Investigating advection control in competitive PDE systems

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OUTLINE
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OPTIMAL CONTROL OF AGENT-BASED MODELS
Introduction

- The reaction of a population for resources is an important concern in ecology.
- With inhomogeneous resources population may tend to move along the spatial gradient of the resource function depending on the initial conditions.
- What about when there is more than one population and there is a competition among them to survive??
The Goal

The Question:

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

- The Goal: To investigate this question with optimal control of PDE
Previous work: Concentrating on Movement

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

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

with zero flux boundary condition.

- \( m(x) \) represents the intrinsic growth rate and measures the availability of the resources.

- “beneficial” means the persistence of the population or the existence of a unique globally attracting steady state.
Previous work: Population Dynamics Model

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

REFERENCE: Finotti, Lenhart, Phan, EECT 2013

- $\Omega \subset \mathbb{R}^n$ 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

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

- $\vec{h} : Q_T \rightarrow \mathbb{R}^n$ is the advection direction.
- $m = m(x, t)$ in $L^\infty(Q_T)$ measures the availability of resources.
- $f : Q_T \times \mathbb{R} \rightarrow \mathbb{R}$ is non-negative and has some smoothness and growth conditions.
- $\mu > 0$ fixed (diffusion coefficient) and $u_0 \in L^\infty(\Omega)$ is smooth.
Seek the advection term $\vec{h}(x, t)$ control that maximizes the total population while minimizing the “cost” due to movement.

Find $\vec{h}^* \in U$ such that

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

$U = \{\vec{h} \in L^2((0, T), L^2(\Omega)^n) : |h_k| \leq M, \quad \forall k = 1, 2, \cdots, n\}.$

$B$ “cost coefficient” due to the population moving along $\vec{h}$.

Limited numerical results with small initial conditions (with little variation) show optimal controls following the gradient of $m$. 
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?

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

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

and

$$S = \partial \Omega \times (0, T).$$
The system of PDE’s describing the dynamics:

\[ u_t - d_1 \Delta u - \nabla \cdot (\vec{h}_1 u) = u[m - a_1 u] - b_1 uv \text{ in } Q \]
\[ v_t - d_2 \Delta v - \nabla \cdot (\vec{h}_2 v) = v[m - a_2 v] - b_2 uv \text{ in } Q \]

\[ d_1 \frac{\partial u}{\partial \eta} + u \vec{h}_1 \cdot \eta = 0 \text{ on } S \]
\[ d_2 \frac{\partial v}{\partial \eta} + v \vec{h}_2 \cdot \eta = 0 \text{ on } S \]

\[ u(x, 0) = u_0(x) \geq 0 \text{ for } x \in \Omega \]
\[ v(x, 0) = v_0(x) \geq 0 \text{ for } x \in \Omega \]
The optimal control problem formulation:

- **Control Set**

  \[ U = \{ (\vec{h}_1, \vec{h}_2) \in ((L^\infty(Q))^d, (L^\infty(Q))^d) : |(h_1)_i| \leq M_1, |(h_2)_i| \leq M_2, i = 1, \ldots, d \} \]

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

- Then, for \( A, B, C, D \geq 0 \) 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,

  \[ J(\vec{h}_1, \vec{h}_2) = \int_Q \left[ Au + Bv - C|\vec{h}_1|^2 - D|\vec{h}_2|^2 \right] \, dxdt \quad (2) \]

  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.
Sensitivity PDE’s

\[(\psi_1)_t - d_1 \Delta \psi_1 - \nabla \cdot (\vec{h}_1 \psi_1 + \vec{l}_1 u) = m \psi_1 - 2a_1 uv \psi_1 - b_1 v \psi_1 - b_1 u \psi_2 \quad \text{in} \; Q\]

\[(\psi_2)_t - d_2 \Delta \psi_2 - \nabla \cdot (\vec{h}_2 \psi_2 + \vec{l}_2 v) = m \psi_2 - 2a_2 v \psi_2 - b_2 v \psi_1 - b_2 u \psi_2 \quad \text{in} \; Q\]

\[d_1 \frac{\partial \psi_1}{\partial \eta} + \psi_1 \vec{h}_1 \cdot \eta = -u \vec{l}_1 \cdot \eta \quad \text{on} \; S\]

\[d_2 \frac{\partial \psi_2}{\partial \eta} + \psi_2 \vec{h}_2 \cdot \eta = -v \vec{l}_2 \cdot \eta \quad \text{on} \; S\]

\[\psi_1(x, 0) = 0 \quad \text{for} \; x \in \Omega\]

\[\psi_2(x, 0) = 0 \quad \text{for} \; x \in \Omega\]
The adjoint PDE's

\[-(\lambda_1)_t - d_1 \Delta \lambda_1 + \vec{h}_1 \cdot \nabla \lambda_1 - m \lambda_1 + 2a_1 u \lambda_1 + b_1 v \lambda_1 + b_2 v \lambda_2 = A \text{ in } Q\]
\[-(\lambda_2)_t - d_2 \Delta \lambda_2 + \vec{h}_2 \cdot \nabla \lambda_2 - m \lambda_2 + 2a_2 v \lambda_2 + b_1 u \lambda_1 + b_2 u \lambda_2 = B \text{ in } Q\]
\[\frac{\partial \lambda_1}{\partial \eta} = 0 \text{ on } S \quad (4)\]
\[\frac{\partial \lambda_2}{\partial \eta} = 0 \text{ on } S\]
\[\lambda_1(x, T) = 0 \text{ for } x \in \Omega\]
\[\lambda_2(x, T) = 0 \text{ for } x \in \Omega .\]
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

\[
0 \geq \lim_{\epsilon \to 0^+} \frac{J((\vec{h}_1, \vec{h}_2)^* + \epsilon(\vec{l}_1, \vec{l}_2)) - J((\vec{h}_1, \vec{h}_2)^*)}{\epsilon} = \int_Q (A\psi_1 + B\psi_2 - 2C\vec{h}_1^* \cdot \vec{l}_1 - 2D\vec{h}_2^* \cdot \vec{l}_2) \, dx \, dt
\]
Characterizing the optimal control $\vec{h}^*$

Hence, for any $(\vec{l}_1, \vec{l}_2)$ we have

$$0 \geq -\int_Q (\vec{l}_1, \vec{l}_2) \cdot (u \nabla \lambda_1 + 2C\vec{h}_1^*, v \nabla \lambda_2 + 2D\vec{h}_2^*) \, dx dt$$

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

$$(h_1)_i^* = \min \left( M_1, \max \left( -\frac{u(\lambda_1)x_i}{2C}, -M_1 \right) \right)$$

$$(h_2)_i^* = \min \left( M_2, \max \left( -\frac{v(\lambda_2)x_i}{2D}, -M_2 \right) \right)$$

(5)
The numerical results

We consider the one dimensional problem corresponds to problem (2):

\[
\begin{align*}
  u_t - d_1 u_{xx} - (h_1 u)_x &= u[m - a_1 u] - b_1 uv & \text{on} & & (0, L) \times (0, T) \\
  v_t - d_2 v_{xx} - (h_2 v)_x &= v[m - a_2 v] - b_2 uv & \text{on} & & (0, L) \times (0, T) \\
  d_1 u_x \cdot \nu + u h_1 \cdot \nu &= 0 & \text{for} & & x = 0 \text{ or } L \text{ and } & t \in (0, T) \\
  d_2 v_x \cdot \nu + u h_1 \cdot \nu &= 0 & \text{for} & & x = 0 \text{ or } L \text{ and } & t \in (0, T) \\
  u(x, 0) &= u_0(x) \geq 0 & \text{for} & & x \in (0, L) \\
  v(x, 0) &= v_0(x) \geq 0 & \text{for} & & x \in (0, L)
\end{align*}
\]

Hence from (5) we have

\[
\begin{align*}
  h_1^* &= \min \left( M_1, \max \left( -\frac{u(\lambda_1)_x}{2C}, -M_1 \right) \right) \\
  h_2^* &= \min \left( M_2, \max \left( -\frac{v(\lambda_2)_x}{2D}, -M_2 \right) \right).
\end{align*}
\]
We used a finite difference scheme to solve the PDE problem and the advection term was modeled using the up wind 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.
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

maximum \( h_i = 4 \) \quad minimum \( h_i = -4 \)

Domain:

spatial length: \( 5 \) units and time length: \( 2 \)

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

Figure 1: Different resource functions $m(x)$

(a) $x/5$  
(b) $\sin(\pi x/5)$  
(c) $6x/5$
Optimal control in PDE systems
Investigating advection control in competitive PDE systems
Optimal control of advection direction in competitive parabolic PDEs systems

Different initial conditions

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
Optimal control in PDE systems
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Without competition: One population only, effects of variation in IC

Figure 3: 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 populations with competition and same small ICs

(a) Optimal control $h_1$  
(b) Population distribution of $u$

**Figure 4:** Populations and optimal controls with same small ICs and the resource function $m = sin(\pi x/5)$ with effect of competition on OC.
Two populations with competition and different small ICs

Figure 5: Population dynamics and optimal control with different small ICs and $m = \sin(\pi x/5)$, Different OCs due to ICs and competition
Two populations with different competition rates: $b_1 = 4$, $b_2 = 0.5$

Figure 6: Population dynamics and optimal control with same small ICs and $m = \sin(\pi x/5)$, Effect of different competition rates
Conclusions

- 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.
Optimal Control for the Sugarscape ABM via a PDE model

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**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

**Prototype 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 function 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
Optimal control in PDE systems

Introduction

Sugarscape ABM

(modified version of Sugarscape in NetLogo)

Landscape is $48 \times 48$ 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.
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.

- **Metabolism**: Each agent burns 2 or 4 sugar per time step.
Optimal control in PDE systems

Introduction

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.
Sugarscape ABM

**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?
Population divided into four classes of agents based on

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

**State Variables**
For $i = 1, 2, 3, 4...$

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

**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 $[0, T]$

$S(x) = \text{sugar available at location } x$
Control Variables: For \( i = 1, 2, 3, 4 \ldots \)

\( u_i(x, t, s) = \) 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 \( i = 1, 2, 3, 4 \ldots \)

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

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 \( m_i \)
State Boundary Conditions
Uniform spatial distribution of agents among sugar levels 0.25 - 10:

\[ N_i(x, s, 0) = \bar{N}_i(x, s) \] (7)

Wrap-around movement in vertical direction:

\[ N_i(x_1, 0, s, t) = N_i(x_1, 48, s, t) \quad \frac{\partial N_i(x_1, 0, s, t)}{\partial x_2} = \frac{\partial N_i(x_1, 48, s, t)}{\partial x_2} \] (8)

No-flux movement in horizontal direction:

\[ \frac{\partial N_i(0, x_2, s, t)}{\partial x_1} = 0 \quad \frac{\partial N_i(48, x_2, s, t)}{\partial x_1} = 0 \] (9)

Death when sugar is depleted:

\[ N_i(x, 0, t) = 0 \quad \text{if} \quad R_i(x, 0, t) \geq 0 \] (10)

Restricted sugar growth at upper bound:

\[ N_i(x, \bar{s}, t) = 0 \quad \text{if} \quad R_i(x, \bar{s}, t) < 0 \] (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

$$\max_{u_i \in U} \sum_{i=1}^{4} \int_{0}^{T} \int_{\Omega} \int_{\bar{\Omega}} (BN_i + Au_isN_i - \epsilon u_i^2) \, ds \, dx \, dt$$

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

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

**Adjoint PDEs:** For \( i = 1, 2, 3, 4 \ldots \)

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

**Adjoint Boundary Conditions**

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

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

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

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

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

\[
P_i(x, \bar{s}, t) = 0 \text{ if } R_i(x, \bar{s}, t) \leq 0 \tag{18}
\]
Optimal Control Characterization
For $i = 1, 2, 3, 4...$

$$u_i^* = \frac{1}{2\epsilon}[sN_i \frac{\partial P_i}{\partial s} + AsN_i^*]$$  \hspace{1cm} (19)

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

- 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.
Optimal control in PDE systems
Results

Thank you....!!!

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