Lecture 3: Systems and Bounds on Controls

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Deterministic OC- ODEs

Find piecewise continuous control $u(t)$ and associated state variable $x(t)$ to maximize

$$\max \int_0^T f(t, x(t), u(t))\, dt$$

subject to

$$x'(t) = g(t, x(t), u(t))$$

$x(0) = x_0$ and $x(T)$ $free$

Contd.

- Optimal Control $u^*(t)$ achieves the maximum
- Put $u^*(t)$ into state DE and obtain $x^*(t)$
- $x^*(t)$ corresponding optimal state
- $u^*(t)$, $x^*(t)$ optimal pair

Using Hamiltonian

Converted problem of finding control to maximize objective functional subject to DE, IC to using Hamiltonian pointwise.

For maximization

$$\frac{\partial^2 H}{\partial u^2} \leq 0 \quad \text{at } u^* \quad \bigcap H(u) \quad \text{as a function of } u$$

For minimization

$$\frac{\partial^2 H}{\partial u^2} \geq 0 \quad \text{at } u^* \quad \bigcup H(u) \quad \text{as a function of } u$$

Two unknowns u^* and x^*
introduce adjoint λ (like a Lagrange multiplier)

Three unknowns u^*, x^* and λ

H nonlinear w.r.t. u

Eliminate u^* by setting $H_u = 0$
and solve for u^* in terms of x^* and λ

Two unknowns x^* and λ
with 2 ODEs (2 point BVP)
+ 2 boundary conditions.

Pontryagin Maximum Principle

If $u^*(t)$ and $x^*(t)$ are optimal for above problem, then there exists adjoint variable $\lambda(t)$ s.t.

$$H(t, x^*(t), u(t), \lambda(t)) \leq H(t, x^*(t), u^*(t), \lambda(t)),$$

at each time, where Hamiltonian H is defined by

$$H(t, x(t), u(t), \lambda(t)) = f(t, x(t), u(t)) + \lambda g(t, x(t), u(t)).$$

and

$$\lambda'(t) = -\frac{\partial H(t, x(t), u(t), \lambda(t))}{\partial x}$$

$$\lambda(T) = 0 \qquad \text{transversality condition}$$

Optimality Cond.-Control Bounds

$$\frac{\partial H}{\partial u} \text{ with } a \leq u \leq b$$

$$u = a \text{ if } \quad \frac{\partial H}{\partial u} < 0$$

$$0 \leq u \leq b \text{ if } \quad \frac{\partial H}{\partial u} = 0$$

$$u = b \text{ if } \quad \frac{\partial H}{\partial u} > 0.$$

Hamiltonian is maximized w.r.t. the controls

Example with bounds

$$\max_u \int_0^2 \left[2x(t) - 3u(t) - u^2(t)\right]\, dt$$

subject to $x'(t) = x(t) + u(t),\ x(0) = 5,$

$0 \le u(t) \le 2.$

Hamiltonian

$$H = 2x - 3u - u^2 + x\lambda + u\lambda.$$

$$\lambda'(t) = -\frac{\partial H}{\partial x} = -2 - \lambda \Rightarrow \lambda = -2 + c_1 e^{-t}$$

$$\lambda(2) = 0 \Rightarrow c_1 = 2e^2 \Rightarrow \lambda = 2e^{2-t} - 2.$$

Consider u^*, taking cases on the sign of $\frac{\partial H}{\partial u}$.

Optimality Conditions

$$\frac{\partial H}{\partial u} = -3 - 2u + \lambda,$$

$$0 > \frac{\partial H}{\partial u} \Rightarrow u = 0 \Rightarrow 0 > -3 + \lambda = -7 + 2e^{2-t}$$

$$0 < \frac{\partial H}{\partial u} \Rightarrow u = 2 \Rightarrow 0 < 7 + \lambda = -7 + (2e^{2-t} - 2)$$

$$0 = \frac{\partial H}{\partial u} \Rightarrow u = \frac{1}{2}(\lambda - 3) \Rightarrow 0 \leq \frac{1}{2}(\lambda - 3) \leq 2$$

Optimal control and state

$$u^*(t) = \begin{cases} 2 & \text{when} \quad 0 \le t < 2 - \ln(\frac{9}{2}), \\ e^{2-t} - \frac{5}{2} & \text{when} \quad 2 - \ln(\frac{9}{2}) \le t \le 2 - \ln(\frac{5}{2}), \\ 0 & \text{when} \quad 2 - \ln(\frac{5}{2}) < t \le 2. \end{cases}$$

Insert values for u^* into DE and solve 3 cases

$$x^*(t) = \begin{cases} k_1 e^t - 2 & \text{when} \quad 0 \le t < 2 - \ln(\frac{9}{2}), \\ k_2 e^t - \frac{1}{2}e^{2-t} + \frac{5}{2} & \text{when} \quad 2 - \ln(\frac{9}{2}) \le t \le 2 - \\ k_3 e^t & \text{when} \quad 2 - \ln(\frac{5}{2}) < t \le 2, \end{cases}$$

details

where k_1, k_2, and k_3 are constants. Using $x(0) = 5$, it follows $k_1 = 7$. Recall, the state must be continuous. So, requiring x^* to agree at $t = 2 - \ln(\frac{9}{2})$ and $t = 2 - \ln(\frac{5}{2})$, we find values for k_2 and k_3, so that

State x*

$$\begin{cases} 7e^t - 2 & , \quad 0 \le t \le 2 - \ln(\frac{9}{2}), \\ (7 - \frac{81}{8}e^{-2})e^t - \frac{1}{2}e^{2-t} + \frac{5}{2} & , 2 - \ln(\frac{9}{2}) \le t \le 2 - \ln(\frac{5}{2}) \\ (7 - 7e^{-2})e^t & , \quad 2 - \ln(\frac{5}{2}) \le t \le 2. \end{cases}$$

Show how to get u* into max min format

$$u^* = min(2, max(0, (\lambda - 3)/2))$$

Bounded Controls

As long as the final position of the state variable is not fixed in advance:
Control $a \leq u(t) \leq b$
Solve for the optimal control using the optimality condition and then impose the bounds on the formula.
In that exercise, suppose for all controls
$0 \leq u(t) \leq 5$
Then $u^*(t) = min(5, max(0, \frac{1}{2\lambda}))$

Multiple States, Controls

$$\max_{\vec{u}} \int_{t_0}^{t_1} f(t, \vec{x}(t), \vec{u}(t))\, dt + \phi(\vec{x}(t_1))$$

subject to $\vec{x}\,'(t) = \vec{g}(t, \vec{x}(t), \vec{u}(t)),$

$\vec{x}(t_0) = \vec{x}_0,\ \vec{x}(t_1)$ free.

States and Adjoints

Each state solves an ODE.
To each state, there corresponds an adjoint.
The first adjoint corresponds to the first state...

Hamiltonian

$$H(t,\vec{x},\vec{u},\vec{\lambda}) = f(t,\vec{x},\vec{u}) + \vec{\lambda}(t)\cdot\vec{g}(t,\vec{x},\vec{u}),$$

one adjoint corresponding to each state

Note that dot product gives a sum of λ_i times the RHS of ODE of i-th state

Necessary Conditions

$$x_i'(t) = g_i(t, \vec{x}, \vec{u}), \;\; x_i(t_0) = x_{i0} \text{ for } i = 1, ..., n,$$

$$\lambda_j'(t) = -\frac{\partial H}{\partial x_j}, \;\; \lambda_j(t_1) = \phi_{x_j}(x(t_1)) \text{ for } j = 1, ..., n,$$

$$0 = \frac{\partial H}{\partial u_k} \text{ at } u_k^* \text{ for } k = 1, ..., m,$$

Example

control the acceleration

$$min \int_0^1 x_2 + u^2 dt$$

$$x_1' = x_2, x_1(0) = 0, x_1(1) = 1$$

$$x_2' = u, x_2(0) = 0, x_2(1) free$$

trajectory starts at 0 position and 0 velocity

$$x_1'' = x_2' = u$$

Example continued

Introduce two adjoint variables, one for each state variable, and form the Hamiltonian,

$$H = x_2 + u^2 + \lambda_1 x_2 + \lambda_2 u.$$

$$\lambda_1'(t) = -\frac{\partial H}{\partial x_1} = 0,$$
$$\lambda_2'(t) = -\frac{\partial H}{\partial x_2} = -\lambda_1 - 1,\ \lambda_2(1) = 0.$$

Solve for adjoints

$$\lambda_1(t) \equiv C,$$
$$\lambda_2(t) = -(C+1)(t-1).$$

Using the optimality condition,

$$0 = \frac{\partial H}{\partial u} = 2u + \lambda_2 \Rightarrow u^* = -\frac{\lambda_2}{2} = \frac{C+1}{2}(t-1).$$

Solve for states

$$x_2' = u \Rightarrow x_2(t) = \frac{C+1}{2}(\frac{t^2}{2} - t), \text{ as } x_2(0) = 0,$$

$$x_1' = x_2 \Rightarrow x_1(t) = \frac{C+1}{2}(\frac{t^3}{6} - \frac{t^2}{2}), \text{ as } x_1(0) = 0.$$

Noting that $x_1(1) = 1$, it follows $C = -7$. Thus, the optimal solution set is

$$u^*(t) = 3-3t, \quad x_1^*(t) = \frac{3}{2}t^2-\frac{1}{2}t^3, \quad x_2^*(t) = 3t-\frac{3}{2}t^2.$$

Optimality Conditions-Control Bou

$$\frac{\partial H}{\partial u_k} = 0 \qquad \text{to} \qquad \begin{cases} u_k = a_k & \text{if} \quad \frac{\partial H}{\partial u_k} < 0 \\ a_k \leq u_k \leq b_k & \text{if} \quad \frac{\partial H}{\partial u_k} = 0 \\ u_k = b_k & \text{if} \quad \frac{\partial H}{\partial u_k} > 0. \end{cases}$$

Hamiltonian is maximized w.r.t. the controls

Bounded Controls

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Numerical Algorithm

1. Make an initial guess for u over the interval. Store the initial guess as u.
2. Using the initial conditions and the stored values for u, solve the state ODEs forward in time.
3. Using transversality conditions and stored values for u and the states, solve adjoints ODEs backward in time.
4. Update the control by entering the new states and adjoint values into the characterization of u.

Check Convergence, Iterate

If values of the variables in this iteration and the last iteration are close, output the current values as solutions. If values are not close, return to Step 2.

Virus and Immune Cells Example

virus population y and a population of immune cells z

$$\begin{aligned} y' &= (1-u)ry\left(1-\frac{y}{k}\right) - ay - pyz, \\ z' &= \frac{cyz}{1+\epsilon y} - qyz - bz, \end{aligned} \tag{1}$$

with $y(0) = y_0$ and $z(0) = z_0$.

The control function u represents a drug treatment to reduce the growth of the virus. The control set U is

$$U = \{u(t) \, : \, 0 \leq a \leq u(t) \leq B < 1, \; u(t) \; \text{ is meas.}\}.$$

Minimize the Objective Functional

$$J(u) = A_1 y(T) + \int_0^T (A_2 y + A u^2)\, dt,$$

take A_1 or A_2 zero and compare

Hamiltonian

The Hamiltonian is:

$$H = (A_2 y + A u^2) + \lambda_1 \left[(1-u) r y \left(1 - \frac{y}{k} \right) - a y - p y z \right]$$
$$+ \lambda_2 \left[\frac{c y z}{1 + \epsilon y} - q y z - b z \right].$$

Adjoints

The form of the first adjoint equation is

$$\lambda_1' = -\frac{\partial H}{\partial y},$$

while the form of the second adjoint equation is

$$\lambda_2' = -\frac{\partial H}{\partial z}.$$

.

where $\lambda_1(T) = A_1$ and $\lambda_2(T) = 0$ are the transversality conditions.

Characterization of OC

$$u^* = \begin{cases} a & \frac{1}{2A}\left[\lambda_1 r y \left(1 - \frac{y}{k}\right)\right] \le a \\ \frac{1}{2A}\left[\lambda_1 r y \left(1 - \frac{y}{k}\right)\right] & a < \frac{1}{2A}\left[\lambda_1 r y \left(1 - \frac{y}{k}\right)\right] < B \\ b & \frac{1}{2A}\left[\lambda_1 r y \left(1 - \frac{y}{k}\right)\right] \ge B \end{cases} \quad (2)$$

Figures

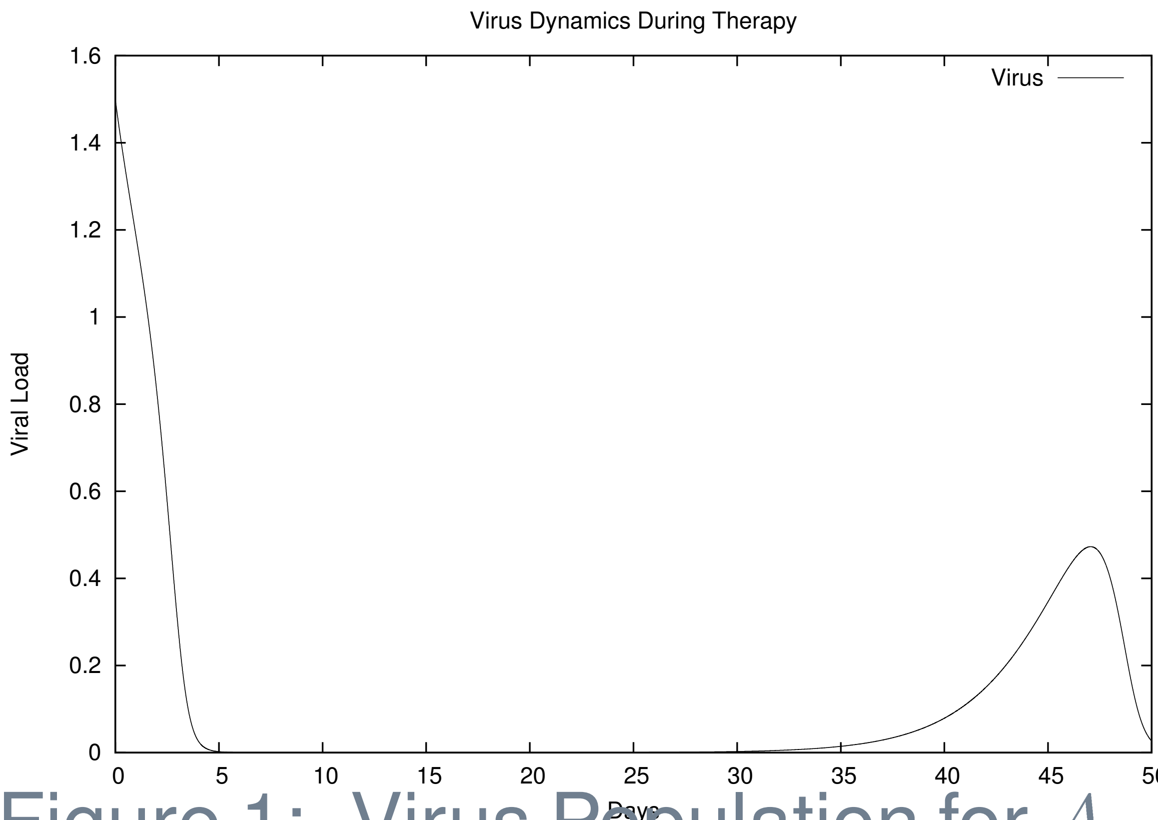


Figure 1: Virus Population for $A_1 = 1, A_2 = 0, A = 70$ and $B = 0.14$

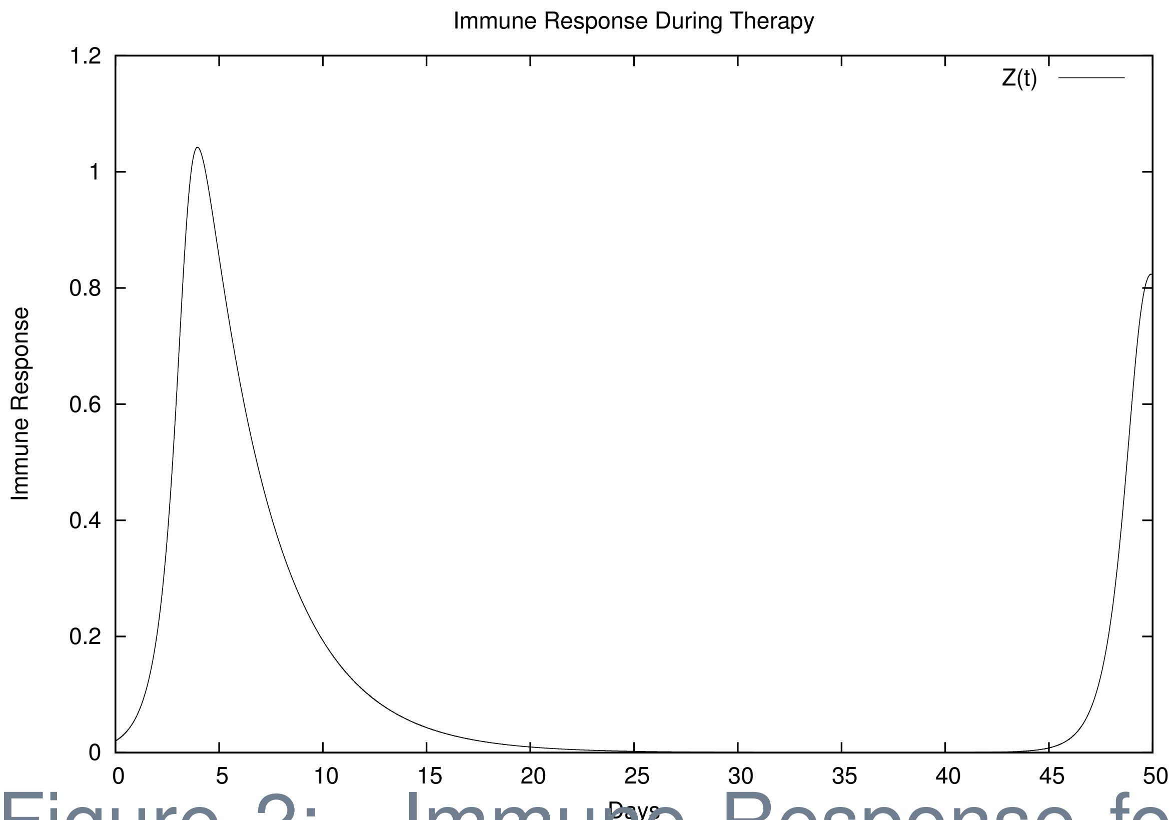


Figure 2: Immune Response for $A_1 = 1, A_2 = 0, A = 70$ and $B = 0.14$

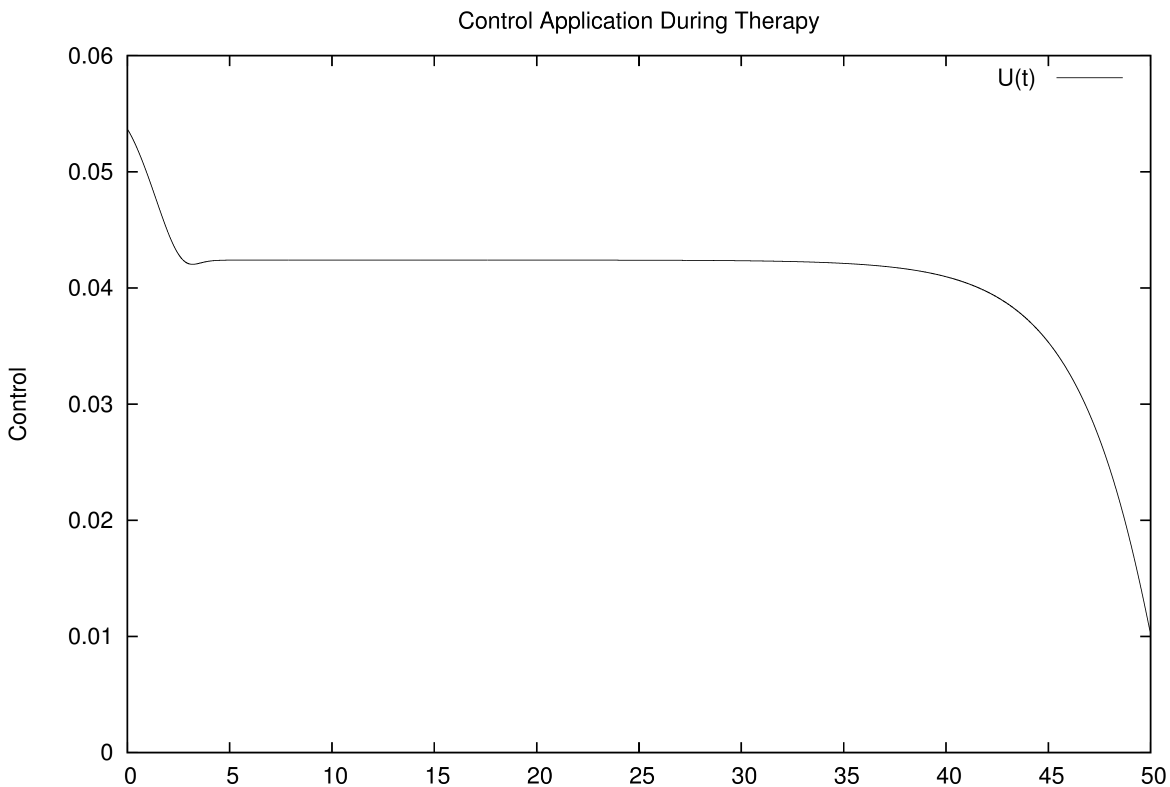


Figure 3: Control for $A_1 = 1, A_2 = 0, A = 70$ and $B = 0.14$

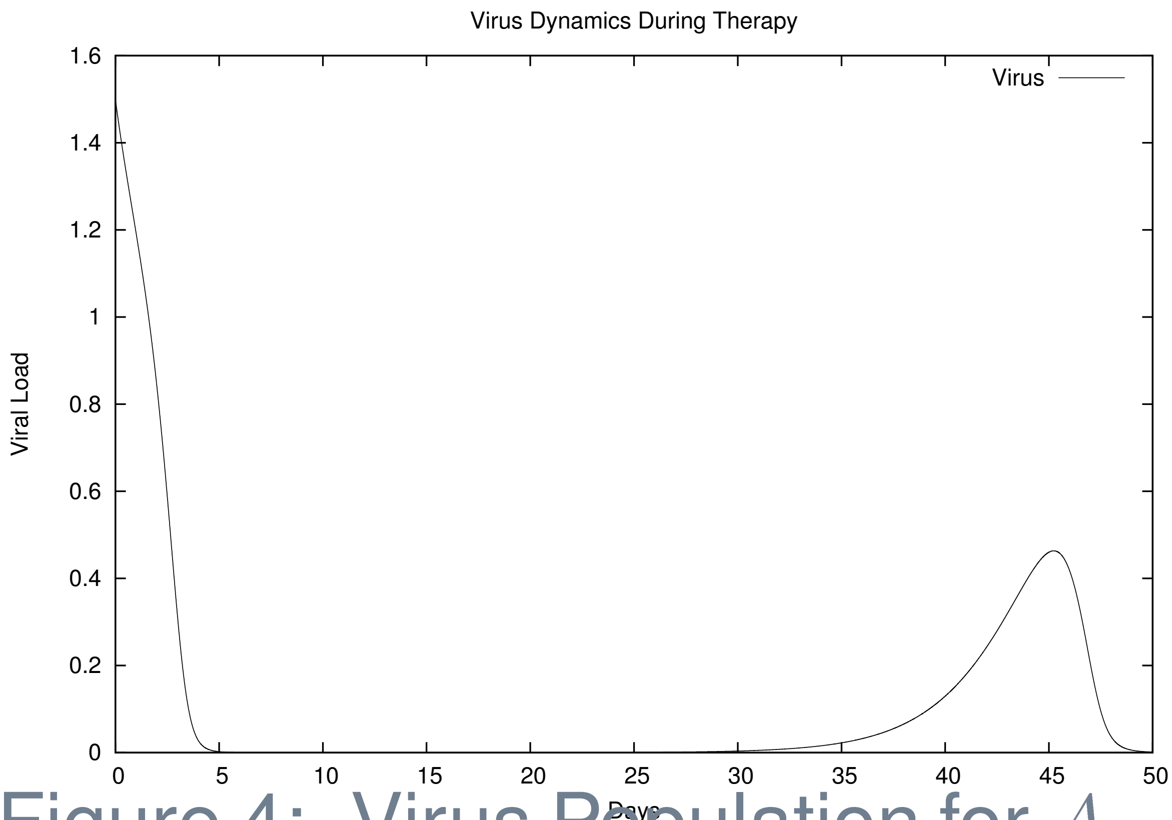


Figure 4: Virus Population for $A_1 = 0, A_2 = 1, A = 70$ and $B = 0.14$

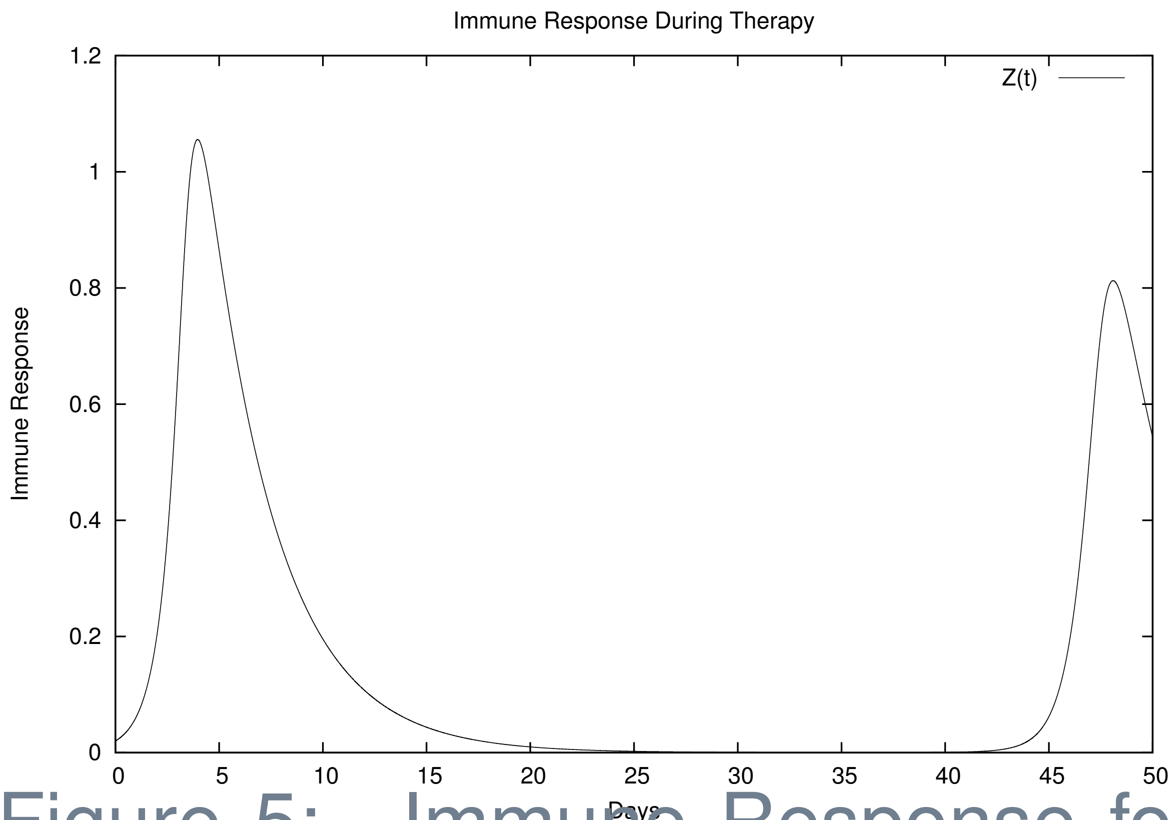


Figure 5: Immune Response for $A_1 = 0, A_2 = 1, A = 70$ and $B = 0.14$

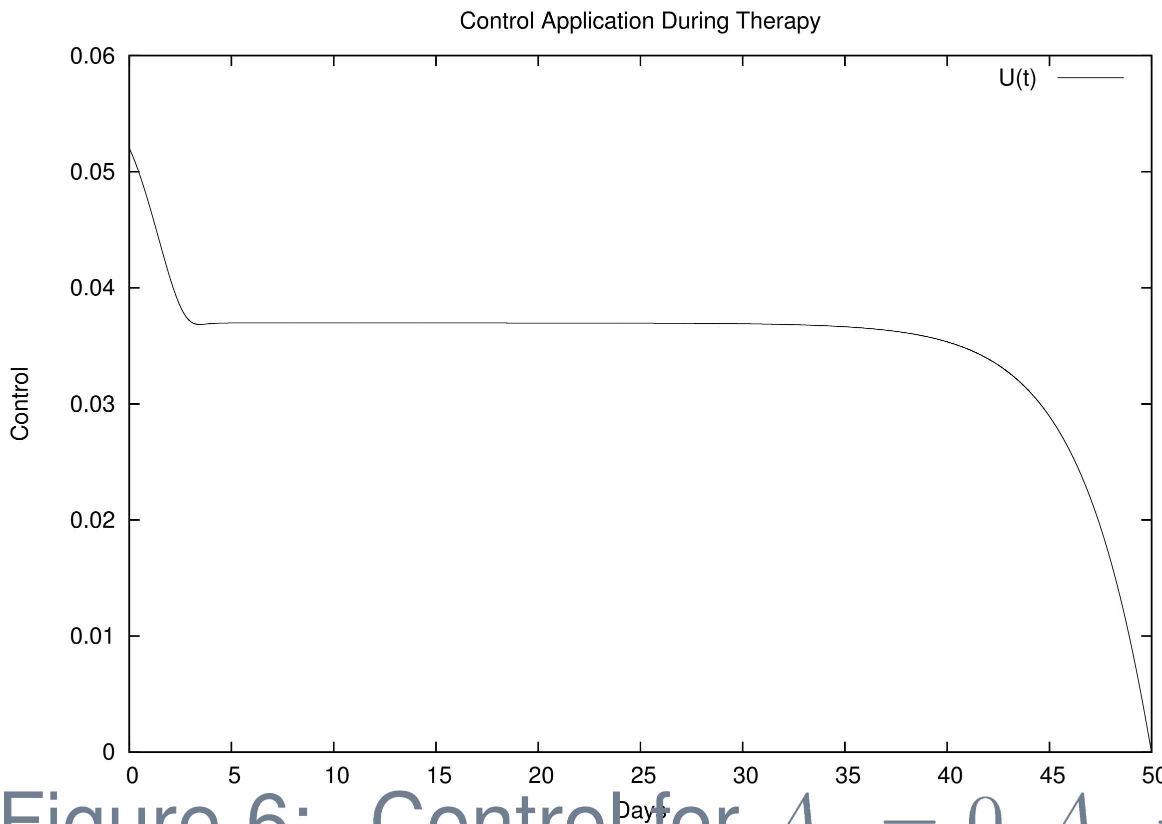


Figure 6: Control for $A_1 = 0, A_2 = 1, A = 70$ and $B = 0.14$

CML Example

This example, taken from the work of Nanda, Moore, and Lenhart, is a model of drug therapy for chronic mylegenous leukemia.

$C(t)$ the cancer cell population

$T_n(t)$ the naive T cell population

$T_e(t)$ the effector T cell population at time t.

Assume that effector T cells are specific to CML, activated by the presence of CML antigen.

Leukemia Model

$$\frac{dT_n}{dt} = s_n - u_2 d_n T_n - k_n T_n \left(\frac{C}{C+\eta} \right), \tag{3}$$

$$\frac{dT_e}{dt} = \tag{4}$$

$$\alpha_n k_n T_n \left(\frac{C}{C+\eta} \right) + \alpha_e T_e \left(\frac{C}{C+\eta} \right) - u_2 d_e T_e - \gamma_e C T_e, \tag{5}$$

$$\frac{dC}{dt} = (1-u_1) r_c C \ln \left(\frac{C_{\text{max}}}{C} \right) - u_2 d_c C - \gamma_c C T_e, \tag{6}$$

Controls

Effect of targeted drug is given by the control $u_1(t)$ which slows the production of cancer cells.

This drug affects only cancer cells, not other cells, $u_1(t)$ appears only in C equation.

$u_2(t)$ term for treatment by a broad chemotherapy, which is cytotoxic to all three cell populations.

u_2 appears in all state equations as a coefficient in the natural attrition terms.

Values of $u_2 > 1$ give treatment with cytotoxic drug.

min J(u1, u2)

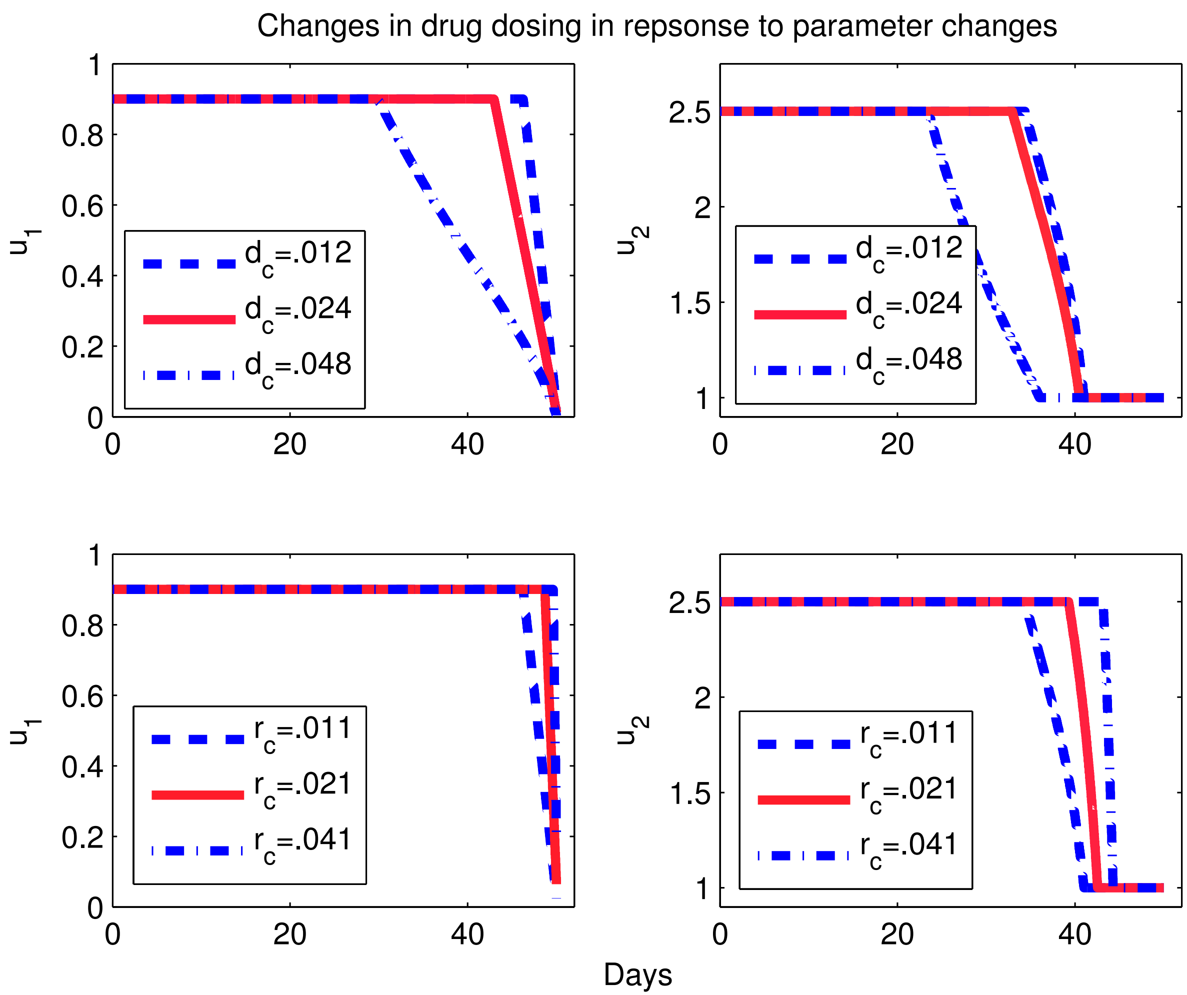
$$\int_0^T \left[C + \frac{B_1}{2} {u_1}^2 + \frac{B_2}{2} {u_2}^2 dt \right] + B_3\, C(T) - B_4\, T_n(T) \tag{7}$$

where

$U = \{(u_1(t), u_2(t)) |\, m_i \leq u_i(t) \leq M_i,$ meas, $i = 1, 2\}.$

$$\lambda_1(T) = -B_4,\ \lambda_2(T) = 0,\ \lambda_3(T) = B_3. \qquad (8)$$

Figures-varying parameters



more info

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Optimal Control Theory in Application to Biology

short course lectures and lab notes

Book: Optimal Control applied to Biological Models

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