

1. Use MATLAB to show that the solution profiles for the example:

$$\begin{aligned} \min \quad & -b(1) \\ \text{s.t.} \quad & \frac{da}{dt} = -a(t)(u(t) + 0.5u(t)^2) \\ & \frac{db}{dt} = a(t)u(t) \\ & a(0) = 1, \quad b(0) = 0, \quad u(t) \in [0, 5] \end{aligned}$$

satisfy the optimality conditions.

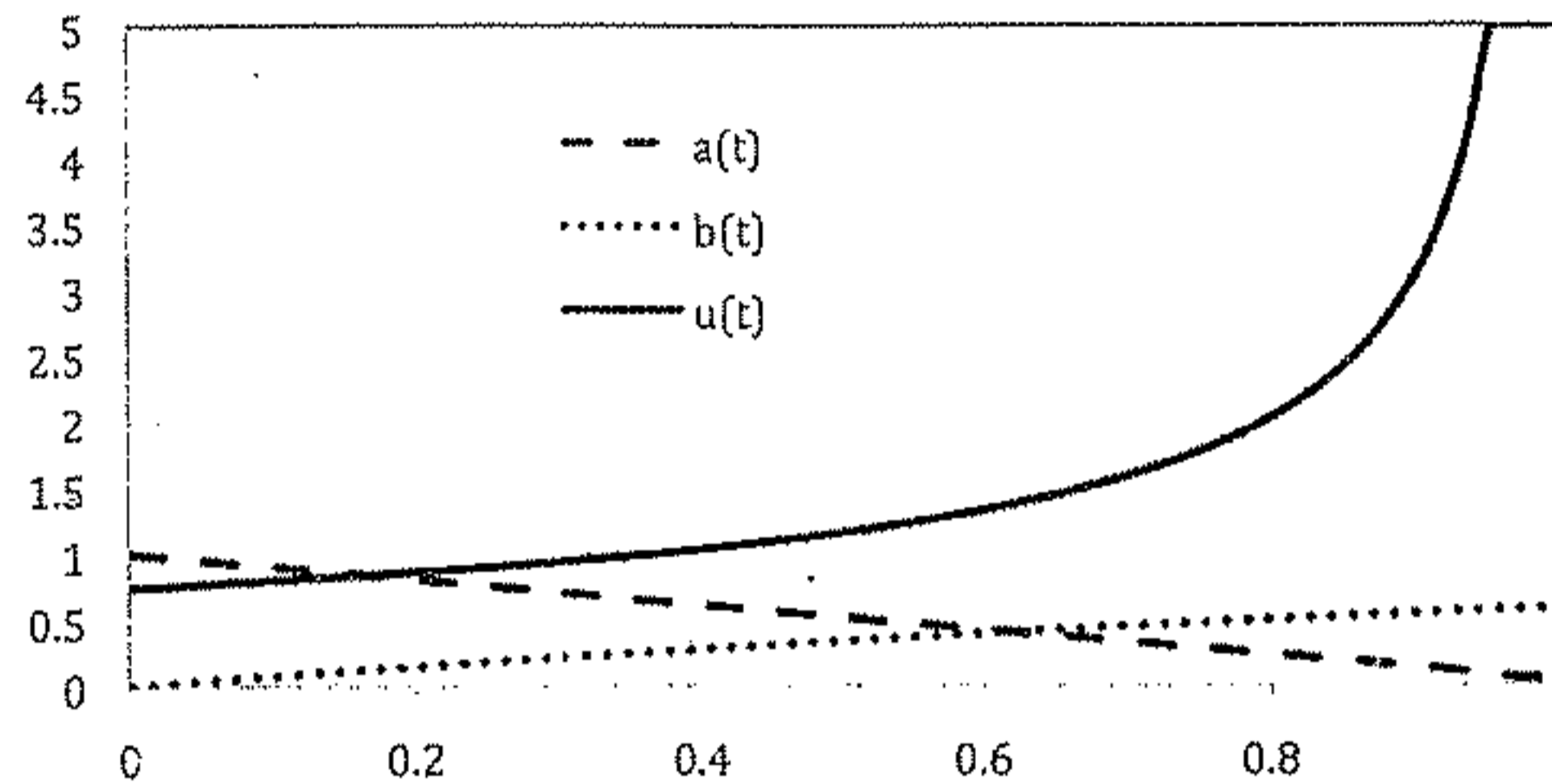


Figure 1: State and Control Profiles for Batch Reactor: $A \rightarrow B, A \rightarrow C$

2. For the singular control problem given by:

$$\min \Phi(z(t)), \quad \text{s.t.} \quad \frac{dz(t)}{dt} = f_1(z) + f_2(z)u(t), \quad z(0) = z_0, \quad u(t) \in [u_L, u_U].$$

Show that $q \geq 2$ in $\frac{d^q H_u(t)}{dt^q} = \varphi(z, u) = 0$.

3. For the problem below, derive the two point boundary value problem and show the relationship of $u(t)$ to the state and adjoint variables.

$$\begin{aligned} \min \quad & z_1(1)^2 + z_2(1)^2 \\ \text{s.t.} \quad & \frac{dz_1(t)}{dt} = -2z_2, \quad z_1(0) = 1 \\ & \frac{dz_2(t)}{dt} = z_1 u(t), \quad z_2(0) = 1 \end{aligned}$$

4. Solve the Catalyst Example given below for the case where the first reaction is irreversible ($k_2 = 0$). Show that this problem has a bang-bang solution.

$$\begin{aligned} \min \quad & a(t_f) + b(t_f) - a_0 \\ \text{s.t.} \quad & \frac{da(t)}{dt} = -u(k_1 a(t) - k_2 b(t)) \\ & \frac{db(t)}{dt} = u(k_1 a(t) - k_2 b(t)) - (1-u)k_3 b(t) \\ & a(0) = a_0, \quad b(0) = 0, \quad u(t) \in [0, 1]. \end{aligned}$$

Solution - Homework 8

1) $\min -b(1)$

$$\text{s.t. } \dot{a} = -a(u + \frac{1}{2}u^2)$$

$$b' = au$$

$$a(0) = 1, b(0) = 0, u \in [0, 5]$$

$$H = -\lambda_1 a(u + \frac{1}{2}u^2) + \lambda_2 au + \gamma_u (u-5) - \gamma_u u$$

$$0 \leq u \perp \gamma_u \geq 0; \quad 0 \leq \gamma_u \perp (5-u) \geq 0$$

$$\dot{\lambda}_1 = (\lambda_1 - \lambda_2)u + \lambda_1 u^2/2, \quad \lambda_1(0) = 0$$

$$\dot{\lambda}_2 = 0, \quad \lambda_2(1) = -1 \Rightarrow \lambda_2(t) = -1$$

$$H_u = -\lambda_1 a(1+u) + \lambda_2 a - \gamma_u + \gamma_u u = 0$$

note

$$H(1) = -a(1)u(1) - \gamma_u + \gamma_u u = 0,$$

so $\gamma_u = a(1)u(1) > 0$ because it is not optimal for $u(1)$ to be zero

$$\text{Hence } \gamma_u > 0 \Rightarrow u(1) = 5.$$

- At t_1 , we have $\gamma_u = 0$ and $u(t)$ moves off bound.
from $H_u = 0$, $u(t) = (\lambda_2/\lambda_1) - 1 = -(1 + \frac{1}{\lambda_1})$
and at $u(t_1) = 5$, $\lambda_1(t_1) = -0.1667$

- Integrate from $t_f = 1 \rightarrow t_1$

$$\dot{\lambda}_1 = 5(\lambda_1 + 1) + 12.5\lambda_1, \quad \lambda_1(0) = 0$$

$$\text{until } \lambda_1(t_1) = -1/6$$

- Integrate from $t_1 \rightarrow 0$ with $u = -(1 + \frac{1}{\lambda_1})$

$$\dot{\lambda}_1 = (\lambda_1 - \lambda_2)u + \lambda_1 u^2/2, \quad \lambda_1(t_1) = -1/6$$

- Integrate a, b forward using $u(t)$

Verification of Profiles:

1. Solve $\dot{\lambda}_1 = 5(\lambda_1 + 1) + 12.5\lambda_1$, $\lambda_1(0) = 0$ (i.e., $u(t) = 5$) until $\lambda_1(t_1) = -1/6$. This occurs at $t_1 = 0.95$.

2. From $t = t_1 \rightarrow 0$, set $u(t) = -(1 + 1/\lambda_1(t))$ and integrate

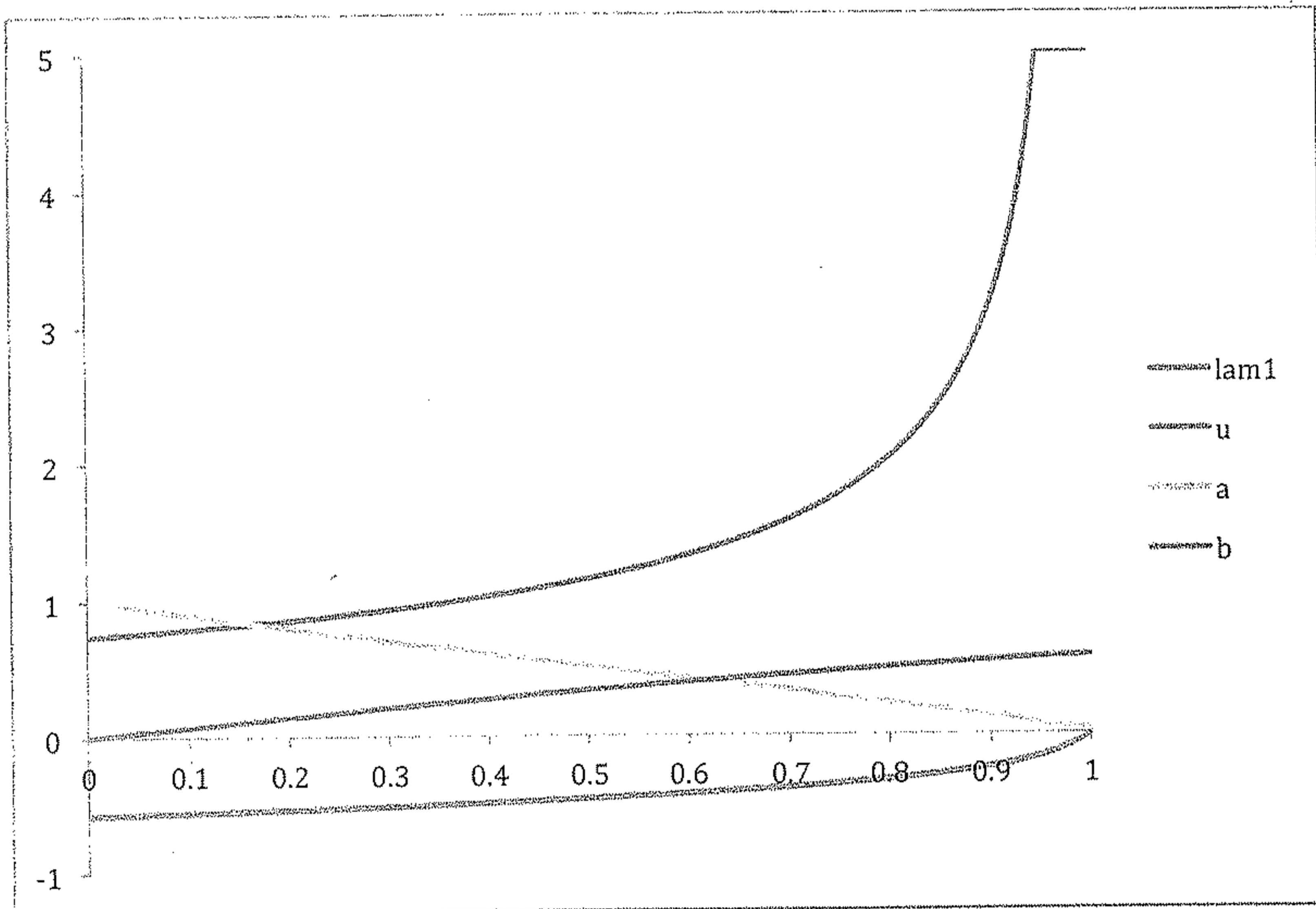
$$\dot{\lambda}_1 = u(t)(\lambda_1 + 1) + u(t)^2 \lambda_1 / 2, \quad \lambda_1(t_1) = -1/6.$$

3. From $t=0$, integrate forward:

$$\dot{a} = -a(u + u^2), \quad a(0) = 1$$

$$\dot{b} = au, \quad b(0) = 0$$

This yields the profiles below.



2. Singular control problem

$$\text{Min } \phi(z(t_f))$$

$$\text{s.t. } \dot{z} = f_1 + f_2 u, \quad z(0) = z_0 \\ u_L \leq u \leq u_U$$

$$H = \lambda^T (f_1 + f_2 u)$$

$$H_u = f_2^T \lambda$$

$$\dot{\lambda} = - \begin{pmatrix} \frac{\partial f_1}{\partial z} & \frac{\partial f_2 u}{\partial z} \end{pmatrix} \lambda$$

$$\lambda(t_f) = \partial \phi / \partial z$$

$$\dot{H}_u = \frac{\partial f_2}{\partial z} (f_1 + f_2 u)^T \lambda - \begin{pmatrix} \frac{\partial f_1}{\partial z} & \frac{\partial f_2 u}{\partial z} \end{pmatrix} \lambda f_2$$

note that since u is a scalar

$$\frac{\partial f_2}{\partial z} (f_2 u)^T \lambda = \frac{\partial f_2}{\partial z} u \lambda f_2$$

so we have

$$\dot{H}_u = \frac{\partial f_2}{\partial z} (f_1^T \lambda) - \frac{\partial f_1}{\partial z} \lambda f_2$$

$$3) \quad \text{Min} \quad z_1^2(1) + z_2^2(1)$$

$$\text{s.t.} \quad \dot{z}_1 = -2z_2, \quad z_1(0) = 1$$

$$z_2 = z_1 u, \quad z_2(0) = 1$$

$$H = -2\lambda_1 z_2 + \lambda_2 z_1 u$$

$$H_u = \lambda_2 z_1 = 0$$

$$\dot{\lambda}_1 = -\lambda_2 u, \quad \lambda_1(1) = 2z_1(1)$$

$$\dot{\lambda}_2 = 2\lambda_1, \quad \lambda_2(1) = 2z_2(1)$$

$$\dot{H}_u = \dot{\lambda}_2 z_1 + \lambda_2 \dot{z}_1 = 0$$

$$= 2\lambda_1 z_1 - 2\lambda_2 z_2 = 0$$

$$\ddot{H}_u = 2(\dot{\lambda}_1 z_1 + \lambda_1 \dot{z}_1 - \dot{\lambda}_2 z_2 - \lambda_2 \dot{z}_2) = 0$$

$$= 2(-\lambda_2 z_1 u - 2\lambda_1 z_2 - 2\lambda_1 z_2 - \lambda_2 z_1 u) = 0$$

$$-2\lambda_2 z_1 u - 4\lambda_1 z_2 = 0$$

$$u = -\frac{2\lambda_1 z_2}{\lambda_2 z_1}$$

4) Catalyst mixing problem

$$\begin{aligned} \text{Min } & a(t_f) + b(t_f) - a_0 \\ \text{s.t. } & \dot{a} = -u k_1 a \\ & \dot{b} = u k_1 a - (1-u) k_3 b \\ & a(0) = a_0, \quad b(0) = 0 \\ & u \in [0, 1] \end{aligned}$$

$$H = (\lambda_2 - \lambda_1) k_1 a u - \lambda_2 k_3 b (1-u) - \gamma_0 u + \gamma_1 (u-1)$$

$$\begin{aligned} \dot{\lambda}_1 &= -(\lambda_2 - \lambda_1) k_1 u & \lambda_1(t_f) &= 1 \\ \dot{\lambda}_2 &= (1-u) \lambda_2 k_3 & \lambda_2(t_f) &= 1 \end{aligned}$$

$$\text{Let } J = (\lambda_2 - \lambda_1) k_1 a + \lambda_2 k_3 b$$

$$\delta H / \delta u = J(t) - \gamma_0 + \gamma_1 = 0$$

$$0 \leq \gamma_0 \perp u \geq 0$$

$$0 \leq \gamma_1 \perp (1-u) \geq 0$$

$$u(t) = 0 \Rightarrow J(t) \geq 0$$

$$u(t) = 1 \Rightarrow J(t) \leq 0$$

$$u(t) \in (0, 1) \Rightarrow J(t) = 0$$

$$\text{at } t = t_f, \lambda_1 = \lambda_2 = 1, J = k_3 b > 0 \Rightarrow u(t_f) = 0$$

$$t = t_0, a = a_0, b = 0, J = (\lambda_2 - \lambda_1) k_1 a_0$$

also

$$H(t) = H(t_f) = -k_3 b(t_f) < 0$$

$$0 > H(0) = (\lambda_2 - \lambda_1) k_1 a_0 < 0$$

$$\Rightarrow u(0) = 1$$

Now is there any point where
 $H_u = \dot{J} = 0$ for $t \in (0, t_f)$?

$$1) \quad J = (\lambda_2 - \lambda_1) k_1 a + \lambda_2 k_3 b = 0$$

$$\begin{aligned} 2) \quad \dot{J} &= (\dot{\lambda}_2 - \dot{\lambda}_1) k_1 a + \dot{\lambda}_2 k_3 b \\ &\quad + (\lambda_2 - \lambda_1) k_1 \dot{a} + \lambda_2 k_3 \dot{b} \\ &= [(\lambda_2 - \lambda_1) k_1 u + (1-u) \lambda_2 k_3] k_1 \dot{a} \\ &\quad - (\lambda_2 - \lambda_1) k_1^2 a u + (1-u) \lambda_2 k_3^2 b \\ &\quad + \lambda_2 k_3 [u k_1 \dot{a} - (1-u) k_3 \dot{b}] \\ &= \lambda_2 k_3 k_1 \dot{a} = 0 \end{aligned}$$

$$\begin{aligned} 3) \quad \dot{J} &= \dot{\lambda}_2 a k_3 k_1 + \lambda_2 \dot{a} k_3 k_1 \\ &= (1-u) \lambda_2 k_3^2 k_1 \dot{a} - \lambda_2 u k_1^2 k_3 \dot{a} \\ &= \lambda_2 k_3 k_1 \dot{a} [k_3 - u(k_3 + k_1)] = 0 \end{aligned}$$

The solution must be bang-bang. From (2) we have $\lambda_2(t) = 0$ if $\dot{J} = 0$. Also from (1) this leads to $\lambda_1(t) = 0$. Both occur since $a(t) > 0$, for $t_f < \infty$. Also, (3) is consistent with $\lambda_2(t) = 0$.

$$\begin{aligned} \text{since } H(t) &= (\lambda_2 - \lambda_1) k_1 a u - \lambda_2 k_3 b (1-u) \\ &= -k_3 b(t_f) < 0 \end{aligned}$$

there is no point in time, t , where
 $\lambda_1(t) = \lambda_2(t) = 0$.

The bang-bang solution can be found with a 2 variable (t_{switch}, t_f) optimization.