Application of optimal control of parabolic PDE systems in biological models

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Thank you for inviting me
to Women in Control Workshop at BIRS in Banff!

OUTLINE
Parabolic Systems for Competitive Population Models

Formulation of optimal control problem

DETOUR in optimal control theory

Optimality Conditions

Numerical results

Parabolic Systems approxmating Agent Based Models

Background of the Sugarscape Agent Based Model

Approximation with PDE system and control application

Choosing Movement Direction

Motivation for first part

- How resource allocation affects the population dynamics of species remains an important issue in conservation biology.
- Given a fixed amount of resources, how can we determine the optimal spatial arrangement of the favorable and unfavorable parts of the habitat for species to survive?
- This question was first addressed by Cantrell and Cosner

$$u_t = \lambda \Delta u + m(x)u - u^2 \qquad \text{in } \Omega,$$

  subject to Dirichlet, Robin, or Neumann BC
  $u(x,t)$ is the density of the species
- $m(x)$ represents the intrinsic growth rate of the species and measures the availability of the resources.
- "beneficial" means the persistence of the population or the existence of a unique globally attracting steady state

Control resources

How does resource allocation affects population size of the species?

Population abundance is clearly a good measurement of conservation effort.

Outside manager controlling **resource** function $m(x)$

REFERENCES: Ding, Finnoti, Y. Lou, Y. Ye, Lenhart, in Nonlinear Analysis: Real World Appl. 2010, ELLIPTIC CASE

Bintz, Finnoti, Lenhart BIOMAT Proceedings 2014, PARABOLIC CASE

The type of boundary condition and the initial condition in the parabolic case make a difference.

Concentrating on Movement

- Ecological question: Given a fixed amount of resources, how does the species react to the habitat to be "beneficial"?
- Movement: Random Diffusion and Directed Advection.
- Belgacem-Cosner and Cantrell-Cosner-Lou studied the effects of the advection along an environmental resource gradient

$$u_t - \nabla \cdot [D\nabla u - \alpha u \nabla m(x)] = u[m(x) - u], \quad \Omega \times (0, \infty)$$

  with zero flux boundary condition.
- $m(x)$ represents the intrinsic growth rate and NOTE advection coefficient $\nabla m(x)$

Concentrating on movement choices

The **movement** of a population in reaction to resources is also an important concern in ecology.

With inhomogeneous resources, a population may tend to move along the spatial gradient of the resource function depending on the initial conditions. **OR maybe not?**

Choosing Movement

If a species could choose the direction for advection movement, how would such a choice be made to maximize its total population?

Would the advection be related to the spatial gradient of m, the resource function? or the spatial gradient of $\ln(m)$?

Population is chosing the advection direction, not an outsider manager.

Population Dynamics Model

- $\Omega \subset \mathbb{R}^n$ is a bounded smooth domain, $Q_T = \Omega \times [0, T]$ and $S_T = \partial\Omega \times [0, T]$ for some fixed $T > 0$.
- Model with $u(x, t)$, population density

$$\begin{cases} u_t - \nabla \cdot [\mu \nabla u + u\vec{h}] & = & u[m - f(x, t, u)], & Q_T, \\ \mu \dfrac{\partial u}{\partial \nu} - u\vec{h} \cdot \nu & = & 0, & \mathcal{S}_T, \\ u(\cdot, 0) & = & u_0 \geq 0, & \Omega. \end{cases}$$

- $\vec{h} : Q_T \to \mathbb{R}^n$ is the advection direction.
- $m = m(x, t)$ in $L^\infty(Q_T)$ measures the availability of resources.
- $f : Q_T \times \mathbb{R} \to \mathbb{R}$ is non-negative and satisfies some natural smoothness and growth conditions.
- $\mu > 0$ is fixed (diffusion coefficient).
- $u_0 \in L^\infty(\Omega)$ is sufficiently smooth.

Problem Formulation

- Seek the advection term $\vec{h}(x,t)$ that maximizes the total population while minimizing the "cost" due to movement.
- Find $\vec{h}^* \in U$ such that

$$J(\vec{h}^*) = \max_U J(\vec{h}), \quad \text{where} \quad J(\vec{h}) = \int_{Q_T} [u(x,t) - B|\vec{h}(x,t)|^2]dxdt.$$

- $$U = \{\vec{h} \in L^2((0,T), L^2(\Omega)^n) : |h_k| \leq M, \quad \forall k = 1, 2, \cdots, n\}.$$
- B "cost coefficient" due to the population moving along $\vec{h}$.
- Denote the dependence of the state on the control by $u = u(\vec{h})$.

REFERENCE: H. Finotti, S. Lenhart, and T. Phan, Optimal control of advection director for reaction-diffusion population models, Evolution Equations and Control Theory 1 (2012), 81-107.


DETOUR

Introduction to Optimal Control of PDEs

After setting up a PDE with a control in a specifed set and an objective functional, proving existence of an optimal control in an appropriate weak solution space is a first step.

To derive the necessary conditions , we need to differentiate the map

control $\rightarrow$ objective functional

Note that the state contributes to the objective functional, so we also must differentiate the map

control $\rightarrow$ state

The "sensitivity" is the derivative of the control-to-state map. The sensitivity solves a PDE, which is linearized version of the state PDE.

How to find and use the adjoint function

The formal **adjoint** of the operator in the sensitivity PDE is found.

Transversality Condition: final time condition $\lambda = 0$ at $t = T$

nonhomogeneous term

$$\frac{\partial(\text{ integrand of J })}{\partial \text{state}}$$

Differentiate the objective functional $J(control)$ with respect to the control.

Use the adjoint problem and the sensitivity problem to simplify and obtain the explicit **characterization** of an optimal control.

END OF DETOUR: Existence Solutions and Estimates

Solution space $u \in L^2((0,T), H^1(\Omega)) \cap L^\infty(Q)$ with $u_t \in L^2((0,T),(H^1(\Omega))^*)$

Theorem

Given $m \in L^\infty(Q_T)$ and u_0 be non-negative, bounded and in $H^1(\Omega)$. Then, for each $\vec{h} \in U$, there is a unique weak solution $u = u(\vec{h})$ of

$$\begin{cases} u_t - \nabla \cdot [\mu \nabla u + u\vec{h}] & = & u[m - f(x,t,u)], & Q_T, \\ \mu \dfrac{\partial u}{\partial \nu} - u\vec{h} \cdot \nu & = & 0, & \mathcal{S}_T, \\ u(\cdot, 0) & = & u_0 \geq 0, & \Omega. \end{cases}$$

Moreover, there is a finite constant $C > 0$ such that

$$0 \leq u(\vec{h}) \leq C, \quad \forall\ (x,t) \in Q_T,$$

and

$$\sup_{0 \leq t \leq T} \int_\Omega u(x,t)^2 dx + \int_{Q_T} |\nabla u(x,t)|^2 dxdt \leq C.$$

Steps in the proof

- Solutions $u \geq 0$ follows from Stampacchia's truncation method (the standard maximum principle is not applicable here).

- The energy estimate
$$\sup_{0 \leq t \leq T} \int_\Omega u(x,t)^2 dx + \int_{Q_T} |\nabla u(x,t)|^2 dxdt \leq C.$$
follows by multiplying the equation with u and using Hölder's inequality, Sobolev embeddings.

- The upper bound for u, i.e. $u \leq C$ is not trivial. It follows from de Giorgi's iteration technique.

- The existence of solution follows by standard method (Galerkin's method).

Existence of an Optimal Control

Theorem

There exists an optimal control $\vec{h}^* \in U$ *such that*

$$J(\vec{h}^*) = \max_{\vec{h} \in U} \int_{Q_T} [u(x,t) - B|\vec{h}(x,t)|^2] dxdt.$$

- Careful analysis of the convergence of maximizing sequence of controls and corresponding states.
- The a-priori estimates of the solutions $u(\vec{h})$ are essential.

We will show details of the necessary condtions in the system case

- The uniqueness of the optimal solutions $\vec{h}^*$
- The stability of the optimal solutions $\vec{h}^*$ with respect to the given resource $m(x,t)$.

We now write
$$\vec{h}^* = \vec{h}^*(m).$$

Theorem

Let $\beta > 0$. There exist $0 < T_1$ and B_1 such that if $B > B_1$ and $0 < T < T_1$, there exists a constant $C = C_T > 0$ such that the estimate
$$||\vec{h}^*(m_1) - \vec{h}^*(m_2)||_{L^2(Q_T)} \leq C||m_1 - m_2||_{L^2(Q_T)},$$
holds for all m_1, m_2 in $L^\infty(Q_T)$ with $|m_1|, |m_2| \leq \beta$.

Movement choices with competition

- With inhomogeneous resources population may tend to move along the spatial gradient of the resource function depending on the initial conditions. Or maybe not?
- What about when there is more than one population and there is a competition among them to survive??
- Several features...confusing.... (even in German)

Competitive Populations: Problem formulation

In an area with two competing populations, if the populations could choose the direction for advection movement, how would such a choice be made to maximize its total population?
Use of optimal control of PDEs

- Let $u(x,t), v(x,t)$ be the population densities of two competing species in a spacial domain Ω in d - dimensional space $\mathbb{R}^d, d \in \mathbb{N}$.
- Assume Ω with smooth boundary $\partial\Omega$ and
- For a given fixed time $0 < T < \infty$ let

$$Q = \Omega \times (0, T)$$

and

$$S = \partial\Omega \times (0, T)$$

.

collaborator: Kokum DeSilva, Tuoc Phan

The system of PDE's describing the dynamics:

$$
\begin{aligned}
u_t - d_1 \Delta u - \nabla \cdot (\vec{h_1} u) &= u[m - a_1 u] - b_1 uv \quad \text{in} \quad Q \\
v_t - d_2 \Delta v - \nabla \cdot (\vec{h_2} v) &= v[m - a_2 v] - b_2 uv \quad \text{in} \quad Q \\
d_1 \frac{\partial u}{\partial \eta} + u\vec{h_1} \cdot \eta &= 0 \quad \text{on} \quad S \\
d_2 \frac{\partial v}{\partial \eta} + v\vec{h_2} \cdot \eta &= 0 \quad \text{on} \quad S \\
u(x,0) &= u_0(x) \geq 0 \quad \text{for} \quad x \in \Omega \\
v(x,0) &= v_0(x) \geq 0 \quad \text{for} \quad x \in \Omega
\end{aligned}
\tag{1}
$$

The optimal control problem formulation:

- Control Set

  $$U = \{(\vec{h_1}, \vec{h_2}) \in ((L^\infty(Q))^d, (L^\infty(Q))^d) : |(h_1)_i| \le M_1, |(h_2)_i| \le M_2, i = 1, ..., d\}$$

  and $(u, v) = (u(\vec{h_1}, \vec{h_2}), v(\vec{h_1}, \vec{h_2}))$ be the solution of (1) for the corresponding $(\vec{h_1}, \vec{h_2})$.

- Then, for $A, B, C, D \ge 0$ we find $(\vec{h_1}, \vec{h_2}) \in U$ such that

  $$J((\vec{h_1}, \vec{h_2})^*) = \sup_{(\vec{h_1}, \vec{h_2}) \in U} J(\vec{h_1}, \vec{h_2})$$

  where, $J(\vec{h_1}, \vec{h_2})$ is the objective functional given by,

  $$J(\vec{h_1}, \vec{h_2}) = \int_Q \left[Au + Bv - C|\vec{h_1}|^2 - D|\vec{h_2}|^2\right] \, dxdt \tag{2}$$

  subject to the PDE system (1).

- We maximize a weighted combination of the two populations while minimizing the cost due to the movements of the populations.
- The cost is due to the "risk" of movements.

Existence and positivity of the state solution and the existence of an optimal control

Solution space $u, v \in L^2((0,T), H^1(\Omega)) \cap L^\infty(Q)$ with
$u_t, v_t \in L^2((0,T), (H^1(\Omega))^*)$

Theorem

Given $m \in L^\infty(Q)$, u_0, v_0 non-negative, $L^\infty(Q)$ bounded and in $H^1(\Omega)$. Then, for each $(\vec{h_1}, \vec{h_2}) \in U$, there is a unique positive weak solution $(u, v) = (u(\vec{h_1}, \vec{h_2}), v(\vec{h_1}, \vec{h_2}))$ of the state system (1).

Theorem

There exists an optimal control $(\vec{h_1}, \vec{h_2})^*$ maximizing the functional $J(\vec{h_1}, \vec{h_2})$ over U. i.e.

$$J(\vec{h_1}, \vec{h_2})^* = \sup_{(\vec{h_1}, \vec{h_2}) \in U} J(\vec{h_1}, \vec{h_2}) .$$

Derivation of the optimality system

To derive the necessary conditions, we need to differentiate the map

- We differentiate the $(\vec{h_1}, \vec{h_2}) \to J(\vec{h_1}, \vec{h_2})$ map and the $(\vec{h_1}, \vec{h_2}) \to (u, v)(\vec{h_1}, \vec{h_2})$ map with respect to the controls $\vec{h_1}$ and $\vec{h_2}$.
- The derivatives of this $(\vec{h_1}, \vec{h_2}) \to (u, v)(\vec{h_1}, \vec{h_2})$ map are the sensitivity functions ψ_1 and ψ_2

The sensitivity PDE's

For a given control $(\vec{h_1}, \vec{h_2}) \in U$, consider another control

$$(\vec{h_1}, \vec{h_2})^\epsilon = (\vec{h_1} + \epsilon\vec{l_1}, \vec{h_2} + \epsilon\vec{l_2})$$

s.t. $(\vec{h_1}, \vec{h_2}) + \epsilon(\vec{l_1}, \vec{l_2}) \in U$ for all sufficiently small $\epsilon > 0$ with $(\vec{l_1}, \vec{l_2}) \in ((L^\infty(\Omega))^d, (L^\infty(\Omega))^d)$ and

$$u^\epsilon = u(\vec{h_1} + \epsilon\vec{l_1}, \vec{h_2} + \epsilon\vec{l_2}) \ \text{ and } \ v^\epsilon = v(\vec{h_1} + \epsilon\vec{l_1}, \vec{h_2} + \epsilon\vec{l_2})$$

We can obtain

$$u^\epsilon \rightharpoonup u \quad , \quad v^\epsilon \rightharpoonup v \quad , \quad u_t^\epsilon \rightharpoonup u_t \quad , \quad v_t^\epsilon \rightharpoonup v_t$$

$$\frac{u^\epsilon - u}{\epsilon} \rightharpoonup \psi_1 \ \text{ and } \ \frac{\mathrm{v}^\epsilon - \mathrm{v}}{\epsilon} \rightharpoonup \psi_2 \ \text{ in } \ \mathrm{L}^2((0,\mathrm{T}),\mathrm{H}^1(\Omega))$$

Sensitivity PDE's

$$
\begin{aligned}
(\psi_1)_t - d_1\Delta\psi_1 - \nabla\cdot(\vec{h_1}\psi_1 + \vec{l_1}u) &= m\psi_1 - 2a_1u\psi_1 - b_1v\psi_1 - b_1u\psi_2 \quad \text{in} \quad Q \\
(\psi_2)_t - d_2\Delta\psi_2 - \nabla\cdot(\vec{h_2}\psi_2 + \vec{l_2}v) &= m\psi_2 - 2a_2v\psi_2 - b_2v\psi_1 - b_2u\psi_2 \quad \text{in} \quad Q \\
d_1\frac{\partial\psi_1}{\partial\eta} + \psi_1\vec{h_1}\cdot\eta &= -u\vec{l_1}\cdot\eta \quad \text{on} \quad S \\
d_2\frac{\partial\psi_2}{\partial\eta} + \psi_2\vec{h_2}\cdot\eta &= -v\vec{l_2}\cdot\eta \quad \text{on} \quad S \\
\psi_1(x,0) &= 0 \quad \text{for} \quad x\in\Omega \\
\psi_2(x,0) &= 0 \quad \text{for} \quad x\in\Omega\ .
\end{aligned} \tag{3}
$$

The adjoint functions:

- To characterize the optimal control, we will use the sensitivity function together with adjoint function to differentiate $(\vec{h_1}, \vec{h_2}) \rightarrow J(\vec{h_1}, \vec{h_2})$ map.
- The adjoint functions show how the states u, v affect the goal
- So, we find the formal adjoint of the operator in the sensitivity PDE s.t.

$$\begin{aligned} & \text{Left hand sides of weak forms of sensitivity equations} \\ & \text{with adjoints as test functions} \\ = \quad & \text{Left hand sides of weak forms of the adjoint equations} \\ & \text{with sensitivities as test functions} \end{aligned}$$

- The non-homogeneous terms on the RHS of the adjoint equations are obtained as,

$$\begin{pmatrix} A \\ \\ B \end{pmatrix} = \begin{pmatrix} \frac{\partial(\text{Integrand of} J)}{\partial u} \\ \\ \frac{\partial(\text{Integrand of} J)}{\partial v} \end{pmatrix} = \begin{pmatrix} \frac{\partial(Au+Bv-C|\vec{h_1}|^2-D|\vec{h_2}|^2)}{\partial u} \\ \\ \frac{\partial(Au+Bv-C|\vec{h_1}|^2-D|\vec{h_2}|^2)}{\partial v} \end{pmatrix}$$

The adjoint PDE's

$$
\begin{aligned}
-(\lambda_1)_t - d_1\Delta\lambda_1 + \vec{h_1}\cdot\nabla\lambda_1 - m\lambda_1 + 2a_1u\lambda_1 + b_1v\lambda_1 + b_2v\lambda_2 &= A \quad \text{in} \quad Q \\
-(\lambda_2)_t - d_2\Delta\lambda_2 + \vec{h_2}\cdot\nabla\lambda_2 - m\lambda_2 + 2a_2v\lambda_2 + b_1u\lambda_1 + b_2u\lambda_2 &= B \quad \text{in} \quad Q \\
\frac{\partial\lambda_1}{\partial\eta} &= 0 \quad \text{on} \quad S \\
\frac{\partial\lambda_2}{\partial\eta} &= 0 \quad \text{on} \quad S \\
\lambda_1(x,T) &= 0 \quad \text{for} \quad x\in\Omega \\
\lambda_2(x,T) &= 0 \quad \text{for} \quad x\in\Omega\ .
\end{aligned} \tag{4}
$$

Characterizing the optimal control $\vec{h}^*$

Suppose there exist an optimal control $(\vec{h_1}, \vec{h_2})^* \in U$ with the corresponding states u^*, v^* and compute the directional derivative of the function $J(\vec{h_1}, \vec{h_2})^*$ with respect to $(\vec{h_1}, \vec{h_2})^*$ in the direction $(\vec{l_1}, \vec{l_2})$ at u^*, v^*.

Since, $J(\vec{h_1}, \vec{h_2})^*$ is the maximum value for the $J(\vec{h_1}, \vec{h_2})$ we have

$$\begin{aligned} 0 &\geq \lim_{\epsilon \to 0^+} \frac{J((\vec{h_1}, \vec{h_2})^* + \epsilon(\vec{l_1}, \vec{l_2})) - J((\vec{h_1}, \vec{h_2})^*)}{\epsilon} \\ &= \int_Q (A\psi_1 + B\psi_2 - 2C\vec{h_1}^* \cdot \vec{l_1} - 2D\vec{h_2}^* \cdot \vec{l_2})\, dxdt \end{aligned}$$

Characterizing the optimal control $\vec{h}^*$

Note that,

$$\int_Q (A\psi_1 + B\psi_2)\ dxdt$$

$=$Sum of the LHS of weak forms of λ_1, λ_2 PDE's with test functions ψ_1, ψ_2

$=$Sum of the LHS of weak forms of ψ_1, ψ_2 PDE's with test functions λ_1, λ_2

$$= -\int_Q (\vec{l_1}, \vec{l_2}) \cdot (u\nabla\lambda_1 + 2C\vec{h_1}^*, v\nabla\lambda_2 + 2D\vec{h_2}^*)\ dxdt$$

Characterizing the optimal control $\vec{h}^*$

Hence, for any $(\vec{l_1}, \vec{l_2})$ we have

$$0 \geq -\int_Q (\vec{l_1}, \vec{l_2}) \cdot (u\nabla\lambda_1 + 2C\vec{h_1}^*, v\nabla\lambda_2 + 2D\vec{h_2}^*) \; dxdt$$

Using cases of $(h_1, h_2)_i^*$ and the sign of variation $(l_1, l_2)_i$,

$$\begin{aligned}(h_1)_i^* &= \min\left(M_1, \max\left(-\frac{u(\lambda_1)_{x_i}}{2C}, -M_1\right)\right) \\ (h_2)_i^* &= \min\left(M_2, \max\left(-\frac{v(\lambda_2)_{x_i}}{2D}, -M_2\right)\right)\end{aligned} \tag{5}$$

Theorem

For sufficiently small T, the solution to the optimality system is unique.

Numerical results

We consider a one spatial dimensional problem:

$$\begin{aligned} u_t - d_1 u_{xx} - (h_1 u)_x &= u[m - a_1 u] - b_1 uv \quad \text{on} \quad (0, L) \times (0, T) \\ v_t - d_2 v_{xx} - (h_2 v)_x &= v[m - a_2 v] - b_2 uv \quad \text{on} \quad (0, L) \times (0, T) \end{aligned}$$

$$\begin{aligned} d_1 u_x \cdot \nu + u h_1 \cdot \nu &= 0 \quad \text{for} \quad x = 0 \ \text{or} \ L \quad \text{and} \quad t \in (0, T) \\ d_2 v_x \cdot \nu + u h_1 \cdot \nu &= 0 \quad \text{for} \quad x = 0 \ \text{or} \ L \quad \text{and} \quad t \in (0, T) \end{aligned}$$

$$\begin{aligned} u(x, 0) &= u_0(x) \geq 0 \quad \text{for} \quad x \in (0, L) \\ v(x, 0) &= v_0(x) \geq 0 \quad \text{for} \quad x \in (0, L) \end{aligned}$$

$$\begin{aligned} h_1^* &= \min\left(M_1, \max\left(-\frac{u(\lambda_1)_x}{2C}, -M_1\right)\right) \\ h_2^* &= \min\left(M_2, \max\left(-\frac{v(\lambda_2)_x}{2D}, -M_2\right)\right) . \end{aligned}$$

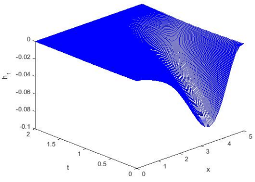
- We used a finite difference scheme to solve the PDE problem and the advection term was modeled using the upwind method.
  - When, the advection control h(i,j) is positive, we used the forward difference for space variable to represent the advection term.
  - When, the advection control h(i,j) is negative, we used the backward difference for space variable to represent the advection term.
- We used the forward backward sweep method to solve the optimal control problem.

First, numerical Illustration, with one population

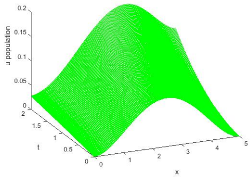
- First an example with

$$\mu = 0.1, \quad T = 2, \quad B = 0.5, \quad \text{and} \quad \textit{logistic} \quad \textit{growth}$$

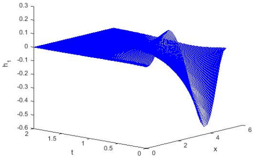
With our notation for the sign of advection terms, h_i being negative (positive) represents movement to right (left).



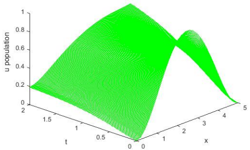
(a)



(b)



(c)



(d)

Figure 1: OC for u with $m = x/5$ and lower IC at top and higher IC at bottom. With higher IC, the OC not driven only by gradient of m

Two population case

Parameter values:

$$a_1 = 1 \quad a_2 = 1$$

$$A = 1 \quad B = 1 \quad C = 0.5 \quad D = 0.5$$

Diffusion Coefficients

$$d_1 = 0.2 \quad d_2 = 0.2$$

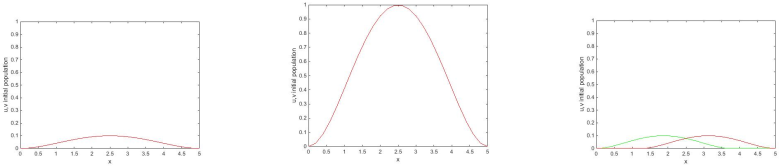
Control limits

$$\text{maximum } h_i = 4 \quad \text{minimum } h_i = -4$$

Domain:

spatial length: 5 units and time length: 2

Different initial conditions



(a) (b) (c)

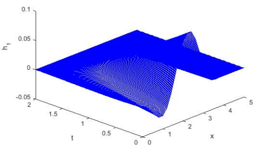
Figure 2: Different initial conditions

2(a)– Smaller initial populations at middle (both same)

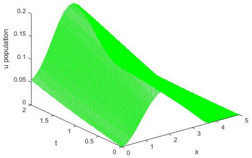
2(b)– Larger initial populations at middle (both same)

2(c)– Two smaller initial populations overlapping in the middle

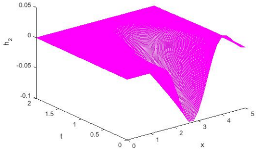
Two populations with resource in middle and different small ICs



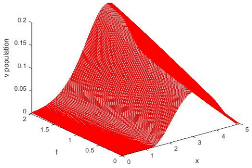
(a) Optimal control h_1



(b) Population distribution of u



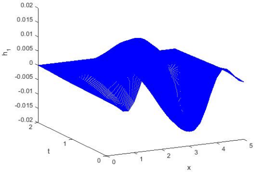
(c) Optimal control h_2



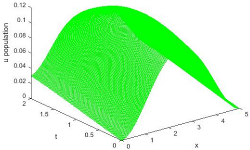
(d) Population distribution of v

Figure 3: Populations and optimal control with different small ICs and $m = sin(\pi x/5)$, Different OCs due to ICs and same competition, movement happens to avoid competition, going towards boundary not to resources

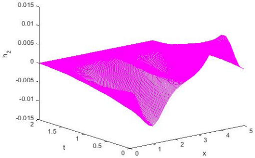
Two populations with different competition rates: $b_1 = 4$, $b_2 = 0.5$



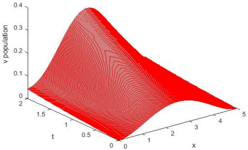
(a) Optimal control h_1



(b) Population distribution of u



(c) Optimal control h_2



(d) Population distribution of v

Figure 4: Population dynamics and optimal control with same small ICs and $m = sin(\pi x/5)$, Effect of different competition rates, better competitor v moves towards resources

Conclusions of first part

- With numerical simulations for one population only, we were able to show the population does not always choose the advection direction to move toward increasing resources.
- When the initial condition has a sufficiently high population with some variation, the movement may be chosen to move to level the population, instead of moving toward increasing resources.
- In the systems case, the level of the competition coefficients can also influence the choice of movement direction.
- Advective directions depend on the initial conditions, diffusion effects, competition rates, and resources.
- Currently working on PDE generalizations including other types of interactions besides competition.

Collaborators: Kokum DeSilva and Tuoc Phan paper appeared in DCDS B 2016

Optimal Control for the Sugarscape ABM via a PDE model

Agent-based model (ABM)

Collaborators: **Scott Christley**, University of Chicago
Matt Oremland, Mathematical Biosciences Institute
Rene Salinas, Appalachian State University
Rachael Neilan, Duquesne University

PAPER: 2016 in Optimal control: applications and methods

Perspective PAPER on optimal control and optimization on ABM: above collaborators and Fitzpatrick, Laubenbacher, An, Kanarek, Federico, Xiong, and Yong, Bulletin of Math Biology 2017

NIMBioS Working Group: Optimal Control for Agent-based Models

National institute for Mathematical and Biological Synthesis

Objective: Explore optimization frameworks for wide range of agent-based models (ABMs)

- Identify prototype ABMs for testing
- Apply different optimization tools to prototype ABMs and evaluate relative success

Outline of Method

Protoype ABM: Sugarscape ABM with control

Goal: Identify control values that steer ABM towards specified objective

Optimization Method

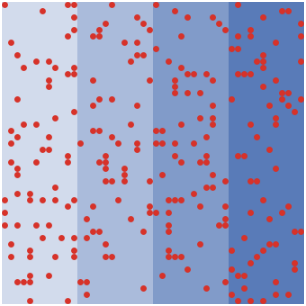
1. Approximate spatio-temporal dynamics of ABM with system of partial differential equations (PDEs)
2. Define objective functional for PDE model
3. Derive optimal control for PDE model using mathematical theory
4. Numerically solve optimality system
5. Discretize optimal control from PDE model and apply it to ABM

Sugarscape ABM

(modified version of Sugarscape in NetLogo (FREE SOFTWARE))

Landscape is 48×48 grid with four vertical regions defining sugar available to agents.

Each agent gains as much sugar as the patch contains per time step. Sugar in patch is not depleted.

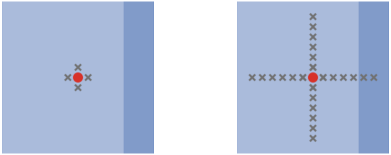


Agents cannot cross left and right boundaries. Wrap-around movement allowed on top and bottom.

Sugarscape ABM

Agents traverse landscape, accumulating or losing sugar.
Agents die when they run out of sugar.

- **Vision**: Each agent can see either 1 or 6 patches up, down, left, and right. Agents move each time step to cell in vision with highest sugar.



Low Vision　　High Vision

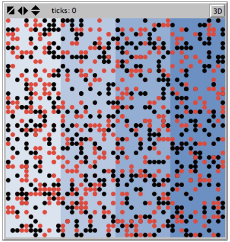
- **Low or High Metabolism**: Each agent burns 2 or 4 sugar per time step.

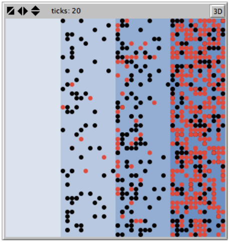
Sugarscape ABM

Initialization

- 4500 agents are placed on a random patch and given a random initial sugar between 0.25 – 10.
- Agents are given metabolism and vision values, chosen randomly. These do not change over the course of the simulation.

Simulations demonstrate wealth inequality over time.





Agents with high vision, low metabolism are able to move to region with high sugar intake and accumulate wealth.

Control: Taxation

- All agents are taxed a percentage of their sugar at the end of every time step.
- Tax rates can vary each time step.
- Tax rates can vary based on vision, metabolism, location, and current sugar held by agent.

Optimization Problem

What tax structure should be implemented to **maximize tax collected** while **minimizing death** over $T = 20$ time steps ?

PDE Model

Population divided into four classes of agents based on

- Metabolism: 2 (low) or 4 (high)
- Vision: 1 (low) or 6 (high)

State Variables

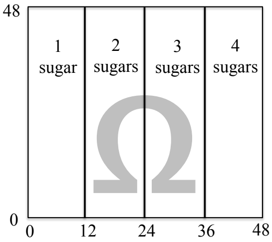
For $i = 1, 2, 3, 4...$

$N_i(x, s, t) =$ density of class i agents in location x with sugar s at time t

Domain

$$Q = \Omega \times (0, T) \times (o, \bar{s})$$

where $\Omega = (0, 48) \times (0, 48)$ and $\bar{s}$ is upper bound on the possible sugar obtained during time [0,T]



$S(x) =$ sugar available at location x

PDE Model

Control Variables: For $i = 1, 2, 3, 4...$

$u_i(x, t, s) =$ proportion of sugar removed from class i agents with sugar s in location x at time t

Set of admissible controls: $U = \{u_i \in L^\infty(Q) \mid u_i : Q \to [0, 1]\}$

State PDEs: For $i = 1, 2, 3, 4...$

$$\frac{\partial N_i}{\partial t} - a_i \sum_{j=1}^{2} \frac{\partial^2 N_i}{\partial x_j^2} + \sum_{j=1}^{2} b_{ij}(x) \frac{\partial N_i}{\partial x_j} + \frac{\partial}{\partial s} (R_i(x, s, t) N_i) = 0 \qquad (6)$$

where

- a_i is spatial diffusion coefficient for class i agents
- $b_{ij}(x)$ is spatial advection coefficient for class i agents
- $R_i(x, s, t) = S(x) - m_i - u_i(x, s, t)s$ is sugar advection coefficient for class i agents with metabolism m_i and $S(x)$ rate of agents gain sugar

PDE Model

State Boundary Conditions

Uniform spatial distribution of agents among sugar levels 0.25 - 10:

$$N_i(x, s, 0) = \bar{N}_i(x, s) \tag{7}$$

Wrap-around movement in vertical direction:

$$N_i(x_1, 0, s, t) = N_i(x_1, 48, s, t) \qquad \frac{\partial N_i(x_1, 0, s, t)}{\partial x_2} = \frac{\partial N_i(x_1, 48, s, t)}{\partial x_2} \tag{8}$$

No-flux movement in horizontal direction:

$$\frac{\partial N_i(0, x_2, s, t)}{\partial x_1} = 0 \qquad \frac{\partial N_i(48, x_2, s, t)}{\partial x_1} = 0 \tag{9}$$

Death when sugar is depleted:

$$N_i(x, 0, t) = 0 \qquad \text{if } R_i(x, 0, t) \geq 0 \tag{10}$$

Restricted sugar growth at upper bound:

$$N_i(x, \bar{s}, t) = 0 \qquad \text{if } R_i(x, \bar{s}, t) < 0 \tag{11}$$

Optimal Control Problem for PDE system

Optimization Problem

What tax structure should be implemented to **maximize tax collected** while **minimizing death** over $T = 20$ units of time?

Objective Functional

$$\max_{u_i \in U} \sum_{i=1}^{4} \int_0^T \int_\Omega \int_0^{\bar{s}} \left(BN_i + Au_i sN_i - \epsilon u_i^2\right) \mathrm{d}s \; \mathrm{d}x \; \mathrm{d}t$$

subject to state PDE (6) and boundary conditions (7-11).

Coefficients B, A, and ϵ balance the importance of maximizing population size (N_i) and taxes collected ($u_i sN_i$) with minimizing impact of high taxation rates (u_i^2).

Optimality System

Adjoint PDEs: For $i = 1, 2, 3, 4...$

$$-\frac{\partial P_i}{\partial t} - a_i \sum_{j=1}^{2} \frac{\partial^2 P_i}{\partial x_j^2} - \sum_{j=1}^{2} \frac{\partial (b_{ij} P_i)}{\partial x_j} - R_i(x, s, t) \frac{\partial P_i}{\partial s} = 1 + A u_i s \tag{12}$$

Adjoint Boundary Conditions

$$P_i(x, s, T) = 0 \tag{13}$$

$$P_i(x_1, 0, s, t) = P_i(x_1, 48, s, t) \tag{14}$$

$$a_i \frac{P_i(x_1, 0, s, t)}{dx_2} + b_{i2} P_i(x_1, 0, s, t) = a_i \frac{P_i(x_1, 48, s, t)}{dx_2} + b_{i2} P_i(x_1, 48, s, t) \tag{15}$$

$$a_i \frac{P_i(0, x_2, s, t)}{dx_1} + b_{i2} P_i(0, x_2, s, t) = 0 \qquad a_i \frac{P_i(48, x_2, s, t)}{dx_1} + b_{i2} P_i(48, x_2, s, t) = 0 \tag{16}$$

$$P_i(x, 0, t) = 0 \text{ if } R_i(x, \bar{s}, t) > 0 \tag{17}$$

$$P_i(x, \bar{s}, t) = 0 \text{ if } R_i(x, \bar{s}, t) \leq 0 \tag{18}$$

Optimality Condition

Optimal Control Characterization

For $i = 1, 2, 3, 4...$

$$u_i^* = \frac{1}{2\epsilon}[-sN_i \frac{\partial P_i}{\partial s} + AsN_i^*] \tag{19}$$

subject to upper and lower bounds, $0 \leq u_i^*(x, s, t) \leq 1$.

Implementation of optimal controls in ABM

Discretization of Space, Time, and Sugar

Numerical solutions of optimal control were found using $dx_1 = 1$, $dx_2 = 1$, $ds = 0.25$, $dt = 0.01$.

- Spatial discretizations of ABM and optimal control matched.
- Optimal control at sugar value s was applied to all agents in ABM with sugar between s and $s + ds$.
- Average value of optimal control between $(t, t + 1]$ was applied to ABM at each time $t + 1$.

Continuous vs. Discrete Rates

Tax collected in ABM from agent class i at time $t + 1$ is

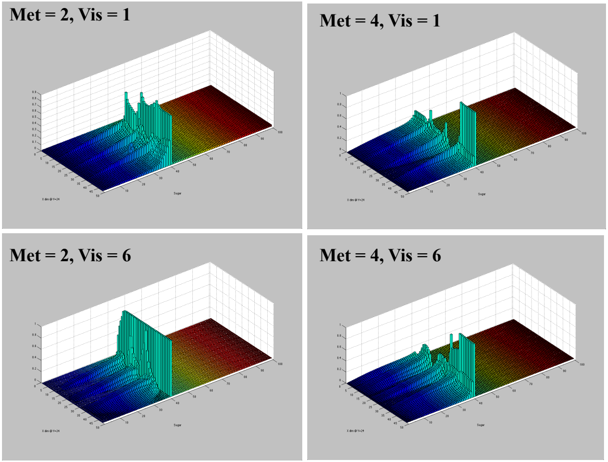
$$(e^{-ut})(\text{sugar at time } t) + \left(\frac{1-e^{-u}}{u}\right)(\text{sugar gained between } t \text{ and } t+1)$$

Results

- **No control**: $u_i(x, s, t) = 0 \;\; \forall (x, s, t) \in Q$
- **Optimal Control**: u_i^* for $B = 1, A = 1, \epsilon = 1$
- **Average optimal control**: $u_i(x, s, t) = \bar{u_i^*} \;\; \forall (x, s, t) \in Q$

Optimal Control

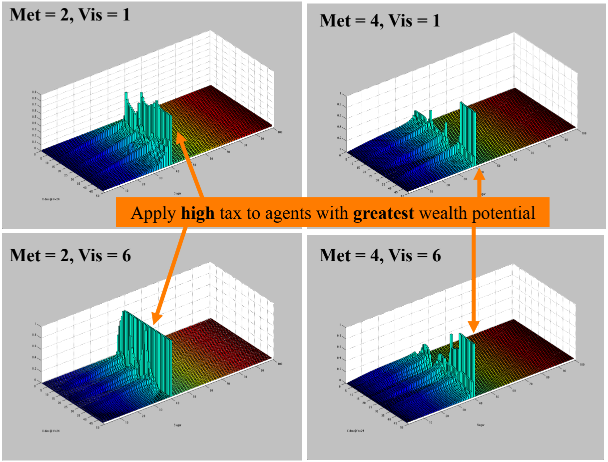
u_i^* **at** $t = 0$



Apply tax to select agents with maximum initial sugar.

Optimal Control

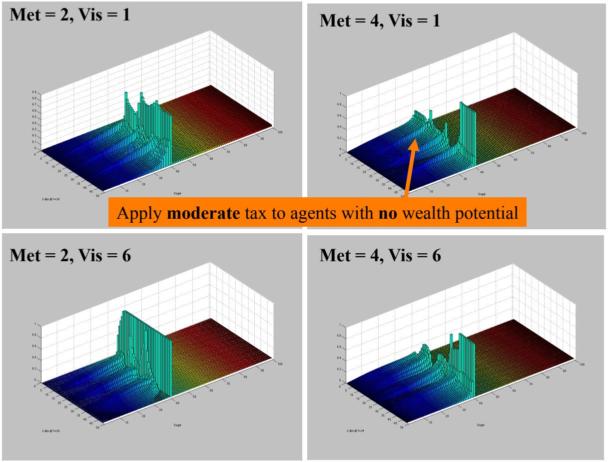
u_i^* **at** $t = 0$



Apply tax to select agents with maximum initial sugar.

Optimal Control

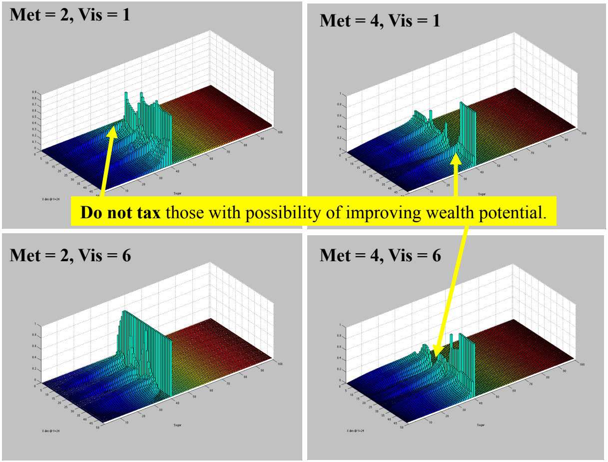
u_i^* **at** $t = 0$



Apply tax to select agents with maximum initial sugar.

Optimal Control

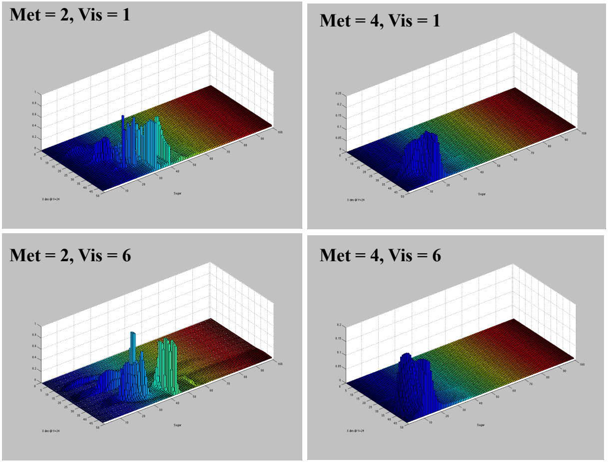
u_i^* at $t = 0$



Apply tax to select agents with maximum initial sugar.

Optimal Control

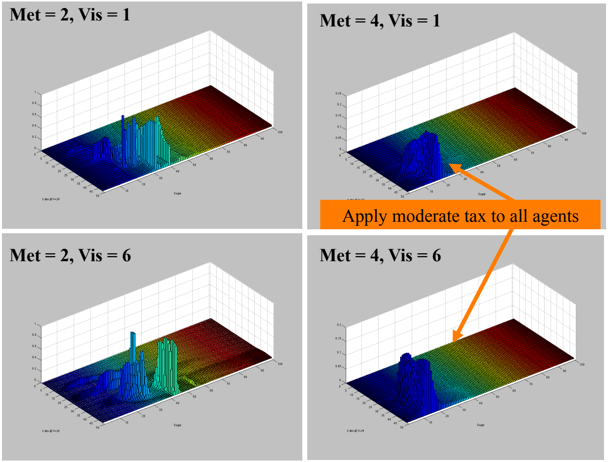
u_i^* **at** $t = 7$



During intermediate times, taxation rates decrease and policy becomes highly selective among remaining agents.

Optimal Control

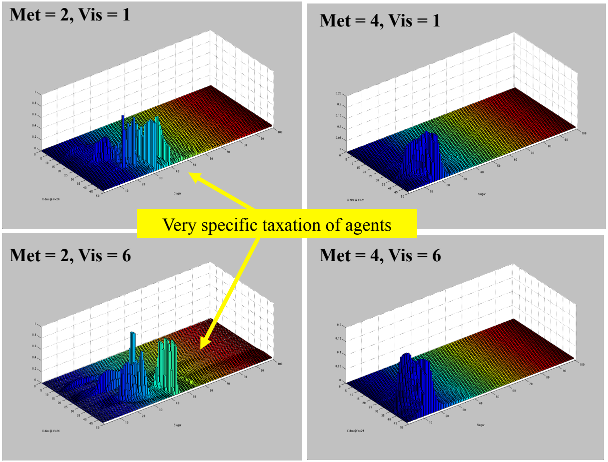
u_i^* **at** $t = 7$



During intermediate times, taxation rates decrease and policy becomes highly selective among remaining agents.

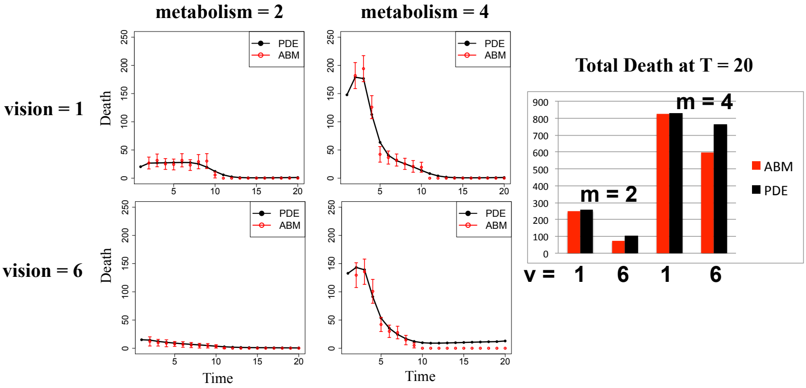
Optimal Control

u_i^* **at** $t = 7$



During intermediate times, taxation rates decrease and policy becomes highly selective among remaining agents.

Optimal Control: Death

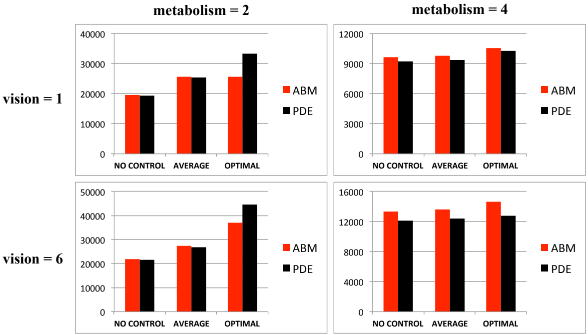


Despite differences in taxation, the two models show similar deaths.

Objective Functional Value

$$\int_0^T \int_\Omega \int_0^{\bar{s}} \left(BN_i + Au_i sN_i - \epsilon u_i^2\right) \mathrm{d}s \; \mathrm{d}x \; \mathrm{d}t$$

Calculate value for no control ($u_i = 0$), optimal control (u_i^*), and average optimal control ($u_i = \bar{u_i^*}$).



Optimal control always performs better than (or the same as) constant controls in the ABM.

Conclusions of second part

- PDE system approximates well the average ABM movement, sugar accumulation, and death in the absence of control.
- Optimal control for PDE system can be highly variable among spatial locations and sugar levels.
- Variability in continuous optimal control from PDE system is challenging to translate accurately back to discrete ABM.
- Implementation of discretized optimal control in the ABM is often better than using a constant control.

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and Thank You...!