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A SMALL PARAMETER METHOD FOR THE CHEMOTAXIS PROBLEM

The paper proposes an iterative method for constructing an approximate analytical solution for the chemotaxis problem in a spatially constrained one-dimensional system. Within the proposed approach, an approximate analytical solution is obtained, sufficient conditions for its applicability are identified, and the approximate and numerical solutions are compared.

Keywords: chemotaxis, attractant, small parameter, distribution, convergence, iteration.

It will take time to restore chaos.

George BUSH

1. Introduction

When solving engineering and physical problems, researchers often encounter mathematically complex problems that lack an analytical solution. In such circumstances, the alternative is either to obtain numerical solutions or to obtain approximate analytical solutions. Each approach has its advantages and disadvantages. A numerical solution can, in principle, be considered “accurate”. More specifically, the accuracy of the solution is determined by the accuracy of the numerical method used to obtain it. In most cases, this accuracy is controllable in the sense that if the numerical method is convergent, it is usually possible to obtain a solution with the required accuracy. However, even this approach is not always acceptable. The fact is that when solving problems in theoretical physics or mathematical biophysics, it

is often necessary to have an analytical solution. It is critically important in cases where the goal of obtaining a solution is further qualitative analysis of the system under study. This is a fairly common and, in a sense, “classical” situation. A numerical solution, no matter how accurate it may be, is usually not suitable for this role. The fundamental impossibility of obtaining an exact analytical solution complicates the situation, but even in its absence, an approximate analytical solution may be quite sufficient. Moreover, an exact solution can be so complex and inconvenient that using an approximate analytical solution becomes a priority. Chemotaxis is an example of a situation in which all of the above is extremely relevant [1–19].

Chemotaxis is a process by which flagellated bacteria move toward higher concentrations of an attractant. *Escherichia coli* bacteria are an example of this, and sugar is the attractant. The whole process is quite complex and multi-stage (see, for example, [20–22]). The bacteria in question can move thanks to the rotation of their flagella. They move uniformly and in a straight line. However, at certain moments, a process called tumbling occurs – the bacterium stops and randomly changes its direction of movement. Bacteria also have specialized receptors that detect attractants. Upon interaction with an attrac-

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tant, the receptors become activated and remain in this state for some time. An important point is that the more receptors are activated in a bacterium, the less likely it is to tumble. In other words, the more attractant a bacterium registers during movement, the less likely it is to change its direction of movement. As a result, the bacterium ends up in the area with a higher attractant concentration. There is a method for studying chemotaxis based on phenomenological models whose core is a system of diffusion-type nonlinear differential equations (see [23–30] and, for comparison and review of models, [31–33]). The specific formulation of the problem depends on the system's dimension, the attractant's distribution characteristics, and the method of injecting bacteria into the system. However, in general, such a system does not admit an exact analytical solution. At the same time, analytical solutions (even approximate ones) are of primary interest, since they are necessary for the qualitative analysis of the corresponding biophysical processes in chemotaxis. Therefore, finding methods to construct approximate analytical solutions to the chemotaxis problem is both relevant and promising.

2. Formulation of the Problem

We consider a one-dimensional system containing bacteria and an attractant. We are interested in finding the stationary distribution of bacteria in such a system. To do this, we formalize the problem. Namely, we assume that the spatial coordinate x varies from 0 to L , i.e., $0 \leq x \leq L$. Let $b(x)$ denote the distribution function of bacteria in the system. Let $a(x)$ denote the distribution of attractant in the system. According to the basic model, the flow $j_b(x)$ of bacteria is determined as follows [23–30]:

$$j_b(x) = -D \frac{db}{dx} + k \frac{b(x) \frac{da}{dx}}{(a_0 + a(x))^2}, \quad (1)$$

where D is the diffusion coefficient, k and a_0 are phenomenological parameters of the model. The first term on the right-hand side of expression (1) describes bacterial diffusion, while the second term describes the contribution to the flow associated with chemotaxis. This term is proportional to the bacterial concentration and the gradient (derivative) of the attractant concentration. The denominator in this term causes saturation in the chemotaxis process, leading to almost all receptors becoming activated and the

bacterium becoming less sensitive to the attractant during movement [21, 22].

The stationarity of the bacterial distribution in the system means that the bacterial flow is constant (including the possibility that it may be zero). However, to finally formulate the problem, it is necessary to set boundary conditions and determine the distribution of the attractant. Boundary conditions are usually chosen based on the experimental setup. We will consider a situation where the number of bacteria at the boundaries of the system is the same and is given:

$$b(0) = b(L) = B, \quad (2)$$

where B is known. As for the attractant, we will consider its concentration to be zero at the left boundary $x = 0$, and at the right boundary $x = L$, the concentration of the attractant will be considered known:

$$a(0) = 0, \quad (3)$$

$$a(L) = A, \quad (4)$$

where the value of A is given. Moreover, under conditions (3), (4), and free distribution of the attractant in the system, it is easy to show that the spatial distribution of the attractant will be linear in the coordinate:

$$a(x) = A \frac{x}{L}. \quad (5)$$

Taking all this into account, we can finally write down the ratio which, together with condition (2), determines the stationary distribution of bacteria in the system:

$$D \frac{db}{dx} - \frac{kA}{L} \frac{b(x)}{(a_0 + \frac{A}{L}x)^2} = \text{const}, \quad (6)$$

where the constant on the right-hand side of equation (6) is found from condition (2).

For further analysis, equation (6) should be written in dimensionless form. To do this, let $x = Lz$ ($0 \leq z \leq 1$), $b(x) = Bm(z)$, and denote $\alpha = \frac{kA}{Da_0^2}$ and $\beta = \frac{A}{a_0}$. Then, we obtain the following equation for determining the profile $m(z)$:

$$\frac{dm}{dz} - \alpha \frac{m(z)}{(1 + \beta z)^2} = C, \quad (7)$$

with boundary conditions

$$m(0) = m(1) = 1, \quad (8)$$

which, among other things, contains the value of the constant on the right-hand side of equation (7).

In principle, problem (7), (8) has an analytical solution, which is given by the relation

$$m(z) = \exp\left(\frac{\alpha z}{1 + \beta z}\right) + C \exp\left(-\frac{\alpha}{\beta(1 + \beta z)}\right) \times \int_0^z \exp\left(\frac{\alpha}{\beta(1 + \beta t)}\right) dt, \quad (9)$$

where the C constant is defined as follows:

$$C = \frac{\exp\left(\frac{\alpha}{\beta(1 + \beta)}\right) - \exp\left(\frac{\alpha}{\beta}\right)}{\int_0^z \exp\left(\frac{\alpha}{\beta(1 + \beta t)}\right) dt}. \quad (10)$$

The problem is that this solution is not very suitable for practical use. Therefore, we propose a method that makes it possible to construct a relatively simple approximate analytical solution for problem (7), (8).

3. Approximate Analytical Solution

First, it is worth noting that the value of the parameter $\alpha = 0$ corresponds to a situation where there is no chemotaxis in the system (i.e., when bacteria do not respond to the presence of a substance we call an attractant). If so, then problem (7), (8) has an obvious, almost trivial solution

$$m(z) \equiv 1, \quad (11)$$

which satisfies relation (7) and boundary conditions (8). As for the approximate solution in the presence of chemotaxis, we will search for it in the form of a series in the small parameter α . For real systems studied in practice, this approach is reasonable. Therefore, we will represent the function being sought in the following form

$$m(z) \approx \sum_{k=0}^n m_k(z) \alpha^k, \quad (12)$$

where the functions $m_k(z)$ ($k = 0, 1, \dots, n$) are unknown. Then, from equation (7), we have the following:

$$\sum_{k=0}^n \frac{dm_k}{dz} \alpha^k - \sum_{k=0}^n \frac{m_k(z) \alpha^{k+1}}{(1 + \beta z)^2} = C, \quad (13)$$

which ultimately boils down to recurrent equations

$$\frac{dm_{k+1}}{dz} = C_{k+1} + \frac{m_k(z)}{(1 + \beta z)^2} \quad (14)$$

for $k \geq 0$ with boundary conditions

$$m_k(0) = m_k(1) = 0, \quad (15)$$

when $k \geq 1$, and the solution for $m_0(z)$ is determined by relation (11). The solution for $m_1(z)$ is quite easy to find. Specifically, to determine this function, we have the equation

$$\frac{dm_1}{dz} - \frac{1}{(1 + \beta z)^2} = C_1 \quad (16)$$

under the condition $m_1(0) = m_1(1) = 0$, from which we get $C_1 = -\frac{1}{1 + \beta}$ and the final solution

$$m_1(z) = \frac{1}{\beta} - \frac{z}{1 + \beta} - \frac{1}{\beta(1 + \beta z)}. \quad (17)$$

Therefore, in a linear approximation with respect to the parameter α , the solution to the problem is as follows

$$m(z) \approx 1 + \alpha \left(\frac{1}{\beta} - \frac{z}{1 + \beta} - \frac{1}{\beta(1 + \beta z)} \right) = 1 + \frac{\alpha \beta z (1 - z)}{(1 + \beta)(1 + \beta z)}. \quad (18)$$

As for the subsequent approximations, considering equality (14) and boundary conditions (15), we can obtain a recursive relation that links the functions $m_{k+1}(z)$ and $m_k(z)$ for $k \geq 0$:

$$m_{k+1}(z) = \int_0^z \frac{m_k(t)}{(1 + \beta t)^2} dt - z \int_0^1 \frac{m_k(t)}{(1 + \beta t)^2} dt. \quad (19)$$

The approximations following the first one are not trivial, but expression (19) can serve as a basis for calculating a certain number of analytical approximations automatically using computer algebra systems such as Maple or Mathematica.

4. Applicability of the Method

If we consider an infinite series

$$m(z) = \sum_{k=0}^{\infty} \alpha^k m_k(z), \quad (20)$$

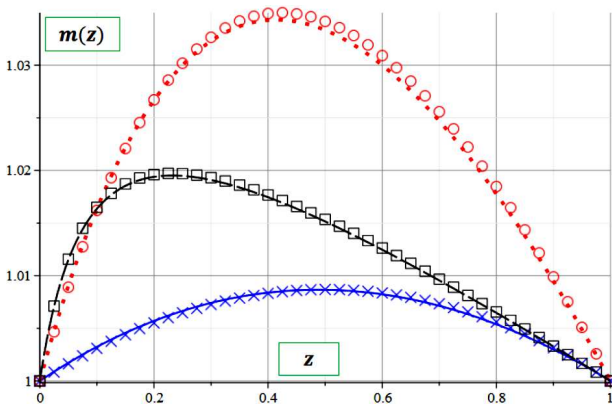


Fig. 1. Numerical solutions for problem (7), (8) and approximate analytical solutions for $\alpha = 0.4$ and different values of β : the crosses and the solid line are for $\beta = 0.1$, the circles and the dotted line are for $\beta = 1$, the squares and the dashed line are for $\beta = 10$

with functions $m_k(z)$ defined according to the recurrence relation (19), the following estimates can be made regarding the uniform convergence of series (20). Thus, if we assume that for some $k \geq 0$ the estimate $|m_k(z)| \leq \mu_k$ holds, where μ_k is a known value, then from (19), we can obtain

$$\begin{aligned}
 |m_{k+1}(z)| &= \left| \int_0^z \frac{m_k(t)}{(1+\beta t)^2} dt - z \int_0^1 \frac{m_k(t)}{(1+\beta t)^2} dt \right| \leq \\
 &\leq \left| \int_0^z \frac{m_k(t)}{(1+\beta t)^2} dt \right| + \left| z \int_0^1 \frac{m_k(t)}{(1+\beta t)^2} dt \right| \leq \\
 &\leq \mu_k \left(\left| \int_0^z \frac{dt}{(1+\beta t)^2} \right| + \left| z \int_0^1 \frac{dt}{(1+\beta t)^2} \right| \right) \leq \\
 &\leq 2\mu_k \left| \int_0^1 \frac{dt}{(1+\beta t)^2} \right| = \frac{2\mu_k}{1+\beta}.
 \end{aligned} \quad (21)$$

Given that $|m_0(z)| \leq \mu_0 = 1$, we have an estimate for the functions included in the expression for functional series (20):

$$|m_{k+1}(z)| \leq \left(\frac{2}{1+\beta} \right)^k. \quad (22)$$

Then, a sufficient condition for the uniform convergence of series (20) will be

$$\frac{2\alpha}{1+\beta} < 1. \quad (23)$$

Considering the natural (arising from the nature of the problem under study) constraints on the parameters $\alpha > 0$ and $\beta > 0$, as well as the fact that the parameter β is determined from the boundary conditions for the attractant (the concentration of the attractant at the right boundary), which can be changed in the experiment, we arrive at another important conclusion, which is that for $\alpha < \frac{1}{2}$, series (20) is uniformly convergent regardless of the value of the parameter β .

5. Analysis of Results

Thus, for the chemotaxis problem (7), (8), an approximate solution has been obtained, and a sufficient condition (23) for its validity has been found. As an illustration, Fig. 1 shows the numerical solutions of the problem (7), (8) compared to the approximate analytical solutions (18), which correspond to the linear approximation in the parameter α and were obtained for the value $\alpha = 0.4 < 1/2$ and several different values of the parameter β .

The results of these and other assessments show that even in a linear approximation in the parameter α , solution (18) for problem (7), (8) gives a qualitatively acceptable result under condition (23) and can therefore be used in practice. As noted, the analytical expression for the bacterial distribution profile in the chemotaxis problem, even if it is approximate, has an undeniable advantage over numerical solutions. First, it enables further qualitative analysis of the corresponding system using the appropriate mathematical apparatus, which is extremely important in theoretical and applied research (see, for example, [10–19] and the references therein). Second, it simplifies the interpretation and visualization of results. As for the criteria for the applicability of an approximate solution, several points are worth noting here. On the one hand, the estimates obtained provide only sufficient conditions for the convergence of the functional series (20) and, accordingly, the possibility of applying an approximate solution instead of a numerical one. Failure to meet the sufficient conditions does not necessarily mean that approximate solutions are invalid. On the other hand, in studies of physical, biophysical, or technical problems, the validity of an approximate solution is usually verified mainly through its practical application. In this sense, the existence

of clear criteria that guarantee the applicability of an approximate solution is a significant result and greatly facilitates further study of the corresponding system.

6. Conclusions

Thus, we have obtained an approximate analytical solution for the chemotaxis problem in a one-dimensional system. An algorithm for constructing subsequent approximations has been proposed, and sufficient conditions have been found under which such an approximate solution can be applied in practice. The results of the analysis are confirmed by comparing numerical solutions with approximate analytical solutions. The results obtained in this work may be useful in further research on chemotaxis systems. They are also of certain value for the confirmation of the correctness and reliability of the results obtained earlier for systems of a similar nature in previous studies.

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МЕТОД МАЛОГО ПАРАМЕТРА
В ЗАДАЧІ ХЕМОТАКСИСУ

У статті пропонується ітераційний метод для побудови аналітичного наближеного розв'язку задачі хемотаксису в просторово обмеженій одновимірній системі. У рамках запропонованого підходу отримано такий розв'язок, знайдено достатні умови його застосовності й виконано порівняння аналітичного наближеного і чисельного розв'язків.

Ключові слова: хемотаксис, аттрактант, малий параметр, розподіл, збіжність, ітерація.