{t_{i,k}} &= -z_{t_{i,j}} + z^0_{t_i} + h_i \sum_{k=1}^{n_c} \mathbf{\Omega}_{k,j} y_{t_{i,k}} \\
\Delta z^0_{c_i} + (1 - \delta_{i,1}) \left(-\Delta z_{c_{i-1,n_c}}\right) &= -\left(z^0_{c_i} + (1 - \delta_{i,1}) \left(-z_{c_{i-1,n_c}}\right) + \delta_{i,1} \left(-\hat{z}_c(\ell)\right)\right) \\
\Delta z^0_{t_i} + (1 - \delta_{i,1}) \left(-\Delta z_{t_{i-1,n_c}}\right) &= -\left(z^0_{t_i} + (1 - \delta_{i,1}) \left(-z_{t_{i-1,n_c}}\right) + \delta_{i,1} \left(-\hat{z}_t(\ell)\right)\right) \\
\nu_{u_{i,j}} \Delta u_{i,j} + \Delta\nu_{u_{i,j}} u_{i,j} &= -\left(\nu_{u_{i,j}} u_{i,j} - \mu\right)
\end{aligned} \tag{11}$$