06-720 Advanced Process Systems Engineering Spring, 2011

Homework 8 Due: 4/11/11

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

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

satisfy the optimality conditions.

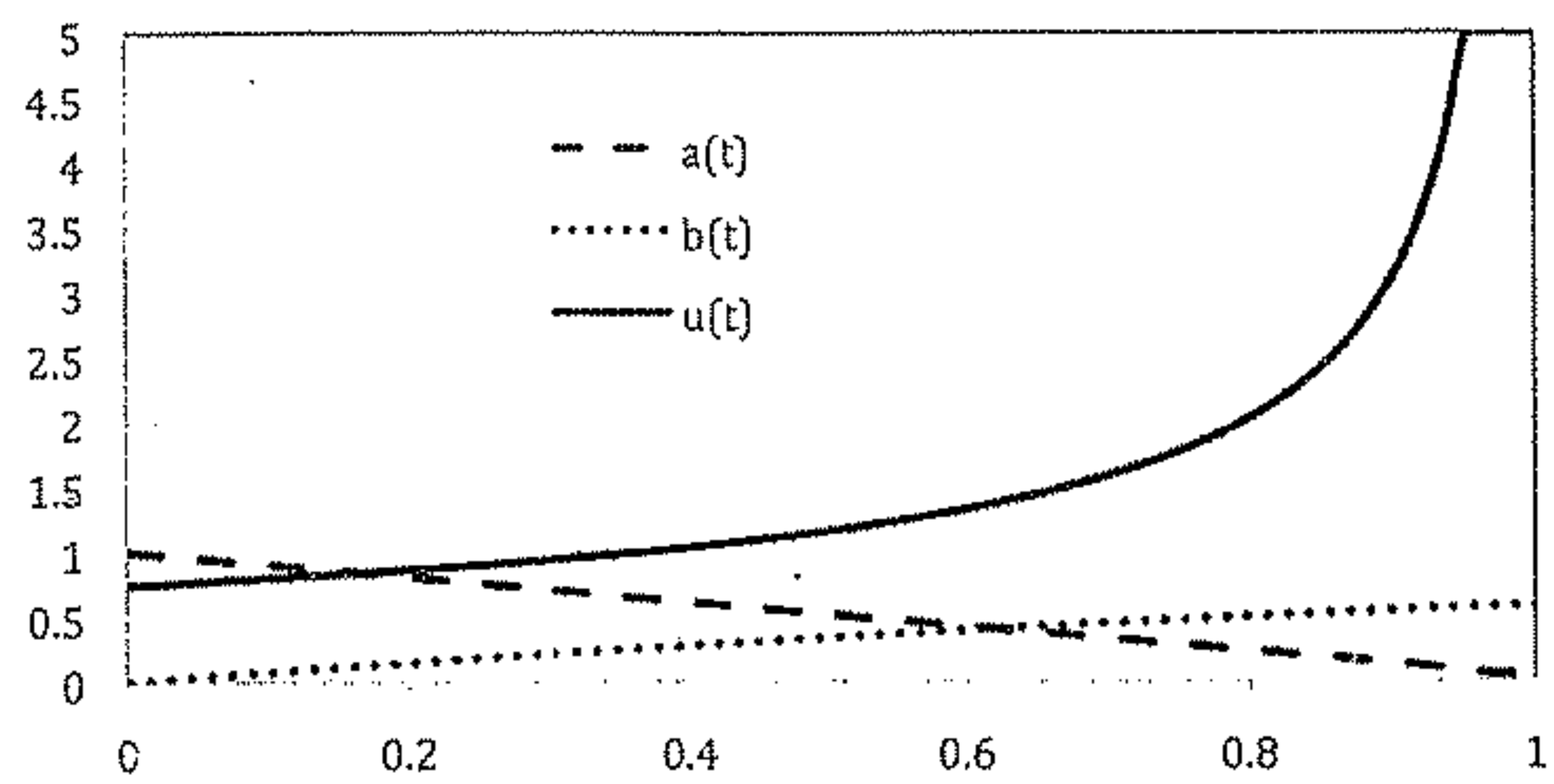


Figure 1: State and Control Profiles for Batch Reactor: $A \to B, A \to C$

2. For the singular control problem given by:

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

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.

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

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.

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

Solution - Hwk 8

1) $\min \; -b(1)$

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

$\dot{b} = a u$

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

$$H = -\lambda_1 a(u + u^2/2) + \lambda_2 a u + \nu_u (u-5) - \nu_\ell u$$

$$0 \le u \perp \nu_\ell \ge 0 \;;\; 0 \le \nu_u \perp (5-u) \ge 0$$

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

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

$$H_u = -\lambda_1 a(1+u) + \lambda_2 a - \nu_\ell + \nu_u = 0$$

<u>note</u>

$H(1) = -a(1)u(1) - \nu_\ell + \nu_u = 0,$

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

Hence $\nu_u > 0 \Rightarrow u(1) = 5.$

- at t_1, we have $\nu_u = 0$ and $u(t)$ moves off bnd.

from $H_u = 0$, $u(t) = (\lambda_2/\lambda_1) - 1 = -(1 + 1/\lambda_1)$

and at $u(t_1) = 5$, $\lambda_1(t_1) = -0.1667$

- Integrate from $t_f = 1 \longrightarrow t_1$

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

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

- Integrate from $t_1 \longrightarrow 0$ with $u = -(1 + 1/\lambda_1)$

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

- 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 $t_1 = 0.95$.

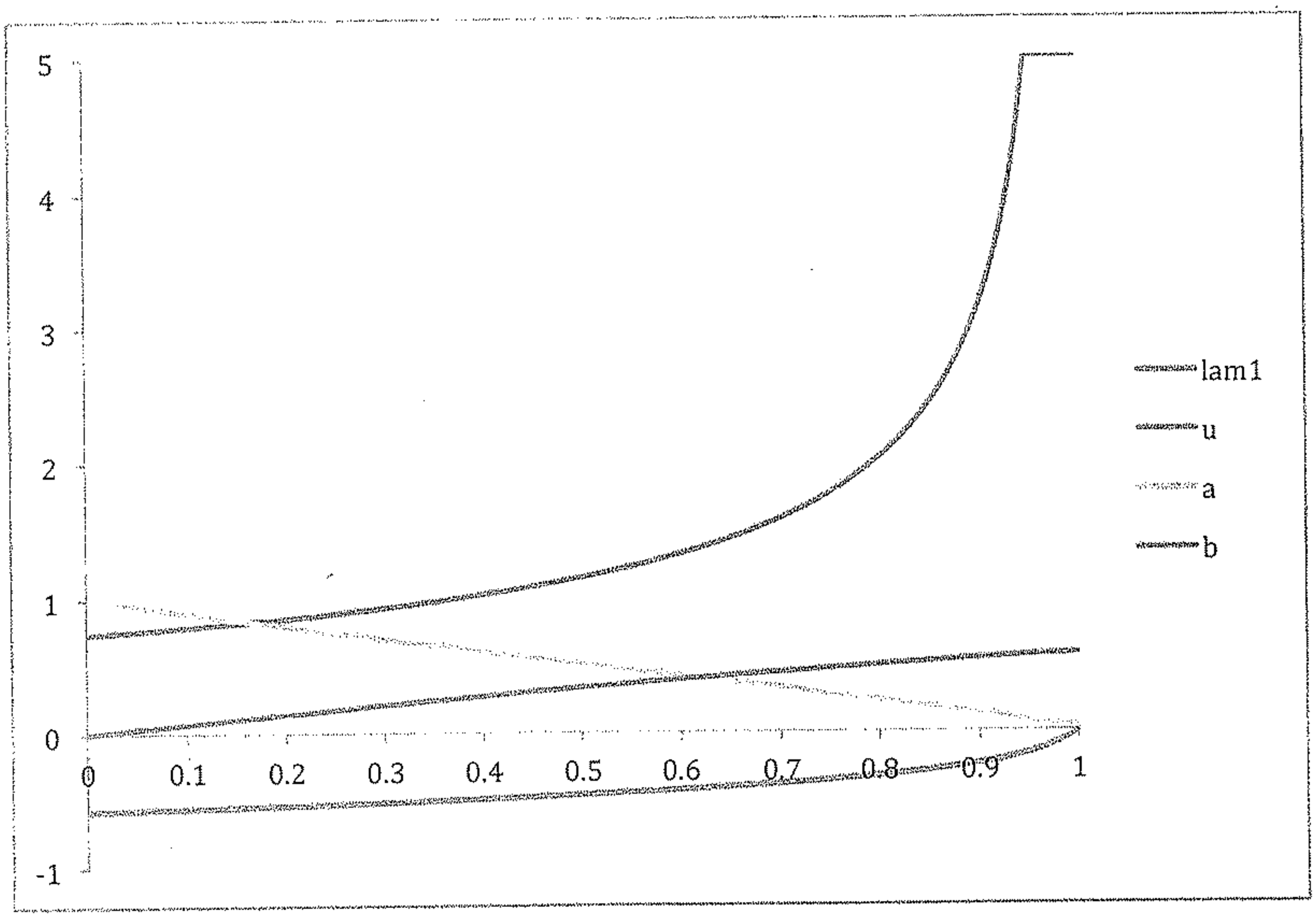
2. From $t = t_1 \rightarrow 0$, set $u(t) = -(1+1/\lambda_1(t))$ and integrate

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

3. From t=0, integrate forward:

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

This yields the profiles below.



2. Singular control problem

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

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

$$H = \lambda^T (f_1 + f_2 u)$$
$$H_u = f_2^T \lambda$$
$$\dot{\lambda} = -\left(\frac{\partial f_1}{\partial z} + \frac{\partial f_2 u}{\partial z}\right) \lambda$$
$$\lambda(t_f) = \partial\phi/\partial z$$

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

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) Min $z_1^2(1) + z_2^2(1)$

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

$\dot{z}_2 = z_1 u, \quad z_2(0) = 1$

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

$H_u = \lambda_2 z_1 = 0$

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

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

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

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

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

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

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

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

4) Catalyst mixing problem

$$\text{Min } a(t_f) + b(t_f) - a_0$$

$$\text{s.t. } \dot{a} = -u k_1 a$$

$$\dot{b} = u k_1 a - (1-u) k_3 b$$

$$a(0) = a_0, \quad b(0) = 0$$

$$u \in [0, 1]$$

$$H = (\lambda_2 - \lambda_1) k_1 a u - \lambda_2 k_3 b (1-u) - \nu_0 u + \nu_1 (u-1)$$

$$\dot{\lambda}_1 = -(\lambda_2 - \lambda_1) k_1 u \qquad \lambda_1(t_f) = 1$$

$$\dot{\lambda}_2 = (1-u) \lambda_2 k_3 \qquad \lambda_2(t_f) = 1$$

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

$$\partial H / \partial u = J(t) - \nu_0 + \nu_1 = 0$$

$$0 \le \nu_0 \perp u \ge 0$$

$$0 \le \nu_1 \perp (1-u) \ge 0$$

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

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

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

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

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

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

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

Now is there any portion where $H_u = J = 0$ for $t \in (0, t_f)$?

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

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

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

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 $\lambda_2(t) = 0$.

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