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"Estudio en la duda. Acción en la fe"

División Académica de Ciencias Básicas
UJAT

JOBS
Journal of Basic Sciences

DACB • UJAT

Volumen 10 • número 29 • septiembre-diciembre 2024

ISSN:2448-4997
https://revistas.ujat.mx/index.php/jobs

En el número 29 del Journal of Basic Sciences, los lectores podrán encontrar reportes de investigaciones en diversos ámbitos del quehacer de las ciencias básicas, que al generar y aplicar el conocimiento científico, se encaminan hacia la atención de problemáticas específicas y también a una mejor comprensión del universo.

Por ejemplo, el desarrollo de procedimientos analíticos para el control de calidad de productos para el consumo humano, es indispensable para asegurar los beneficios, así como disminuir los riesgos potenciales que puedan estar asociados. Es así que se presenta un estudio dirigido a la optimización de un método de preconcentración dirigido a la determinación de contaminantes derivados del ácido ftálico, que pueden estar presentes en bebidas embotelladas. El método reportado presenta una buena precisión y buenos límites de detección, por lo que se considera una buena opción en el pretratamiento de muestras. Por otro lado, se incluye una aportación dirigida a evaluar la calidad microbiológica de dos bebidas ancestrales: el aguamiel y el pulque, cuyo consumo puede representar un beneficio por el aporte de probióticos y prebióticos, aunque es necesario el establecimiento de parámetros normados de calidad e inocuidad, que puedan dar certeza a los procesos de fabricación de las mismas.

Una problemática actual en la química ambiental, son los denominados contaminantes emergentes, los cuales no están regulados en su disposición final por encontrarse en bajas concentraciones, pero que tienen la propiedad de ser bioacumulables, representando un riesgo potencial para la salud. Este es el caso de colorantes industriales como el naranja ácido 52, para el cual se presenta un estudio de su procesos de degradación mediante diversas tecnologías avanzadas de oxidación, con resultados efectivos para su remoción. En otro orden de ideas, el diseño de materiales con propiedades específicas es también un área de gran interés, como lo muestra el artículo relacionado con la evaluación de hidrogeles de carboximetilcelulosa como agentes para la liberación controlada de fármacos.

Además, en este número se presenta un estudio relacionado con la estimación de parámetros para la interacción de tres especies en un nicho ecológico: planta, plaga y agente de biocontrol, empleando la modelación matemática por un método multipasos. No menos importante, es la contribución presentada para la determinación numérica de los estados ligados de un sistema cuántico, con un pozo de potencial triangular, lo que permitió profundizar en la comprensión de este tipo de sistemas.

Así, con este número del Journal of Basic Sciences, se difunde el quehacer científico en diferentes vertientes, esperando sea de utilidad para nuestros lectores.

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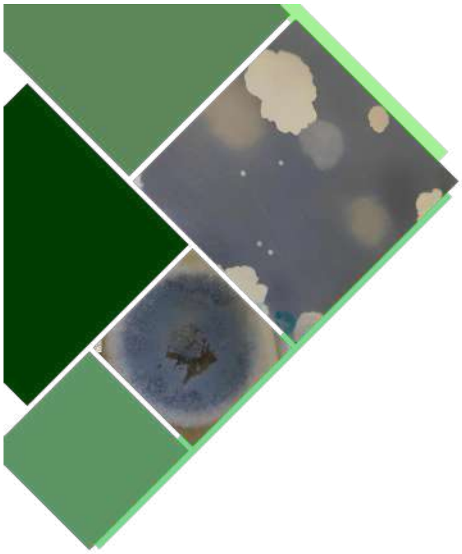

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CONTENIDO

Vol. 10 (29), p. 50-63, septiembre-diciembre 2024,e-ISSN: 2448 4997
JOURNAL OF BASIC SCIENCES

NUMERICAL ESTIMATION OF PARAMETERS IN MATHEMATICAL MODELS FOR PEST CONTROL

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Resumen

En este trabajo nos centramos en la estimación de parámetros de un modelo matemático para la interacción de tres especies, (planta, plaga, agente de bio control), con el objetivo de garantizar la sobrevivencia de todas las especies. Se lleva a cabo un análisis cualitativo del modelo matemático para mostrar la dinámica del mismo. El modelo se resuelve utilizando un esquema numérico basado en los métodos multi pasos, el código obtenido se acopla con el entorno de trabajo Spux para estimar, mediante simulaciones estocásticas, los parámetros desconocidos del modelo. Los resultados obtenidos muestran que Spux da valores esperados de los parámetros, porque los resultados de las simulaciones hechas, con los valores de los parámetros estimados recrean de manera satisfactoria los datos proporcionados.

Palabras claves: *Comensalista, Punto de equilibrio, Métodos multi pasos, Estimación de parámetros, Spux*

Abstract

In this work we focused on the estimation of the parameters belonging to a mathematical model for the interaction between three species (plant, plague and bio control agent), with the goal to guaranty the survival of all them. A qualitative analysis of the model is carried out to show the dynamic of it. As well, the model is solved by using a numerical scheme based on multi step method. The obtained code is coupled with the Spux framework to estimate, by stochastic simulations, the unknown parameters of the model. Numerical results show that Spux gives a correct approximation of the parameters because the model simulations with the approximated parameters are in good agreement with the data.

Keywords: *Conmesalist, Equilibrium points, Multi-Stept Method, Parameter Estimation, Spux*

Recibido: 04 de junio de 2024, Aceptado: 22 de septiembre de 2024, Publicado: 16 de diciembre de 2024

1. Introducción

A usual strategy for the pest control is to do a combination of several method in a framework known as Integrated Pest Management (IPM). This approach focuses on the reduction of the pest up to levels where both plant and pest can survive, and the minimization of both the economical cost for the producer and the risk for the people and the environment [11]. Several works were focused on the analysis of mathematical models into the IPM approach by supposing that there is not exist interaction between the predators, then the functional and numerical responses just depend on the number of the prey population. However, it is natural to take into account the interactions between the predators, [1, 3]. First, a summary of the mathematical model analysis for the interaction between the plant, parasite and the bio-control agent, is presented. This análisis has been developed in [11]. The mathematical model has several numerical parameters, which has to be estimated due to they are essential in the numerical solution. The estimation of parameter is usually done by manual tuning or by optimization processes with the goal of reproduce the data phenomenon. With this way to estimate the parameters, the computational cost increases and the uncertainties of the parameters is dismissed [17]. Nowadays, an efficient alternative to carry out the estimation of the parameters, by taking into account the effects of the uncertainties, is the Bayesian inference [6]. To carry out the Bayesian inference is needed to define a model M, which is the problem to be solved, and formulate the so called likelihood function of that model M. The model M is formulated as a probability distribution of the observations data D, for given parameter values θ. In this sense the model M shall depend on the parameters to be estimated. Additional to the model, to do the Bayesian inference, it is needed to have some prior information of the modeled by a probabilistic distribution $\pi(\theta)$. We also need a probabilistic distribution of the error in the data, because the data usual have errors, such as, observation errors, measurements errors, among others.

In this work, we shall estimate the parameter of the mathematical model by using the framework Spux, [17]. This software offers a framework that is open to a large class of model structure and it is possible to use any programming language, for instance, C/C++, java, Python, Fortran, among others. The framework was programmed in Python due to it is simple, popular, flexible and it has been constantly updated. To carry out the parameter estimation, in this work, the mathematical model will be solved by using a multi step numerical scheme. The chosen numerical scheme is the predictor corrector one.

The Adams Moulton method is employed to predict a preliminar solution, [9]. In order to do that, this method computes the integral of the right hand system, over a certain time interval,by using the polimial approximation of such that right hand site. After that, the correction is done by using the Adams-Bashfort method, [9]. This method computes the approximation by employing a fourth degree polynomial approximation of the right hand site of the system, this approximation, is used to compute the integral. In order to compute the solution at wished time is needed to solve a non linear system, to avoid this difficulty, the obtained preliminar approximation is used to compuete the right hand site of the system in the correction processes. In order to obtain the solution at the first two instants, the fourth order Runge Kutta numerical scheme will be employed. The numerical scheme, to compute the global solution, is implemented in a code developed in the language C++, because the computational time to solve the problem is less than the compute time spent by other programming languages. The final code is coupled with the framework Spux to do the numerical estimation of the parameters.

2. Mathematical model and qualitative análisis

A system of differential equations is proposed to model the interaction of three populations: plants, pests, and biocontrol agents, with population densities denoted by x, y and z, respectively. We assume that the pest predates the plant, the relationship between the plant and the biocontrol agent is commensalism and the biocontrol agent predates the pest. In the literature, to the best knowledge of the authors, models that include a commensalism between biocontrol and the host have not been analyzed. Explicitly, we study the following differential equations system:

$$\dot{x} = r_1 x\left(1 - \frac{x}{k_1 + \beta_1 z}\right) - \alpha\frac{xy}{b + cyz},$$

$$\dot{y} = \gamma\frac{xy}{b+cyz} - \mu y - v yz, \qquad (1)$$

$$\dot{z} = r_2 z\left(1 - \frac{z}{k_2\beta_2 y}\right).$$

In this system we assume that:

- α is the predation rate of pest on plant.
- μ is the mortality rate of the pest.
- v is the predation rate of biocontrol agent on pest.
- γ is the conversion rate of consumed plant biomass into pest biomass.
- r_1 is the plant intrinsic growth rate.
- r_2 is the biocontrol agent intrinsic growth rate.
- k_1 and k_2 are the carrying capacities of plant and biocontrol agent, respectively.
- β_1 is the profit rate that receive plant of biocontrol agent, as a consequence of the commensalism between plants and biocontrol agent.
- β_2 is the increment of carrying capacity of biocontrol agent due to the pest predation.
- b is the half-saturation constant.
- c measures the interference of biocontrol agent in the plant predation.
- The pest is specialist and its relationship with biocontrol agent is predator-prey type with Lotka-Volterra functional response.

For biological reasons, we consider that all parameters in system (1) are positive, then dynamics is analyzed in the positive octan which is denoted by Ω.

2.1 Local analysis of the model

The following statements holds, [11].

The trivial equilibrium points of the system are those equilibrium points that have at least one coordinate equal to zero. Then system (1) presents the following trivial equilibrium points

1 $* \tilde{P}_0 = (0,0,0),$

2 $* \tilde{P}_1 = (k_1, 0,0),$

3 $* \tilde{P}_2 = (0,0,k_2),$

4 $* \tilde{P}_3 = (k_1 + k_2\beta_1, 0, k_2),$

$$* \tilde{P}_2 = \left(\frac{b\mu}{\gamma}, \frac{br_1(\gamma k_1 - b\mu)}{\alpha\gamma k_1}, 0\right).$$

From all of the trivial equilibrium points, the most important of them is $\tilde{P}_3$, as it is where the eradication of the pest occurs.

- The coexistence equilibrium points (CEP) of the system (1) are those equilibrium points with positive coordinates. In section 2 of [11] the authors demonstrate that system (1) has at most four CEPs
- The trivial equilibrium points $\tilde{P}_0$, $\tilde{P}_1$, $\tilde{P}_2$ and $\tilde{P}_4$ of system (1) are saddle points.
- The equilibrium point $\tilde{P}_3 = (k_1 + k_2\beta_1, 0, k_2)$, of system (1) is locally asymptotically stable, if $\frac{\mu + v k_2}{k_1 + k_2\beta_1} > \frac{\gamma}{b}$. In other words, the pest population becomes extinct if the ratio between the potential maximum mortality rate of the pest population ($\mu + v k_2$) and the potential máximum carrying capacity of the plant population ($k_1 + k_2\beta_1$) exceeds the benefit the pest receives from consuming plant biomass. Thus, a relatively inefficient pest is driven to extinction.
- The equilibrium $\tilde{P}_3$ is locally asymptotically stable if only if system (1) has four, two or no CEPs.

Additionally, examples are provided where system (1) exhibits bistability and tristability. Bistability is demonstrated when the system has three CEPs, two of which are locally asymptotically stable. Tristability is shown when the system has four CEPs, two of which are locally asymptotically stable, along with the trivial equilibrium $\tilde{P}_3$, which is also locally asymptotically stable.
System (1) presents the following bifurcations:

- A transcritical bifurcation at $\tilde{P}_1$ with respect to parameter b.
- A transcritical bifurcation or a pitchfork bifurcation at $\tilde{P}_3$ with respect to parameter b.
- A transcritical bifurcation or a pitchfork bifurcation at $\tilde{P}$ with respect to parameter μ.
- A saddle-node bifurcation at $P = \left(\frac{5(689-\sqrt{324305}}{2212}, \frac{1}{2}, \frac{3}{5}\right)$ with bifurcation parameter μ and bifurcation value $\mu = \frac{544}{553}$.
- A saddle-node bifurcation at P = (0.5465, 0.7864, 1.7864) with bifurcation parameter μ and bifurcation value μ= 1.0934.

The proofs of previous results can be consulted at [11].

3. Numerical solution of the system

In this section we present the numerical solution of the mathematical model introduced in Section 2 and the numerical estimation for the parameters of the model.

3.1 Multi-step method

In this section we present the numerical solution of the mathematical model (1). In order to do that, we follow the work presented in [12, 13, 18]. In this work we have chosen the Adams-Moulton method, because of the classical ones, like Euler method [4] and the Runge Kutta method [5], they were tested and they can not reach the stable state of the mathematical model, which has been shown in Section 2.

The mathematical model can be considered as

$$\dot{\mathbf{X}}=\mathbf{F}(t,\mathbf{X}), \tag{2}$$

where

$$\mathbf{X}=\begin{pmatrix} x \\ y \\ z \end{pmatrix},$$

and

$$\boldsymbol{F}(t,\boldsymbol{X}) = \begin{pmatrix} r_1 x\left(-\dfrac{x}{k_1\beta_1 z}\right) - \alpha\dfrac{xy}{b+cyz} \\ \gamma\dfrac{xy}{b+cyz} - \mu y - \nu yz \\ r_2 z\left(1-\dfrac{z}{k_2\beta_2 y}\right) \end{pmatrix}.$$

We want to approximated the solution of initial problema value

$$\dot{\mathbf{X}}=\mathbf{F}(t,\mathbf{X}), \qquad \mathbf{X}(0)=\mathbf{X}_0. \tag{3}$$

Let be t_n the *nth* time, $\mathbf{X}_n = \mathbf{X}(t_n)$ the solutionat time t_n, $\mathbf{F}_n = \mathbf{F}(t_n, \mathbf{X}_n)$ the right hand side evaluated at time tn and $h = t_n - t_{n-1}$ the time step, which is considered constant. Classical methods use information at time tn to compute the solution at time t_{n+1}. Semi-implicit or implicit methods use the information at time t_n and t_{n+1} to get the solution at time t_{n+1}, but this kind of methods imply to solve a nonlinear equation to know the solution at time t_{n+1}. Multi-step methods give more efficiency by taking into account the information of previous steps, an example of a multi-step method is

$$\mathbf{X}_{n+1} = \mathbf{X}_n + h\sum_{i=1}^{r}\beta_i\mathbf{F}_{n+1-i}, \tag{4}$$

where r is the numbers of steps. The constants β_i satisfy the condition

$$\sum_{i=0}^{r}\beta_i = 1.$$

This condition guaranty the right solution to problema (3) when $\mathbf{F}(t,\mathbf{X})=\alpha$, for $\alpha \in \mathbb{R}$. A special type of the multi-step methods is called Adams methods [9]; these methods holds that

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \int_{t_n}^{t_{n+1}}\mathbf{F}(t,\mathbf{X}(\tau))d\tau. \tag{5}$$

Different Adam methods are based approximating $\mathbf{F}$ with a polynomial of degree s – 1 at points t_{+1-s}, $t_{n+2-s},\ldots,t_n$, then, the integral in the right-hand site of (5) is computed by using that polynomial approximation. Le tus consider the interpolating third degree polynomial of Lagrange

$$P_3(\tau)=F_{n-2}L_{n-2}(\tau)+F_{n-1}L_{n-1}(\tau)+F_nL_n(\tau), \tag{6}$$

where L_n is *nth* polynomial in the basis of Lagrange. In this case, we get

$$L_{n-2}(\tau) = \frac{1}{2h^2}(\tau - t_{n-1})(\tau - t_n), \tag{7}$$

$$L_{n-1}(\tau) = \frac{1}{h^2}(\tau - t_{n-2})(\tau - t_n), \tag{8}$$

$$L_n(\tau) = \frac{1}{2h^2}(\tau - t_{n-2})(\tau - t_{n-1}). \tag{9}$$

By substituting the interpolating polynomial of Lagrange in (5) we obtain

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \mathbf{F}_{n-2}\int_{t_n}^{t_{n+1}} \boldsymbol{L}_{n-2}(\tau)\boldsymbol{d}\tau + \mathbf{F}_{n-1}\int_{t_n}^{t_{n+1}} \boldsymbol{L}_{n-1}(\tau)d\tau + \mathbf{F}_n\int_{t_n}^{t_{n+1}} \boldsymbol{L}_n(\tau)d\tau. \tag{10}$$

This integral is evaluated by doing the change of variable

$$u = \frac{\tau - \tau_n}{h} \quad 0 \leq u \leq 1.$$

Thus, equation (10) becomes in

$$\mathbf{X}_{n+1} = \mathbf{X}_n \frac{h}{12}(5\mathbf{F}_{n-2} - 16\mathbf{F}_{n-1} + 23\mathbf{F}_n). \tag{11}$$

This last equation give us the three-steps Adams-Basforth method. Notice that computing solution $\mathbf{X}_3$ needs to know the solutions $\mathbf{X}_0$, $\mathbf{X}_1$ and $\mathbf{X}_2$. From the initial conditions of the problem, the solution $\mathbf{X}_0$ is given, but the solutions $\mathbf{X}_1$ and $\mathbf{X}_2$ have to be computed by other numerical scheme. In this case we will compute those by using the fourth order Runge-Kutta method.

3.1.2. Adams-Moulton method

This method implements the fourth degree polynomial interpolating approximation for $\mathbf{F}$, given by

$$P_4(\tau) = \mathbf{F}_{n-2}\mathrm{L}_{n-2}(\tau) + \mathbf{F}_{n-1}\mathrm{L}_{n-1}(\tau) + \mathbf{F}_n\mathrm{L}_n(\tau) + \mathbf{F}_{n+1}\mathrm{L}_{n+1}(\tau) \tag{12}$$

Where the Lagrange polynomial are

$$L_{n-2}(\tau) = \frac{1}{6h^3}(\tau - t_{n-1})(\tau - t_n)(\tau - t_{n+1}), \tag{13}$$

$$L_{n-1}(\tau) = \frac{1}{2h^3}(\tau - t_{n-2})(\tau - t_n)(\tau - t_{n+1}), \tag{14}$$

$$L_n(\tau) = \frac{1}{2h^3}(\tau - t_{n-2})(\tau - t_{n-1})(\tau - t_{n+1}), \tag{15}$$

$$L_{n+1}(\tau) = \frac{1}{6h^3}(\tau - t_{n-2})(\tau - t_{n-1})(\tau - t_n). \tag{16}$$

So, applying the same procedure as previous section, the Adams Moulton method reads

$$\mathbf{X}_{n+1} = \mathbf{X}_n + \frac{h}{24}(\mathbf{F}_{n-2} - 5\mathbf{F}_{n-1} + 19\mathbf{F}_n + 9\mathbf{F}_{n+1}). \tag{17}$$

Notice that this method is a implicit method, so that, we need to solve a non linear equation every time step in order to know the solution at time t_{n+1}.

3.1.3. Predictor-corrector method

An alternative method to avoid the solution of the non linear equation every step in the Adams Moulton method is to pair both Adams Bashforth Adams Moulton methods to obtain the the Adams Moulton predictor-corrector method, such as follows:

- Predict: Compute the approximation $\widehat{\mathbf{X}}_{n+1}$ by using the Adams Bashforth method.
- Evaluation: Evaluate $\mathbf{F}(t_{n+1}, \widehat{\mathbf{X}}_{n+1})$,
- Correct: Use the Adams Moulton method to compute $\widehat{\mathbf{X}}_{n+1}$ by using the evaluation $\mathbf{F}(t_{n+1}, \widehat{\mathbf{X}}_{n+1})$,

3.2. Stochastic approximation of the parameters

In this section we describe the way as the parameters of the model (1) are estimated. In order to carry out the Bayesian estimation, the framework Spux is used [17]. This framework has been widely used for the estimation of the parameters, for instance we refer to the works [16, 14]. Spux is a modular framework which can be coupled to any model written in any programming language. In this case, we will couple spux with the code described in Section 3.

3.2.1. Mathematical concepts

Following [16], for a given model M, let us consider the parameter vector θ, such that the model depends on the vector θ, we shall define the state m as $m \sim M(\theta)$ and D is the observation data for a given model parameter values θ. The so called likelihood $L(D|\theta, M) = \mathbb{P}(D|\theta, M)$ of the model M defines a probability distribution or the observation data.

Let us suppose that the initial information of the parameters θ is known and it is described by the prior distribution $\pi(\theta|M) = \mathbb{P}(\theta|M)$. The prior knowledge on the model and the information about the parameters D, is combine via the likelihood $L(D|\theta, M)$ to get the posterior distribution $\mathbb{P}(D|\theta, M)$ of the model parameter θ,

$$\mathbb{P}(D|\theta, M)=\frac{L(D|\theta, M)\pi(\theta|M)}{\mathbb{P}(D|M)} \propto L(D|\theta, M)\pi(\theta|M). \tag{18}$$

Due to the Bayesian inference cannot be solved analytically for a posterior distribution $\mathbb{P}(\theta|D, M)$, numerical methods have been developed to sample from the posterior distributions of the model parameters. Usually, Metropolis or Metropolis Markov Chain Monte Carlo (MCMM) sampling schemes are applied [7, 10, 6]. These methods are based on the simulation of several parameters samples and the evaluation of the likelihood and prior to these parameter values.

In a general model M, a set of parameters with a vector θ is mapped to the model prediction, as is shown in the left-hand hand side of figure 1, then such model prediction is categorized into the full model state $m = M(\theta)$ and its hidden part as the model output $y = h(m, \theta)$.

Many realistic models have an explicit temporal dimensions (it is a time evolution phenomenon), as it is show in the right hand site of figure 1. In this case we denote that time dependence of the model, for any time t, as M_t and the specific model state by mt,as well, the output model is denoted by $y_t = h(m_t, \theta)$.

A stochastic time dependent model M is called a hidden-Markov model if, for any increasing sequences of time $s_1 < s_2 < \cdots s_N$ its corresponding states $m_t \sim M_t(\theta)$ satisfy the Markov property, for all θ and all $1 \leq k \leq N$

$$\mathbb{P}(m_{s_k}|m_{s_{k-1}}, \dots m_{s_1}, \theta, M). = \mathbb{P}(m_{s_k}|m_{s_{k-1}}, \theta, M). \tag{19}$$

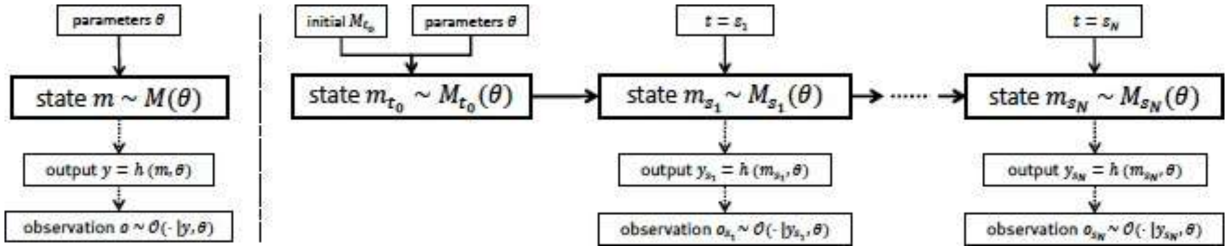

Figura. 1. Generic model and hidden-Markov model, mapping parameters θ to the state m

In certain situation, to be modeled by M, the output y, also called the exact or true output, are often not measured completely accurately during the data generation. Particularly the corresponding data observations o are assumed to follow a probabilistic distribution $O(\cdot|y, \theta)$. It is also called the observational error model. This error can depends on some uncertain parameter, included within vector θ.

Due to Bayessian inference cannot be solved analitically, in approximate the posterior distribution $\mathbb{P}(\theta|D, M)$, as well, in the case of stochastic model, both the likelihood distribution $L(D|\theta, M)$ and the posterior model states $\mathbb{P}(m|D, M)$, numerical methods have been developed to sample from posterior distributions of the model parameters θ, obtained by running several simulations of the model M, for instance, Metropolis or Metropolis-Hastings Markov Chain Monte Carlo (Markov-type), see [8], Approximate Bayesian Computation (ABC-type) see [2], among others. In the fra- mework Spux the ABC-type samplers are already available.

3.3. Spux framework

Spux is a framework which provide a high level interface to perform Bayesian inference, also it is highly customized and adaptive due to it is based in Python programming language [19]. The Spux framework is a collection of optimized modular components. The basic key component implemented in Spux, together with available specific numerical methods is provided in the table 1

Tabla 1. Components of modular framework Spux

$\mathbb{P}(\theta|D, M)$	**Sampler**	**EMCEE,MC**	**Parameter smpling**
$L(D|\theta, M)$	Likelihoo	Direct, PF	State sampling
$\rho(D|\theta, M)$	Distance	Norm, Regression	Distance for ABC sampler
$m_t \sim M_t(\theta)$	Model	Mathematical EDO	Model for user's application

Every component of Spux can be assigned to each other following the required dependencies, together with the asociated mathematical object introduced before.

3.4. Deterministic and stochastic models

In Bayesian inference, for a deterministic model M a simple directly likelihood can be analytically computed by using the specified error

$$L(D|\theta, M) = O(D|y,\theta)$$

where

$$y = h(m) \text{ and } m = M(\theta)$$

For stochastic models *M*, in addition to uncertain model parameters θ, also the uncertain model states $m \sim M(\theta)$ needs to be inferred. In this case, the error *O* is often not enough to compute analitically the likelihood $L(D|\theta, M)$, this happen when the model is time-independent.

3.5. Spux configuration

In order to carry out the parameter estimation by using Bayesian inferences, it is needed to give to Spux the following information [15]:

- Model: It is solved the mathematical model (1) by using the numerical scheme described in Section 3.1.3.
- Data Set: In this file, is the data set is built to be used in the inference process the Pandas library of Python.
- Error: In this file, the probabilistic distribution of the error, for the data set, are given.
- Prior Distribution: In case of know the distribution for the different parameters, in this file, it is loaded. If the distribution is unknown, it is possible to use a uniform distribution if the knowledge of a value approximation for the parameter is given.
- Exact: This file is optional, usually it is employed in academical test. In this file we load the information of the exact values for the parameters

4. Numerical Results

In this section, we present the numerical results by using the multi-step numerical scheme coupled together with Spux.

4.1. Steady states

In this experiment, we want to calibrate the multi-step numerical scheme we introduce as input the obtained values for the parameters in the qualitative analysis which guaranty the survival of the three species.

- Initial conditions: $x_0 = 24$, $y_0 = 5$, $z_0 = 168$.
- Initial time $t_0 = 0$. Final time $t_f = 500$.
- Values for the parameters: $r_1 = 1$, $k_1 = 5$, $\beta_1 = 0.33333333$, $\alpha = 71.45862713545837$, $b = 26$, $c = 0.5$, $\mu = 0.272507803139913$, $v = 0.0000152587890625$, $\beta_2 = 217.5605468750000$, $k_2 = 6$, $\gamma = 1$, $r_2 = 1$. These parameters were obtained in work [11].

In figure 2, we can see the results obtained by the numerical multi-step scheme when the equilibrium states are reached. These equilibrium states are in accordance with the qualitative analysis, which holds that, for the set of given parameter values, the density of the plague decrease, as can be seen in the orange line. As well, we can see that the density of both plant and Trichoderma increase at the first 10 seconds to decrease until reaching the equilibrium states. It is important to note that the plant density is greater than the parasite one at the equilibrium.

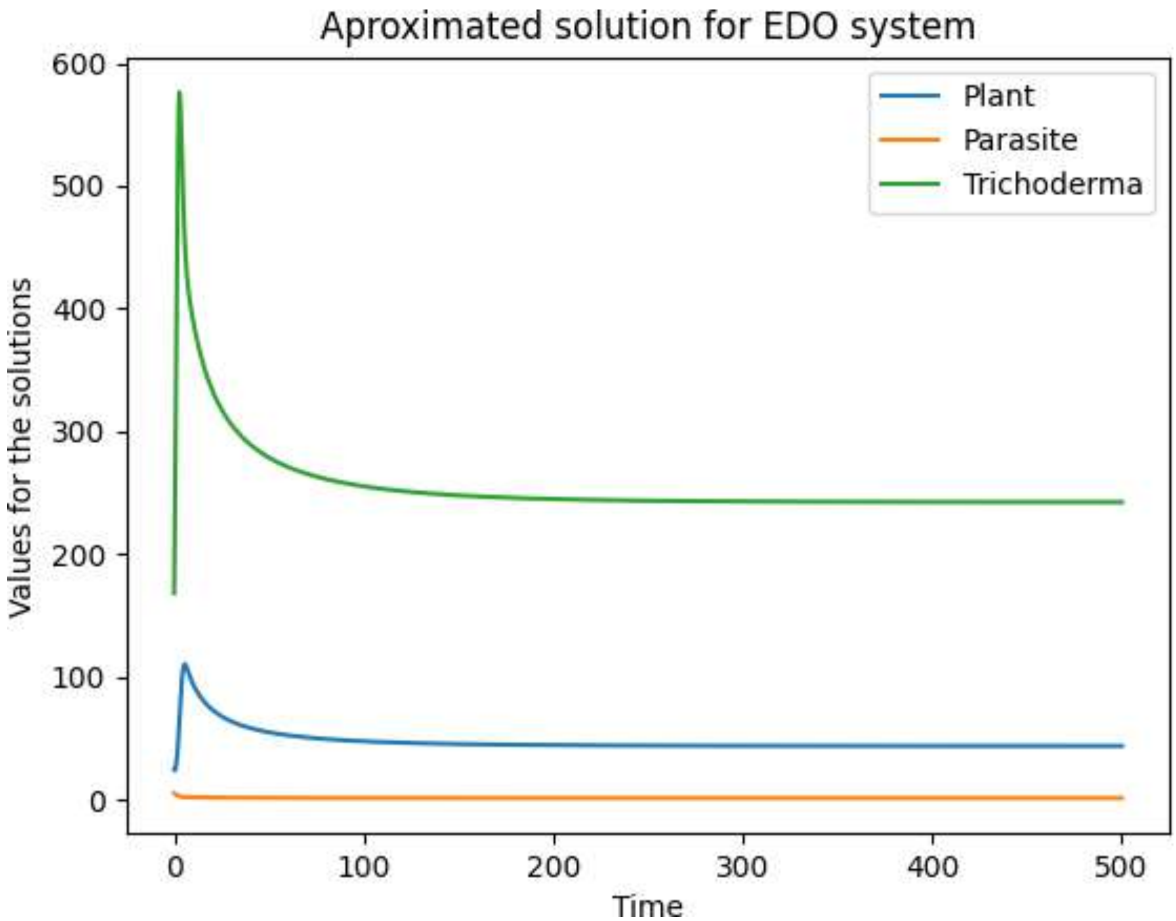

Figura. 2. Numerical result for the three species after 500 s of simulation

4.1. Parameter estimation

In this example, we estimate the mathematical model parameters (1) by using Spux together with code developed in the Section 3.1.3. To do so, we define the following assumptions to be used by Spux.

- Data set. Due to there is not any data available, we have decided to to use our own data set, in order to build this data set we introduce noise into the exact solution by supposing that the data have an error which is model by a normal distribution with mean equal to the exact solution and standard deviation equal to 0.01. The data set can be seen in figure 3.
- Prior information. A uniform distribution for every parameter has been chosen. These distribution can be seen in figure 4.
- Error information. In this case, we have considered a normal N (xi, 0.01), where xi is a prior value of the solution system (1).

The parameter estimated by Bayesian inference are showed in tables 2 and 3. Making a comparison between the exact parameters and the computed ones, we can notice that some parameter are well approximated, whiles the approximation for other ones has to be improved. For example, a well approximation is obtained for the the predation rate of pest on plant α, the profit rate that receive plant of biocontrol agent β_1, the conversion rate of consumed plant biomass into pest biomass γ, the biocontrol agent intrinsic growth rate r_2, this can be seen in figure 5.

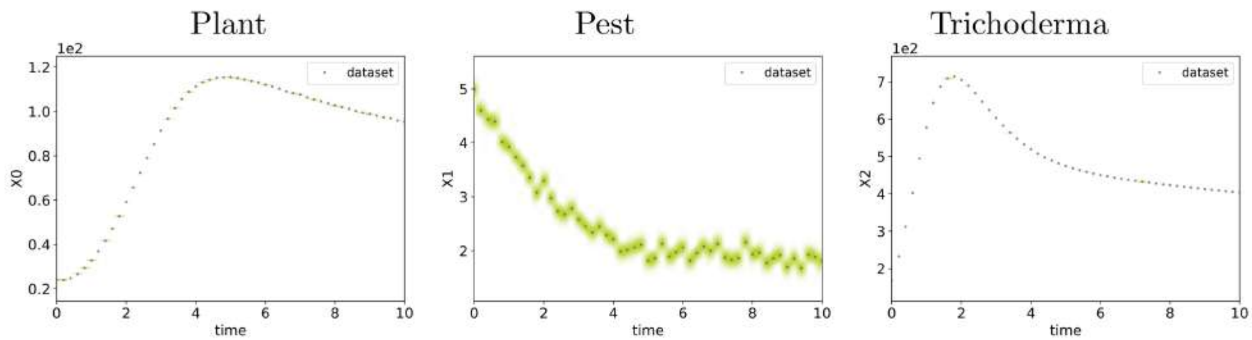

Figura. 3. Data set for every variable in the mathematical model. The dots indicates the data values, the green region indicate the density of the error model distribution

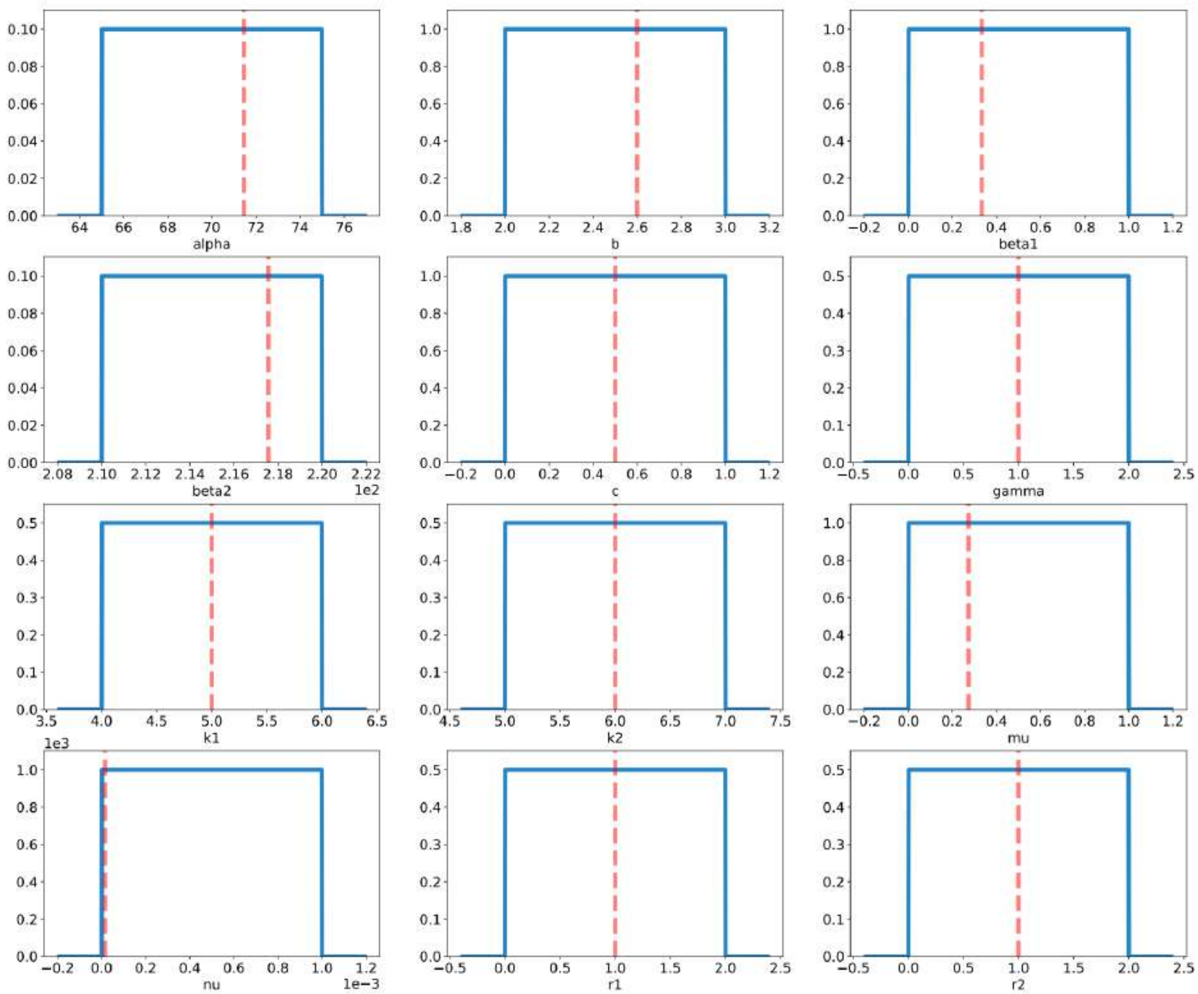

Figura. 4. Prior information about the parameters (Solid blue line) and exact parameter values (Orange dashed line)

Tabla 2. Estimated parameter by using Spux

α	b	β_1	β_2	c	γ
$7.30e+01$	$2.73e+00$	$2.44e-01$	$2.13e+02$	$2.91e-01$	$9.19e-01$

Tabla 3. Estimated parameter by using Spux

k_1	k_2	μ	v	r_1	r_2
$4.20e+00$	$6.91e+00$	$1.43e-01$	$3.72e-04$	$1.83e+00$	$8.43e-01$

Making use of these parameters the computed solution of the mathematical model is showed in figure 6 and the posterior distribution for every parameter is depicted in figure 5. From the figure 6 we can see that the better approximation is obtained for the parasite and the trichoderma, while the approximation for the plant is good enough in qualitative way but in quantitative way there is some minimal difference.

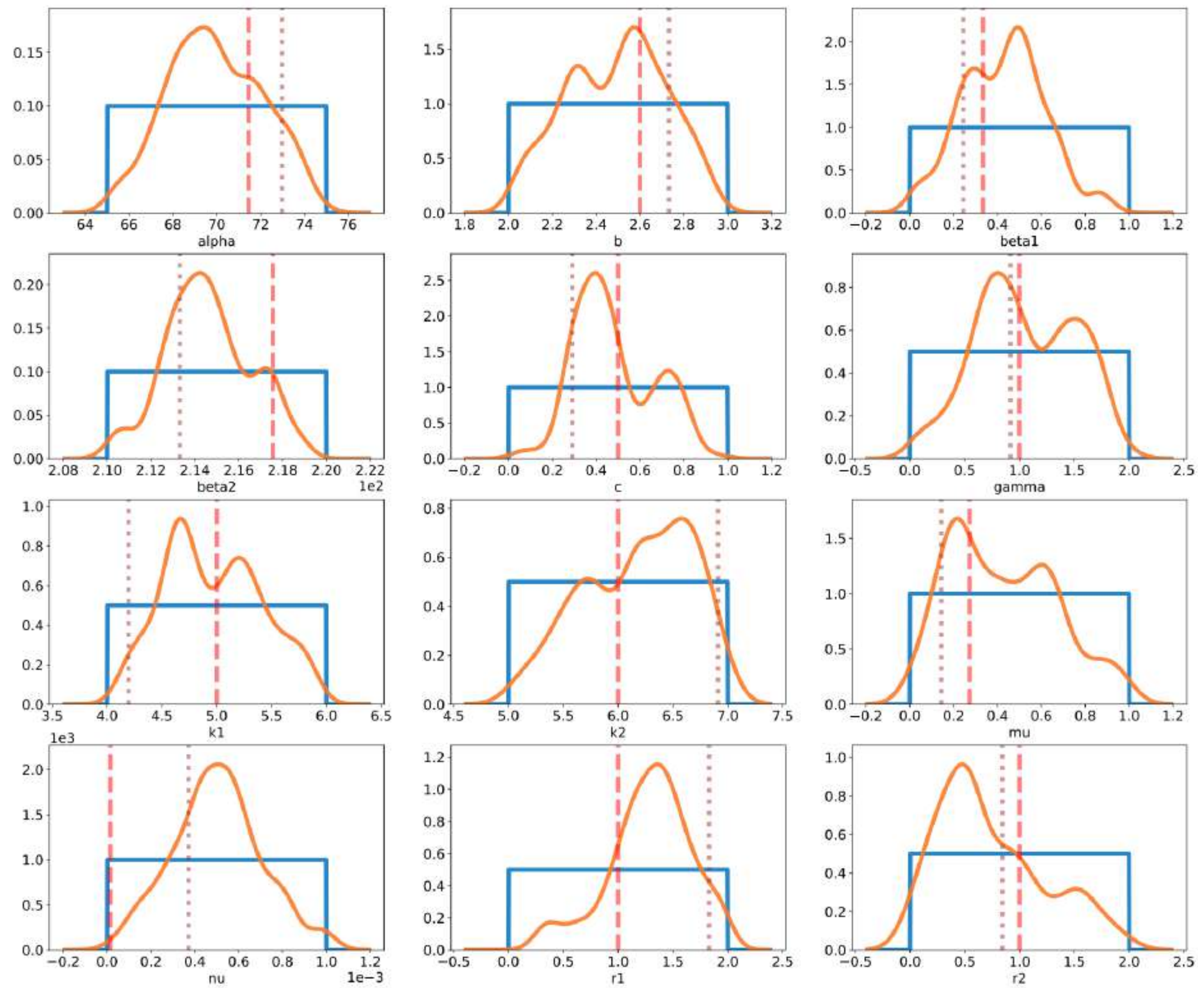

Figura. 5. Marginal posterior distribution (solid orange line), prior distribution (solid blue line), estimated maximum a posterior parameter values (doted brown line) and exact parameter values (orange doted line)

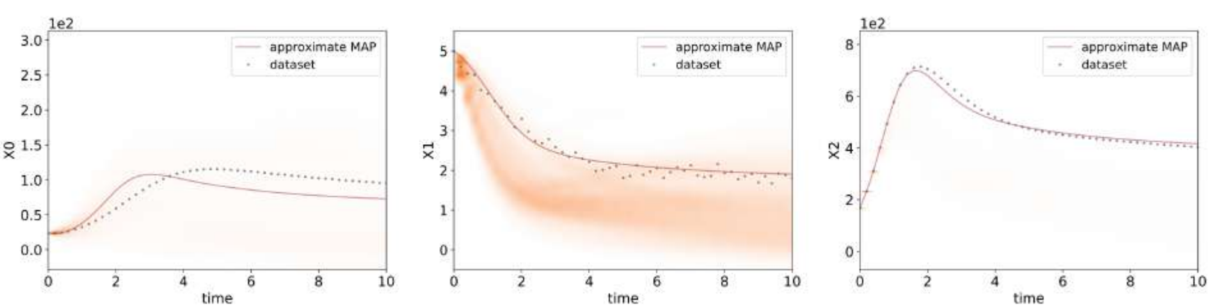

Figura. 6. Comparison between the data set (dots) and the approximated solution by using the estimated maximum a posterior parameter value (solid orange line). The shade orange region indicates the log-density of the posterior model prediction at the corresponding time points

5. Conclusión

In this work, we have studied a mathematical system to model the interaction between three species, (plant, plague and biocontrol agent). We have studied the equilibrium points of the system getting that at most there are four CEP for the studied system. As well, it was developed a numerical scheme to solve the mathematical model, to do that, a multi-step method was employed.

That method is based on the Adams Bashforth method to computed a prediction of the solution at time t_{n+1}, later, by using the Adams Moulton method, the correction for the solution at time t_{n+1} is computed. This method has showed good results, over all, it computes the correct steady state for the system, this state was showed in the bibliography reference cited in the section where the mathematical model is introduced. The estimation of the parameters was carried out, but due to the lack of the data information for studied phenomenon, we have used a perturbation of the steady state approximated solution, as a data information. Making comparison between the exact values for the parameters and the estimated ones by the framework Spux, we can notice a good agreement. This is verified when the estimated parameters values are used to compute the solution of the system and agree with the proposed solution. This work gives a methodology to compute the values of certain parameter for the mathematical model studied, but this technique is able to be used in several types of problems where the parameter estimation is needed. To know the values of the parameters with a degree of certainty allows to do predictions of the studied phenomena without expensive compute time, because usually the parameters are tuned to reproduce the known solution of the phenomenon.

6. Agradecimientos

The authors of this work want to say thank to the authorities of the Instituto Tecnológico Superior de Comalcalco for the given facilities to carry out this research under the project entitled "Estimación numérica de parámetros en modelos matemáticos para el control de plagas" with reference ITSC-CB01-1

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