Numerical Approximation of a Free Boundary Problem for a Predator-Prey Model

Răzvan Ştefănescu and Gabriel Dimitriu

University of Medicine and Pharmacy "Gr. T. Popa",
Department of Mathematics and Informatics,
700115 Iasi, Romania
rastefanescu@yahoo.co.uk, dimitriu.gabriel@gmail.com

Abstract. This paper is concerned with the numerical approximation of a free boundary problem associated with a predator-prey ecological model. Taking into account the local dynamic of the system, a stable finite difference scheme is used, and numerical results are presented.

1 Introduction

In recent years, the two-species predator-prey ecological models have received increasing research attention. Various forms of the systems have been proposed, especially on the following coupled systems of two reaction-diffusion equations:

$$\begin{cases} P_t - d_1 \Delta P = P(a_1 - b_{11}P + c_{12}Q), & x \in \Omega, t > 0, \\ Q_t - d_2 \Delta Q = Q(a_2 - b_{21}P - c_{22}Q), & x \in \Omega, t > 0, \end{cases} \tag{1}$$

where $d_i,\ a_i,\ b_{ij},\ c_{ij}$ are positive constants. In biological terms, P and Q represent, respectively, the spatial densities of predator and prey species that are interacting and migrating in the habitat Ω, d_i denotes its respective diffusion rate, and the real number a_i describes its net birth rate. b_{11} and c_{22} are the coefficients of intra-specific competitions, and b_{21} and c_{12} are the coefficients of inter-specific competitions. In the case that c_{12} is replaced by $-c_{12}$, (1) is the well-known Lotka-Volterra competition model.

Movement plays a role in structuring the interactions between individuals, their environment and their species. Next to the first passage time concept (in the context of animal movement, first passage time is the time taken for an animal to reach a specified site for the first time), the free boundary predator-prey models represent a new modality of understanding the effect of the landscape on animal movement and search time.

The remainder of the article is organized as follows. In the next section we briefly describe the free boundary predator-prey model. Section 3 is devoted to the description of the numerical approach. The numerical results are presented and discussed in Section 4. Finally, Section 5 is dedicated to the presentation of some conclusions and objectives for future work.

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2 Free Boundary Problem

The asymptotic behavior of species have been known in the literature for domains with fixed boundary. In what follows, we consider that the predator species are initially limited to a specific part of the domain. To be more specific, let us consider the one-dimensional case. Assume that the prey species migrates in the habitat $(0, l)$ and the predator disperses through random diffusion only in a part of the habitat $(0, l)$, namely $0 < x < h(t)$, then there is no predator in the remaining part.

Let the diffusivity of the predator be d_1. Then the number of predator populations flowing across the boundary $x = h(t)$ from time t to time $t + \Delta t$ is $J\Delta t = -d_1(\partial P/\partial x)\Delta t$. These predators disperse from $x = h(t)$ to $x = h(t+\Delta t)$ during the time interval $[t, t + \Delta t]$ and the size of the population decides the length $h(t + \Delta t) - h(t)$. Supposing

$$-d_1 \frac{\partial P}{\partial x} \Delta t = f[h(t + \Delta t) - h(t)],$$

we know that the function f is increasing and $f(0) = 0$. Ecologically, this means that the size is increasing with respect to the moving length. Using the Taylor expansion of the function f one obtains

$$f[h(t+\Delta t) - h(t)] = 0 + f^{'}(0)[h(t+\Delta t) - h(t)] + \frac{1}{2} f^{''}(0)[h(t + \Delta t) - h(t)]^2 + ...$$

and therefore

$$-d_1 \frac{\partial P}{\partial x} = f^{'}(0) \frac{[h(t + \Delta t) - h(t)]}{\Delta t} + \frac{1}{2} f^{''}(0) \frac{[h(t + \Delta t) - h(t)]^2}{\Delta t} + ...$$

Now, letting $\Delta t \to 0$, we arrive at

$$-d_1 \frac{\partial P}{\partial x} = f^{'}(0) h^{'}(t).$$

Here, $f^{'}(0)$ is a positive constant since f is increasing and depends on the diffusivity of the predator in the part where no predator exists. If $f^{'}(0)$ is big enough, then the predator can disperse easily in the new area.

Denoting $\mu = d_1/f^{'}(0)$, then the conditions on the interface (free boundary) are

$$P = 0, \qquad -\mu \frac{\partial P}{\partial x} = h^{'}(t).$$

If all populations do not attempt to emigrate from inside, then there is no flux crossing the fixed boundary, that is, the homogeneous Neumann boundary conditions hold

$$\frac{\partial P}{\partial x}(0, t) = \frac{\partial Q}{\partial x}(0, t) = \frac{\partial Q}{\partial x}(0, t) = 0.$$

In such case, we have the problem for $P(x,t)$ and $Q(x,t)$ with a free boundary $x = h(t)$ such that

$$(P) \quad \begin{cases} P_t - d_1 P_{xx} = P(a_1 - b_{11}P + c_{12}Q), & 0 < x < h(t),\ t > 0, \\ Q_t - d_2 Q_{xx} = Q(a_2 - b_{21}P - c_{22}Q), & 0 < x < l,\ t > 0, \\ P(x,t) = 0, & h(t) < x < l,\ t > 0, \\ P = 0,\ h'(t) = -\mu \frac{\partial P}{\partial x}, & x = h(t), \quad t \geq 0, \\ \frac{\partial P}{\partial x}(0,t) = \frac{\partial Q}{\partial x}(0,t) = \frac{\partial Q}{\partial x}(l,t) = 0, & t > 0, \\ h(0) = b, \quad (0 < b < l), & \\ P(x,0) = P_0(x) \geq 0, & 0 \leq x \leq b, \\ Q(x,0) = Q_0(x) \geq 0, & 0 \leq x \leq l, \end{cases}$$

where the initial values P_0, Q_0 are nonnegative and satisfy $P_0(x) \in C^2[0,b]$, $P_0(x) > 0$, for $x \in [0,b)$, $P_0^{'} < 0$, $Q_0(x) \in C^2[0,l]$ and the consistency conditions $P_0^{'}(0) = Q_0^{'}(0) = Q_0^{'}(l) = 0$.

In the absence of Q, the problem is reduced to the one-phase Stefan problem, which accounts for phase transitions between solid and fluid states such as the melting of ice in contact with water. The existence, uniqueness and asymptotic behavior of the solution for (1) are known ([8]).

The results for free boundary problems have been applied to many areas, for example, the decrease of oxygen in a muscle in the vicinity of a clotted bloodvessel, the etching problem, the combustion process, the American option pricing problem ([6]), chemical vapour deposition in a hot wall reactor, image processing ([1]), wound healing and tumour growth ([4], [5] and [7]), the temperature distribution for polythermal ice sheets ([3]).

3 Numerical Approximation

The discretization is carried out by finite differences. The grids with equidistant nodes are denoted by:

$$0 = x_1 < x_2 < ... < x_{2n+1} = l,\ x_{n+1} = b; \qquad 0 = t_1 < t_2 < ... < t_{m+1} = T.$$

Furthermore, we choose : $x_j = (j-1)h, \quad j = 1, 2, ..., 2n+1$ with $h = \frac{1}{n}$, and $t_i = (i-1)k, \quad i = 1, 2...., m+1$, with $k = \frac{T}{m}$.

To obtain the numerical approximation of problem (P), we use the standard implicit scheme which is unconditionally stable.

Let $P_j^{(i)}$ and $Q_j^{(i)}$ be the approximations of $P(t_i, x_j)$ and $Q(t_i, x_j)$. The initial conditions yield:

$$P_j^{(1)} = P_0(x_j), \quad j = \overline{1,n}; \qquad Q_j^{(1)} = Q_0(x_j), \quad j = \overline{1, 2n+1}.$$

Our next goal is to pass from some level i $(t = t_i)$ to the next level *i+1* $(t = t_{i+1})$, for $i = \overline{1,m}$. First, we need to determine the free boundary $h(t_{i+1})$, before calculating the solution of the system (P) at time level t_{i+1}. Thus, we search for an interval $[x_p, x_{p+1}]$ such that $h(t_i) \in [x_p, x_{p+1}]$. Then, in order to match the points from the free boundary with the grid points, we evaluate and compare the distances between $h(t_i)$ and x_p and $h(t_i)$ and x_{p+1}, respectively. The lowest value of this distance gives us the point x_f which represents the corresponding grid boundary point at time level t_i.

From the free boundary conditions we get:

$$h(t_{i+1}) = -\mu\frac{k}{h}[P(x_f,t_i) - P(x_{f-1},t_i)] + h(t_i).$$

Using a Taylor's series expansion we get the following discretization for the system equations:

$$-d_1kP_{j-1}^{(i+1)} + (h^2 + 2d_1k - a_1kh^2)P_j^{(i+1)} - kh^2c_{12}P_{j+1}^{(i+1)}Q_{j+1}^{(i+1)}$$

$$+b_{11}kh^2(P_j^{(i+1)})^2 - d_1kP_{j+1} - h^2P_j^{(i)} = 0, \qquad j = \overline{2, f-1},$$

for the first equation, and

$$-d_2kQ_{j-1}^{(i+1)} + (h^2 + 2d_2k - a_2kh^2)Q_j^{(i+1)} + b_{21}kh^2Q_{j+1}^{(i+1)}P_{j+1}^{(i+1)}$$

$$+c_{22}kh^2(Q_j^{(i+1)})^2 - d_2kQ_{j+1}^{(i+1)} - h^2Q_j^{(i)} = 0, \qquad j = \overline{2, 2n},$$

for the second one.

The discretization of equation corresponding to the boundary condition leads to

$$Q_2^{(i+1)} = Q_1^{(i+1)}; \qquad Q_{2n+1}^{(i+1)} = Q_{2n}^{(i+1)}; \qquad P_2^{(i+1)} = P_1^{(i+1)};$$

Moreover, we have $P_j^{(i+1)} = 0,\ j = \overline{f, 2n}$.

If we denote by $\alpha_1 = h^2 + d_2k - a_2kh^2$, $\alpha_2 = h^2 + 2d_2k - a_2kh^2$, $\beta_1 = h^2 + d_1k - a_1kh^2$ and $\beta_2 = h^2 + 2d_1k - a_1kh^2$, we obtain the discrete problem (P_h):

$$\begin{cases} \alpha_1Q_2^{(i+1)} + b_{21}kh^2Q_2^{(i+1)}P_2^{(i+1)} + c_{22}kh^2(Q_2^{(i+1)})^2 - d_2kQ_3^{(i+1)} - h^2Q_2^{(i)} = 0, \\ -d_2kQ_{j-1}^{(i+1)} + \alpha_2Q_j^{(i+1)} + b_{21}kh^2Q_{j+1}^{(i+1)}P_{j+1}^{(i+1)} + c_{22}kh^2(Q_j^{(i+1)})^2 \\ -d_2kQ_{j+1}^{(i+1)} - h^2Q_j^{(i)} = 0, \qquad j = \overline{3, 2n-1}, \\ -d_2kQ_{2n-1}^{(i+1)} + \alpha_1Q_{2n}^{(i+1)} + b_{21}kh^2Q_{2n}^{(i+1)}P_{2n}^{(i+1)} + c_{22}kh^2(Q_{2n}^{(i+1)})^2 - h^2Q_{2n}^{(i)} = 0, \\ \beta_1P_2^{(i+1)} - c_{12}kh^2P_2^{(i+1)}Q_2^{(i+1)} + b_{11}kh^2(P_2^{(i+1)})^2 - d_1kP_3^{(i+1)} - h^2P_2^{(i)} = 0, \\ -d_1kP_{j-1}^{(i+1)} + \beta_2P_j^{(i+1)} - c_{12}kh^2P_j^{(i+1)}Q_j^{(i+1)} + b_{11}kh^2(P_j^{(i+1)})^2 \\ -d_1kP_{j+1}^{(i+1)} - h^2P_j^{(i)} = 0, \qquad j = \overline{3, f-2}, \\ -d_1kP_{f-2}^{(i+1)} + \beta_2P_{f-1}^{(i+1)} - c_{12}kh^2P_{f-1}^{(i+1)}Q_{f-1}^{(i+1)} + b_{11}kh^2(P_{f-1}^{(i+1)})^2 - h^2P_{f-1}^{(i)} = 0, \\ P_j^{i+1} = 0, \qquad j = \overline{f, 2n}, \end{cases}$$

which is a nonlinear algebraic system with $4n-2$ equations and $4n-2$ unknowns.

Remark 1. We use $P_j^{(i+1)}$ for $j = \overline{f, 2n}$ as unknowns, even if these are equal to zero, in order to get an algebraic system which has the number of equations equal to the number of unknowns.

To solve this nonlinear system, we use the Newton-Raphson method. We introduce the unknowns x_i according to

$$x_i = Q_{i+1},\ i = \overline{1, 2n-1}; \qquad x_j = P_{j-(2n-2)},\ j = \overline{2n, 4n-2}$$

Next, the problem (P_h) can be rewritten as:

$$f_l(x_1, x_2, ..., x_{4n-2}) = 0, \qquad l = \overline{1, 4n-2}, \tag{2}$$

where f_l represents the equation (1) of the discretized system.

If we denote by $X = (x_1, x_2, ..., x_{4n-2})$, then in the neighborhood of X, each of the functions f_l can be expanded in Taylor series as

$$f_l(X + \delta X) = f_l(X) + \sum_{v=1}^{4n-2} \frac{\partial f_l}{\partial x_v}\delta x_v + O(\delta X^2).$$

By neglecting the terms of order δX^2 and higher, we obtain a set of linear equations for the correction δX, that move each function closer to zero simultaneously:

$$\sum_{v=1}^{4n-2} a_{lv}\delta x_v = \beta_l, \qquad l = \overline{1, 4n-2},$$

where

$$a_{lv} = \frac{\partial f_l}{\partial x_v};\ \beta_l = -f_l(X).$$

This linear system can be solved by a direct method or an iterative one. The corrections are then added to solution vector:

$$x_i^{new} = x_i^{old} + \delta x_i.$$

To start this algorithm, we have to choose an initial estimate of the system's solution(at every time level i), and also a stopping criterion for ending the iteration process, which in our case was defined by

$$||\delta X||_{max} \le 10^{-3}.$$

In the sequel, we present the Jacobian matrix corresponding to the system (2).

$$J = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

where:

$$A = \begin{pmatrix} q_2 & q_1 & 0 & 0 & \cdots & \cdots & 0 \\ q_1 & q_3 & q_1 & 0 & \cdots & \cdots & 0 \\ 0 & q_1 & q_4 & q_1 & 0 & \cdots & 0 \\ 0 & 0 & q_1 & q_5 & q_1 & 0 & \cdots \\ \cdots & \cdots & \cdots & \ddots & \ddots & \ddots & \cdots \\ 0 & 0 & \cdots & \cdots & q_1 & q_{2n-1} & q_1 \\ 0 & 0 & \cdots & \cdots & 0 & q_1 & q_{2n} \end{pmatrix},\ B = \begin{pmatrix} p_2 & 0 & \cdots & \cdots & 0 \\ 0 & p_3 & 0 & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots & \cdots \\ 0 & \cdots & \cdots & p_{2n-1} & 0 \\ 0 & 0 & \cdots & 0 & p_{2n} \end{pmatrix},$$

$$C=\begin{pmatrix} s_2 & 0 & \cdots & \cdots & \cdots & \cdots\cdots & 0 \\ 0 & s_3 & 0 & \cdots & \cdots & \cdots\cdots & 0 \\ \cdots\cdots & \ddots & \cdots & \cdots & \cdots\cdots\cdots \\ 0 & \cdots\cdots & s_{f-2} & 0 & \cdots\cdots & 0 \\ 0 & 0 & \cdots & 0 & s_{f-1} & 0 \cdots & 0 \\ 0 & \cdots\cdots & \cdots & \cdots & 0 & \cdots\cdots \\ 0 & \cdots\cdots & \cdots & \cdots & \cdots\cdots & 0 \end{pmatrix}, D=\begin{pmatrix} r_2 & r_1 & 0 & 0 & \cdots & \cdots\cdots\cdots & 0 \\ r_1 & r_3 & r_1 & 0 & \cdots & \cdots\cdots\cdots & 0 \\ 0 & r_1 & r_4 & r_1 & 0 & \cdots\cdots\cdots & 0 \\ \cdots\cdots & \ddots & \ddots & \ddots & \cdots\cdots\cdots \\ 0 & 0 & \cdots & r_1 & r_{f-1} & 0 & \cdots\cdots & 0 \\ 0 & 0 & \cdots\cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & \cdots\cdots\cdots & \cdots & \cdots & 1 & \cdots & 0 \\ \cdots\cdots\cdots\cdots & \cdots & \cdots\cdots\cdots\cdots \\ 0 & \cdots\cdots\cdots & \cdots & \cdots\cdots\cdots & 1 \end{pmatrix},$$

with

$$\begin{cases} q_1 = -d_2k, \\ q_2 = h^2 + d_2k - a_2kh^2 + b_{21}kh^2P_2 + 2c_{22}kh^2Q_2, \\ q_l = h^2 + 2d_2k - a_2kh^2 + b_{21}kh^2P_l + 2c_{22}kh^2Q_l, & l = \overline{3, 2n-1}, \\ q_{2n} = h^2 + d_2k - a_2kh^2 + b_{21}kh^2P_{2n} + 2c_{22}kh^2Q_{2n}, \\ p_l = b_{21}kh^2Q_l, \quad l = \overline{2, 2n}, \\ s_l = -kh^2c_{12}P_l, \quad l = \overline{2, f-1}, \\ r_1 = -d_1k, \\ r_2 = h^2 + d_1k - a_1kh^2 - kh^2c_{12}Q_2 + 2b_{11}kh^2P_2, \\ r_l = h^2 + 2d_1k - a_1kh^2 - kh^2c_{12}Q_l + 2b_{11}kh^2P_l, & l = \overline{3, f-1}. \end{cases}$$

Remark 2

a) Matrices C and D have a special form, owing to the free boundary $h(t)$.
b) The overall error satisfies :

$$(i).\ ||Q_j^{(i)} - Q(x_j, t_i)||_{max} = O(h^2) + O(k), \qquad j = \overline{1, 2n+1}, i = \overline{2, n+1},$$

$$(ii).\ ||P_j^{(i)} - P(x_j, t_i)||_{max} = O(h^2) + O(k), \qquad j = \overline{1, 2n+1}, i = \overline{2, n+1}.$$

These error estimates are deduced from the Taylor series expansions of $Q(x_j, t_i)$ and $P(x_j, t_i)$.

4 Numerical Results

The numerical tests have been performed with the following values of the parameters: $l = 2$, $T = 1$, $d_1 = 0.31$, $d_2 = 0.7$, $a_1 = 0.5$, $a_2 = 1.5$, $b_{11} = 0.9$, $c_{22} = 1.3$, $b_{21} = 0.4$, $c_{21} = 1$, $maxit = 100$, $eps = 0.001$, $\mu = 0.35$, $k_1 = 1$, $k_2 = 0.5$, $b = 1$, $P_0(b) = 0.3$, $n = m = 31$.

Here $maxit$ is the maximum number of iterations for Newton-Raphson method, eps the stopping criterion also for Newton-Raphson method, k_1 and k_2 the initial values (at time step $t = 1$) for Q and P.

The free boundary corresponding to the prey and predator is shown in Figure 1.

We used the Newton Raphson method for nonlinear systems to get these results. As we told before, this algorithm needs, at every time step, some initial

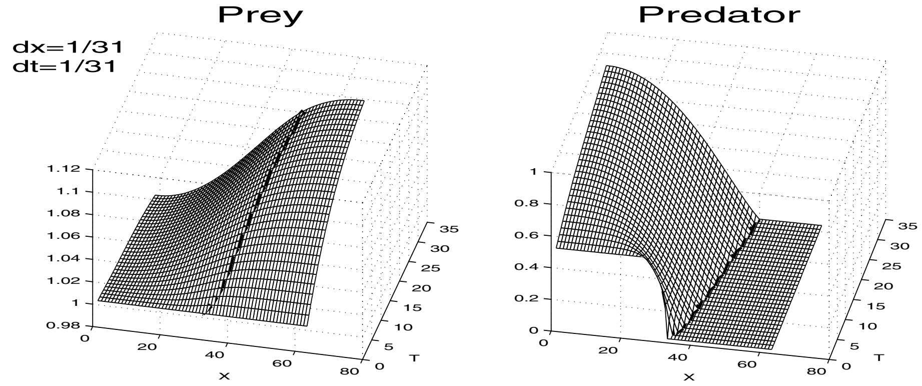

Fig. 1. The profiles of the state variables Q (left side) and P (right side), respectively

values for the solutions Q and P, in order to start it. In our case, at time level *i+1*, we choose as initial estimations to be the values of Q and P obtained at time step i.

Next, if we analyze the results in a different way (for a similar interpretation of the inverse Stefan problem see [2], pp. 132-137), separating the values of P respectively Q depending on the initial values, we see that a new free boundary arises. The behavior of this free boundary is shown in Figure 2. The meaning of the symbols in these figures is specified as

I : a grid node (t_i, x_j) such that $Q(t_i, x_j) = k_1,\ P(t_i, x_j) = k_2$;
$+$: a grid node (t_i, x_j) such that $Q(t_i, x_j) > k_1,\ P(t_i, x_j) > k_2$;
$-$: a grid node (t_i, x_j) such that $Q(t_i, x_j) < k_1,\ P(t_i, x_j) < k_2$;
0 : a grid node (t_i, x_j) such that $P(t_i, x_j) = 0$;

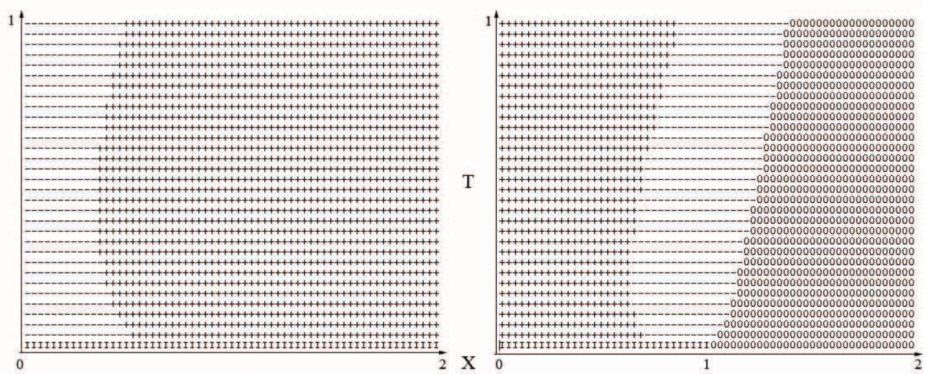

Fig. 2. The projection on the horizontal plane (x, t) of the variation profiles for Q (left side) and P (right side), respectively. The free boundary delimits the areas between negative and positive values for state variables.

5 Conclusions

In this study we focused on the numerical approximation of a free boundary problem for a predator-prey model. Using an implicit scheme, we obtained a nonlinear system of algebraic equations, which was solved with Newton-Raphson method. The numerical solution was determined by using Matlab software.

For the model considered here, it is assumed that the number of predators flowing across the free boundary is increasing with respect to the moving length. Similar free boundary condition can be found in [4] for modeling the corneal stimulus cell density in the healed region. From ecological point of view, one more reasonable assumption is possibly that the motion of predators relies on the prey. In other words, the higher the density of the prey at the free boundary, the larger the flux of the predators should be.

Compared with the existing models such as tumor growth, to the best of our knowledge, there are very few results from the free boundary problems describing ecological models. As a future task, we intend to discretize this problem using spectral methods both in 1D and 2D cases, and also, in order to manipulate the free boundary, we want to place the problem into an optimal control framework.

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