Phase Plane Analysis of Linear Systems in Dynamic Mathematical Models

By

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Date: May 2018

This mini dissertation is submitted in partial fulfilment of the requirements of the Master of Science Degree

University of Fort Hare

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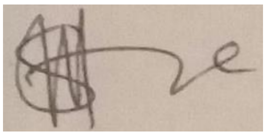
Declaration

I, the undersigned, solemnly declare that the work contained in this thesis is my own original work and has not been submitted in its entirety or in part to any other university for a degree. The use of both published and unpublished work from other sources has been fully acknowledged in the text and a list of references is provided.



12 April 2019

S.D Marange **Date**

Acknowledgements

I would like to convey my gratitude to my fellow postgraduate students (Ebenezer, Israel and Simba) for their immense support that I could not do without. I am grateful to my wife, son and daughter. Finally, special thanks go to Mathematics Department.

Dedication

I dedicate this thesis to my wife Faith, son Danfer, daughters Dannielle and Deanne and lastly my parents (Mrs T. Marange and the late Mr A. T Marange).

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Abstract

A plethora of dynamic mathematical models exist and to understand and master all of them would be a gargantuan task. The author had, nonetheless, attempted to outline some of the methods used to analyse linear systems in modeling. Systems techniques are fundamental to current research in molecular cell-biology. The systems-approach stands in stark contrast to the historically, reductionist paradigm of molecular biology. Field work can be very dangerous. The main purpose of this study was to come up with the best analysis that would be used without going to the real field and thus saving time, money and risks associated with remote field localities. This research showed that the best analysis depends on the nature of the objectives intended to be solved by the model. Phase plane analysis on linear systems assisted in gaining deeper knowledge on the characteristics of such systems. This work analysed some dynamic models looking at phase planes, bifurcation, sensitivity and stability. The research provided a qualitative analysis of the processes not a numerical analysis.

Chapter 1 Introduction

1.1 Introduction

The research seeks to address the phase plane analysis of linear systems. A background of modeling is discussed in this chapter. Also, the statement of the problem is outlined, as well as aims of the study, rational of the study, significance of the study and a summary of the chapter will be looked at.

1.2 Background

Model analysis provides us with an insight into how and why a system behaves in the way it does, providing a linkage between network's structure and behaviour. Since a model is a hypothesis, so the outcomes of the investigation are also a hypothesis. Some models have limited portending power, however they will be futile for guiding the choice of components and suggesting the most compelling experiments for testing system completion. Systems and synthetic biology represent unique opportunities. In health, agriculture, manufacturing, energy production, and environmental remediation, the use of mathematical models is leading to rapid progress in a wide range of human endeavours (Ingalls, 2012).

Balance equations and constitutive equations resulting in a set of Differential Algebraic Equations (DAE) are currently used in mathematical-process modeling and simulation. DAE are systems of differential equations with algebraic constraints that can be expressed in terms of an initial value problem such as

$$F(t\,;x\,(t)\,;x^{I}(\,t))=0,$$

$$G(t\,;x\,(t))=0, \quad x(t_0)=x_0,\ x^{I}(t_0)=x_1, \tag{1}$$

in which F represents differential equations, containing differential terms, G represents algebraic constraints, which are equations without differential terms; so, G may be considered as initial, or boundary conditions to the Ordinary Differential Equations (ODEs).

Commercial software packages are available that assist with simulation models. Unfortunately, many of the more effective software packages are exorbitantly expensive. MATLAB, for instance is one such package that is very good in simulation. More recently, packages such as Freemat and Octave, that can be used for simulation have become freely available. The end goal of most modeling exercises is to provide, at least, qualitatively correct, preferably quantitatively correct information, thus we prefer accurate simulations of real behaviour. The accurate representations are then used in model-based designs, which will then result in faster and most efficient developments of systems. For example, the Boeing 777 jet was executed and tested broadly in computer simulations before any physical manufacture began (Ingalls, 2012).

Recently, more and more assembly projects use three-dimensional/four-dimensional (3D/4D) models to support management tasks. The propensity of 4D modeling technology used in the Architecture, Engineering and Construction (AEC) Industry has been studied and documented in recent years. 4D modeling allows project teams to visualize construction plans, identify construction consequences and space conflicts, identify safety issues and improve communication of the project team members (Koo and Fischer 2000). The implementation in engineering education is still limited, despite an increasing number of successful applications of 4D modeling in the AEC Industry (McKinney et al.1998). 3D visualisation, 4D models and virtual reality models can be utilised for more effective generation, communication and evaluation of schedule information.

The main aids that a 4D model provides are,

- a visualisation tool that assist in conveying information on planning
- an analysis tool that will enhance collaboration among project participants
- an integration medium that will support users to conduct additional analyses.

4D modeling also enables the identification of potential conflicts between building elements and workspaces, safety hazards created due to proximity of construction activities, and the visualization of construction plans (McKinney et al.1998). There are so many constructions in Dubai, for example, that were extensively tested using computer simulations long before the actual construction work even commenced (Baker W.F and Irwin P.A 2006).

A deeper understanding of cellular networks comes from using model-based design in synthetic biology. Engineers need to be able to build, re-use and interconnect mathematical models from different physical domains into one common simulation platform. Despite the fast developments in different fields of software programming and hardware availability, industrial practice shows that there are still several problems to be solved on dynamic model building and model interconnection (Ingalls, 2012). The available simulation tools in the market provide several alternatives for model representations, model aggregation and model interconnectivity of processes from different physical domains (Soetjahjo, 2006).

Some of the fundamental concepts in dynamic mathematical modeling are explained below.

Deterministic and Stochastic Models

A **deterministic** mathematical model is exactly reproducible, while **stochastic model** allows for randomness in their behaviour. Deterministic models are far more compliant for both simulation and model analysis, than stochastic models are.

Global and Local Behaviour

Nonlinear dynamic systems can display a wide variety of behaviours. Local behaviour analysis involves paying attention to the near, particular points, therefore providing comprehensive insight into global behaviour. The approximations locally allow one to apply linear analysis tools and gather more information about the system. Biological modeling uses local approximations in particular, since self-regulating (homeostatic) systems spend much of their time operating around specific nominal conditions.

Linearity and Nonlinearity

A linear relationship has direct proportionality (Ingalls, 2012). Linearity allows for effortless extrapolation; that is, if the independent variable is tripled, the outcome will also be tripled. A linear, dynamic mathematical model is one that has all the interactions among its components linear and they have a limited range of behaviour. A nonlinear relation does not follow any specific pattern and is difficult to address in generality. A hyperbolic saturation (as independent variable increases, the dependent decreases) and sigmoidal saturation (the dependent variable starts slowly, then rapidly increases before saturating the rate of growth) are examples of nonlinear relationships (Ingalls, 2012).

State Variables and Model Parameters

The distinction between state variables (free/primary components of the model) and parameters (fixed values) is clear cut, although it depends on an individual model's context, as well as the time scale over which simulations run. The model parameters can be varied so as to explore system behaviour under perturbations, or in altered environments (Ingalls, 2012).

Steady-state and Transient Behaviour

Biological models display a persistent operating state referred to as steady state (Ingalls, 2012). Transient behaviour is the evolution that leads from an initial state to the long-term behaviour. Steady-state behaviour reflects the prevailing condition of the system, while transient behaviour shows the immediate response of a system to perturbation.

When reliable simulations related to the behaviour of the real system are available, it may be possible, in most cases, to reduce the time devoted to observation and experiments. Bearing in mind the above reasoning, one can state that there exists a strong link between applied sciences and mathematics, represented by mathematical models designed and applied, with the aid of computers and other devices, for the simulation of systems in the real world. Mathematical models are designed to describe physical systems by equations, or more generally, by logical and computational structures.

1.3 Statement of the Problem

Selecting the best method to analyse a linear system in mathematical dynamic model is always a challenge. The purpose of the study is to analyse the different ways mathematical dynamic systems operate so as to gather deeper understanding of different models.

1.4 Significance of Study

This research was done in order to understand different analyses used in dynamic mathematical problems. Modeling performs an important role in biological systems, engineering and construction. The analysis of the dynamic mathematical model is crucial, as this will aid in improving the lifestyles of human kind. It will also assist in saving costs and human life. Since models are used to predict the future, means more understanding of models will enable predictions to be refined. Making predictions about the behaviour of a system is an important idea since many of the mathematical models, of the world around us, are in the form of rules and they are of much greater use if accurate predictions can be made on the basis of the model and its initial conditions.

The act of creating a model forces the modeler to think deeply about the setting. Translating an imprecise, complex, multivariate real-world situation into a simpler, more-clearly-defined mathematical structure; such as a function or a system of rules for a simulation yields several benefits (Adams J.P, 2001). Problems as diverse as the simulation of planetary interactions, fluid flow, chemical reactions, biological pattern formation and economic markets can all be modeled as dynamic systems. The main goal of doing this research was to seek a deeper understanding of how dynamic models operate. Furthermore, it is to assist others to understand the different dynamic systems.

1.5 Aims of the study

The main aim of the study is to analyse the linear systems in mathematical modeling using phase plane. Other types of analysis such as sensitivity, bifurcation and stability will be discussed as well. Nonlinear systems will also be analysed. The analysis that will be done should be cost effective and produce reliable results.

1.6 Rational of the study

The reason behind studying analysis is to assist modelers in selecting the best method to use when they want to do a valid modeling. A good understanding of linear systems will aid in gaining deeper understanding of nonlinear systems as there tend to be some similarities with linear systems when local analysis is done. For example, at a point of contact a tangent has the same characteristics as the nonlinear systems.

1.7 Research outline

The fundamentals of dynamic modeling will be outlined in chapter one. Chapter two is a literature review. An outline of model construction is presented in chapter three. A few examples of the models outlined in chapter three are solved in chapter four. Chapter five is an introduction to the XPPAUT software, a free program written specifically for dynamic modeling; and MATLAB, which is a more comprehensive computational tool. XPPAUT is more accessible to readers without any computational background. The researcher could not run the program due to unavailability of data. Chapter six will give a conclusion and recommendations.

Hopefully, many readers will be able to use this research to enrich themselves with a deeper understanding of dynamic mathematical modeling.

Summary

The author outlined the background of the study and the fundamental principles of dynamic mathematical modeling have been discussed. The following chapter delves in modeling cycle.

Chapter 2 Modeling Cycle

Introduction

In modeling, there is a need to identify a problem and then look for different ways to solve it mathematically. The solution should be able to assist to avoid the same problem occurring again in future.

Mathematical Models

A dynamical mathematical model of a real-world system is an equation or system of equations to describe the evolution of a state with suitable variable which encapsulates the physical state of the system. A real physical system is closed if it does not interact with the outer environment, while it is open if it does (Ingalls, 2012).

The theory of dynamical systems is concerned primarily with making qualitative predictions about the behaviours of systems, which evolve in time; as parameters, which control the system, and the initial state of the system itself, are varied. Modeling is done to aid the conceptualisation and measurement of complex systems and sometimes to predict the consequences of an action that would be expensive, difficult or destructive to do in the real-life scenario.

Models are necessary, as they form a link between the observational and theoretical levels. They are manifestation of the simplifications, devaluation, actualisation, experimentation, extension of globalisation theory formation and explanation.

Dynamic and Static Models

The most notable difference between static and dynamic models of a system is that while a dynamic model refers to runtime model of the system, static model is the model of the system not during runtime. Another difference lies in the use of differential equations in dynamic model which are conspicuous by their absence in static model. Dynamic models keep changing with reference to time whereas static models are at equilibrium of in a steady state.

Static model is more structural than behavioural while dynamic model is a representation of the behaviour of the static components of the system. Static modeling includes class diagram and object diagrams and help in depicting static constituents of the system. Dynamic modeling on the other hand consists of sequence of operations, state changes, activities, interactions and memory.

Static modeling is more rigid than dynamic modeling as it is a time independent view of a system. It cannot be changed in real time and this is why it is referred to as static modeling. Dynamic modeling is flexible as it can change with time as it shows what an object does with many possibilities that might arise in time (Blower S, Bernoulli D, 2004).

Discrete and Continuous Models

Continuous modeling is a mathematical practice of applying a model to continuous data. A mathematical model is discrete if it is based on discrete data. A probable classification can be related to the above definitions and to the structure of the state variable, as it is shown in the following table:

Discrete	Static	$u = u_e$
Discrete	Dynamic	$u = u(x)$
Continuous	Static	$u = u(t)$
Continuous	Dynamic	$u = u(t; x)$

Table 1: Discrete and continuous dynamic models.

Where u is the output variable, $u(x)$ is the state variable, $u(t; x)$ is the variable depending on time and state.

Linear, static and deterministic models are usually easier to compute than nonlinear, dynamic and stochastic models. Continuous variable models appear to be more amenable to computation than the discrete variable models, due to the development of calculus and differential equations, however, continuous models are simpler only when analytical solutions are available (Kapur, 1994). Otherwise one has to approximate a continuous model by a discrete model so that it can be dealt with numerically (Kapur, 1994). There are some models that involve both discrete and continuous variables simultaneously.

Modeling is a symbol representation of a real-life scenario. One may as well define mathematical modeling as a mathematical construction designed to study a particular real-world system or phenomenon. Some will refer to it as transforming a real life situation into a mathematical problem that can be solved using different techniques. The solutions then need to be thoroughly checked initially to see if they corroborate with real world data. The model can then be modified accordingly, depending on its deficiencies. If the solutions are satisfactory then the made model can be implemented in real life scenarios.

A biological model can be devised to gain a deeper understanding of an organism, an ecosystem, a genetic lineage, or a wide variety of other topics in biology (Ingalls, 2012). Using mathematics, people can set up and test a model. Many topics require a mathematical framework. For example, population growth and population dynamics are topics, which lend themselves favourably to mathematical modeling.

Modeling dynamic systems with mathematics, furthermore, allows one to entertain hypothetical parameters and variables to predict what would happen if such changes occurred in the real world. For example, a group of scientists working on an insect pest control project might take a mathematical model of the pests in question and then start adding variables like the use of insecticides, genetic manipulation of the population to create sterility, and other factors to investigate an effective strategy for pest control, or extirpation.

A model organism can provide data that may be applicable to other organisms. The lab rat is a time-honoured favourite, studied with the goal of learning more about the nature of other mammals, especially humans (Ingalls, 2012). Fruit flies are also commonly used, as is *Escherichia coli*, a bacterium widely studied in labs all over the world. These biological models are chosen because of the similarities between them and other organisms, or for traits such as rapid reproduction or genomes that are easy to manipulate (Singleton P. 1999).

A system is a collection of objects joined in some regular synergy. Studying different systems will help us to accurately model any real-world phenomenon. Future predictions can be obtained from the understanding of systems.

There is a procedure to be followed when modeling:

1. Abstraction or Simplification – focusing on important characteristics of a system will help to determine the primary factors indicated by the real-world behaviour. This is where information is abstracted into a mathematical context.
2. Logical argument – solving the mathematical system generated and deriving mathematical conclusions. It also involves analysis and conjecture.
3. Interpretation – depicting in terms of the real-world problem and making predictions based on the mathematical conclusions.
4. Verification or Experiments or Simulations – results are tested in real life situations, or computer programs are used to simulate the real-world phenomenon.

The above procedure is represented diagrammatically in Figure 1.

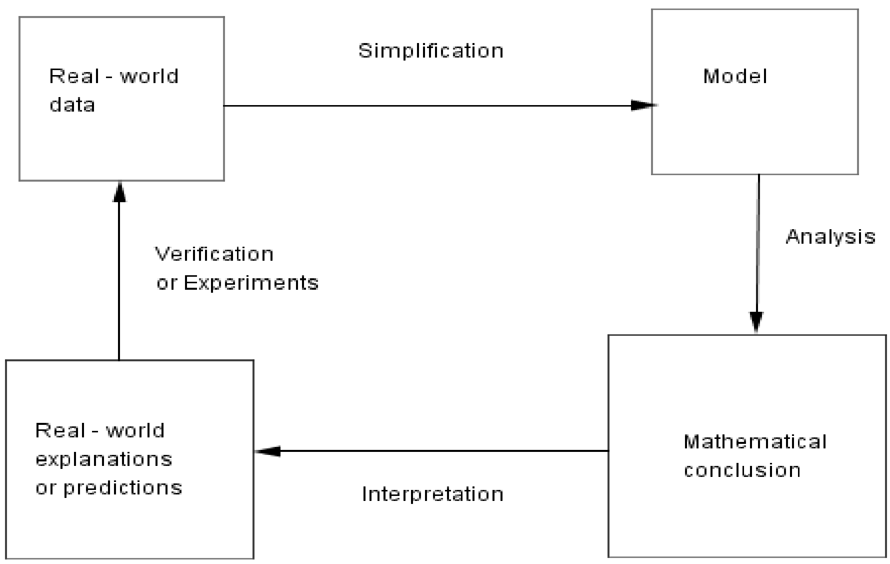


Figure 1: The modeling cycle

Models are used since they are easier to study than real life situation, cheaper and enable the desired results to be obtained faster. Models elucidate real-life problems, they can also be manipulated and studied. They are also, useful to science as they assist in conceptualising, organising and communicating complicated phenomena. Lastly, models can be used to make predictions and help people with information. For example, a model can be used to predict bad weather, and people will be warned well in advance to vacate an area to avoid injury, or loss of life.

There are three main properties of a model that should be considered when devising one:

- Fidelity: The preciseness of a model's representation of reality.

  Real-world observations demonstrate the greatest fidelity even though they might have bias in testing and errors in measurement. Experiments will also show greatest fidelity since behaviour is observed in a controlled environment such as the laboratory. Simulations will lose fidelity because of indirect observation. Mathematically it will also lose fidelity because real-world conditions that have been abstracted are simplified. Every model will have additional simplifications thereby losing more fidelity.
- Costs: The total cost of the modeling process. Experiments and simulation are very expensive to set up and operate. Computer software, for example can be expensive and so is the maintenance of computers.
- Flexibility: The ability to change and control conditions affecting the model.

  Mathematical models are generally more flexible since different assumptions and conditions can be selected relatively easily. Experiments are less flexible because some factors are very difficult to control beyond specific ranges. Real-world observations have little flexibility because the observer is limited to the specific conditions that pertain at the time of the observation. Other conditions might be impossible to create.

Mathematical models are used in many areas of science to elucidate a system's behaviour through the imitation of specific system behaviour. A dynamic system is one in which its centralised properties, or quantities, undergo a change over the course of time. Finkelstein (1985) stated that a dynamic system is one in which the present value of one of the output variables in the system depends, not only on the current value of the input signal being applied to the system, but also the history of the system. It is a mathematical description of a dynamic system that consists of aspects such as time and behaviour equations (Willems, 1996). Behaviour B of a dynamic system manifests as a set of signal trajectories $z(t) \in R^n$ on some time interval $t \in (a;b); a,b \in R$, satisfying behaviour equations,

$B = \{z(t) : R \to R^n$ such that behaviour equations are satisfied$\}$ (2)

Modeling complicated processes involves an interconnection of sub-models, each represented by a set of behaviour equations (2). Mathematical modeling of a system is always subject to assumptions. The assumptions are made to reduce complexity in modeling. Mathematical models are driven by questions; and we seek solutions to these questions by using the models. In most cases models are designed to focus on certain aspects of the object of study, making other aspects irrelevant. There are, however, still many instances, which have not yet been mathematically modeled, either because the situations are sufficiently complicated or since the resulting mathematical models are mathematically intractable.

Summary

Chapter two gave a summary of different types of models. It is the author’s desire to assist different people on the types of models that exist. It is important for modelers to outline the objectives of each model so that an effective analysis will be done that will assist in cutting costs. There is no satisfaction in life other than cutting costs in everyday survival. Chapter three will analyse different types of analysis that will be useful in choosing a model.

Chapter 3 Analysis of Dynamic Mathematical Models

Introduction

In this chapter different types of analysis will be discussed. There are four types of analysis that the author will discuss that is phase plane, bifurcation, sensitivity and stability analysis. Linear and nonlinear systems will both be looked at.

3.1 Phase plane analysis

Phase plane analysis is a graphical method for studying autonomous second-order systems. The method involves plotting the time derivatives of the system's position as a function of position for various values of initial conditions. The equations of the type:

$$\frac{dx}{dt} = P(x, y)$$
$$\frac{dy}{dt} = Q(x, y), \tag{3}$$

where x and y are the state variables of the system, $P(x, y)$ and $Q(x, y)$ are functions that satisfy the conditions for the existence and uniqueness of solutions and are the time independent variables. Phase plane analysis provides for motion trajectories corresponding to various initial conditions, examining of qualitative features of trajectories and obtaining information regarding the stability of the equilibrium points (Keshmir, 1995).

A singular point is a point at which a given function of a complex variable has zero derivative but of which every neighbourhood contains points at which the function has derivatives. A singular point is an equilibrium point in the phase plane, since it is defined as a point where the system states can stay forever. For a linear system, there is usually only one singular point, although in some cases there can be a set of singular points. Singular points are very important features in the phase plane. Examining the singular points can reveal a great deal of information about the properties of a system. In fact, the stability of linear systems is uniquely characterized by the nature of their singular points. Although the phase plane method was developed primarily for second-order systems, it can also be applied to the analysis of first-order systems. The difference is that the phase is composed of a single trajectory. At the equilibrium point the system can either be stable or unstable. There are a number of methods for constructing phase plane trajectories for a linear or a nonlinear system, for example, the so-called analytical method, the method of isoclines, the delta method, Lienard's method and Pell's method (Slotine, 1991).

Phase Plane Analysis of Linear Systems

The general form of a linear second-order system is,

$$\begin{aligned} \dot{x}_1 &= ax_1 + bx_2 \\ \dot{x}_2 &= cx_1 + dx_2, \end{aligned} \qquad a, b, c, d \epsilon \mathbb{R}. \tag{4}$$

The equations are transformed into a scalar, second-order differential equation of the form,

$$b\dot{x}_2 = bcx_1 + d\left(\dot{x}_1 - ax_1\right). \tag{5}$$

Differentiation and substitution lead to

$$\ddot{x}_1 = (a + d)\dot{x}_1 + (cb - ad)x_1. \tag{6}$$

The second-order linear system is

$$\ddot{x} + a\dot{x} + bx = 0. \tag{7}$$

To obtain the phase portrait of this system, we solve for time history.

$$x(t) = k_1 e^{\lambda_1 t} + k_2 e^{\lambda_2 t} \quad \text{for } \lambda_1 \neq \lambda_2$$
$$x(t) = k_1 e^{\lambda_1 t} + k_2 t e^{\lambda_2 t} \quad \text{for } \lambda_1 = \lambda_2, \tag{8}$$

where the constants λ_1 and λ_2 are the solutions of the characteristic equation

$$s^2 + as + b = (s - \lambda_1)(s - \lambda_2) = 0. \tag{9}$$

They (λ_1 and λ_2) are the eigenvalues of the system's Jacobian.

$$J = \begin{bmatrix} a & b \\ c & d \end{bmatrix}. \tag{10}$$

The Jacobian is constructed from (4).

The roots λ_1 and λ_2 can be explicitly represented as

$$\lambda_1 = \frac{-a + \sqrt{a^2 - 4b}}{2} \text{ and } \lambda_2 = \frac{-a - \sqrt{a^2 - 4b}}{2}. \tag{11}$$

For a linear system there is only one singular point $(b \neq 0)$, namely the origin. The trajectories in the vicinity of the singular point can display quite different behaviour, depending on the values of a and b. The following cases occur

- λ_1 and λ_2 are both real and have the same sign (+/-). This corresponds to a node that can be stable $(\lambda_1, \lambda_2 < 0)$ or unstable $(\lambda_1, \lambda_2 > 0)$. There will be no oscillation in the trajectories.
- λ_1 and λ_2 are both real and have opposite sign. This corresponds to a saddle point.
- λ_1 and λ_2 are complex conjugates with non-zero real parts. This corresponds to a focus that can be a stable focus $\{\mathrm{Re}\ (\lambda_1, \lambda_2) < 0\}$ or unstable focus

$\{\text{Re }(\lambda_1, \lambda_2) > 0\}$.

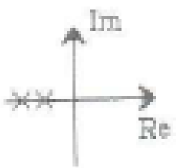
- λ_1 and λ_2 are complex conjugates with real parts equal to 0. This corresponds to a centre point. All trajectories are ellipses and the singular point is the centre of these ellipses.

It should be noted that the stability behaviour of linear systems is uniquely determined by the nature of their singularity points. This is not true with nonlinear systems. Figure 2 gives a summary of phase plane-portraits for linear systems.

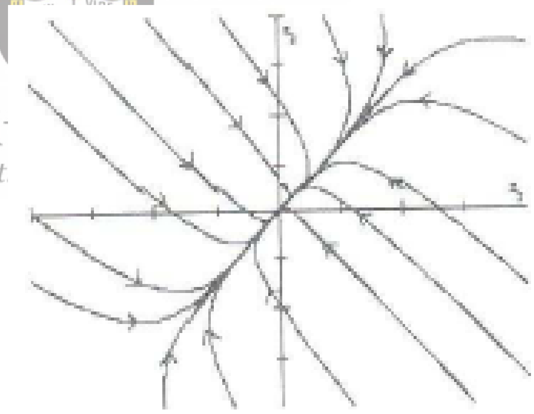
Phase-portraits of linear systems

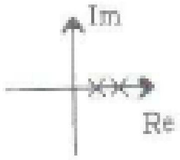
Eigenvalues

Phase Plane Plot

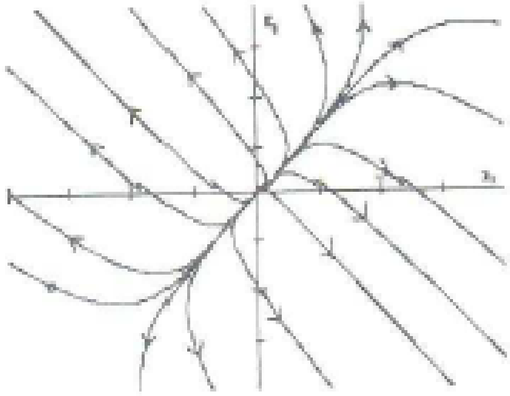


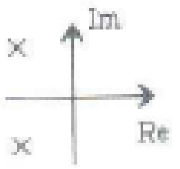
stable node



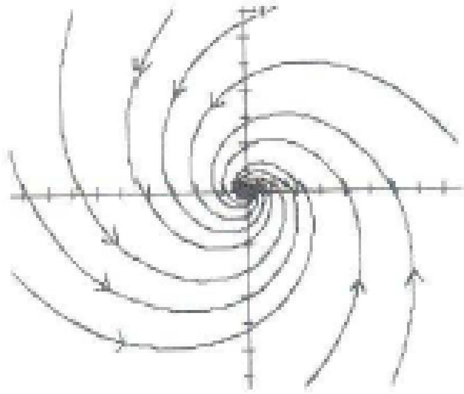


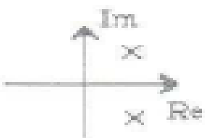
unstable node

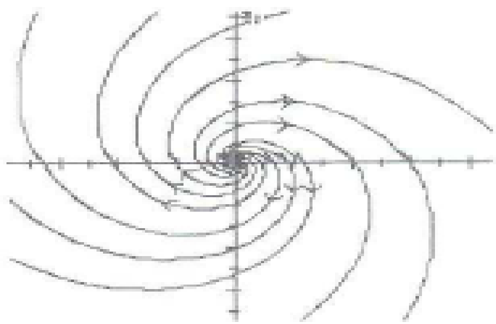




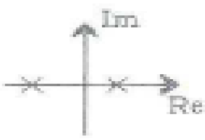
stable focus



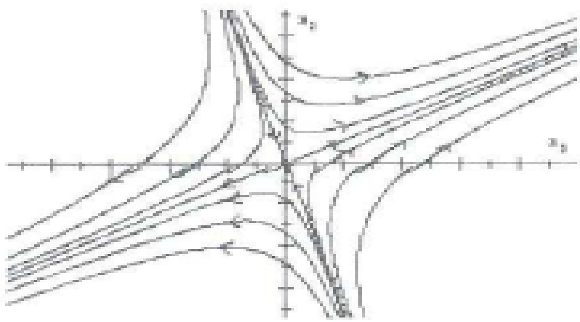


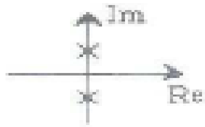


unstable focus



saddle





centre

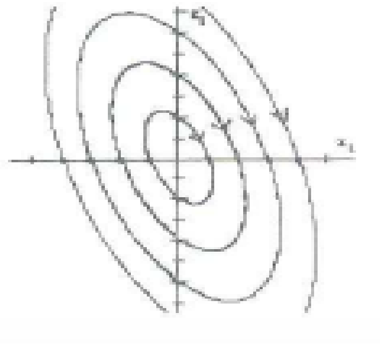


Figure 2: Phase-portraits of linear systems **Source: Slotine J.J.E (1991).**

Phase Plane Analysis of Nonlinear Systems

The analysis is related to that of linear systems because the local behaviour of a nonlinear system can be approximated by the behaviour of a linear system. Nonlinear system can exhibit much more complicated patterns in the phase plane, for example, multiple equilibrium points and limit cycles. The Hartman–Grobman theorem, or linearization theorem, is a theorem about the local behavior of dynamical systems in the neighbourhood of a hyperbolic equilibrium point. It asserts that linearization (which is a natural simplification of the system) is effective in predicting qualitative patterns of behaviour (Hartman, P. 1960).

When the singular point is not at the origin, it must be shifted to the origin. Using Taylor expansion, equation (3) can be rewritten in the form

$$\dot{x}_1 = ax_1 + bx_2 + g_1(x_1, x_2)$$

$$\dot{x}_2 = cx_1 + dx_2 + g_2(x_1, x_2), \tag{12}$$

in which g_1, g_2 contain higher order terms.

The higher order terms can be neglected in the locality of the origin and the nonlinear system trajectories therefore satisfy the linearised equation (4). As a result, the phase portraits of linear systems can approximate the local behaviour of the nonlinear system.

A limit cycle is an isolated, closed curve (Nguyen, 2002). The trajectory has to be both closed, indicating the periodic nature of the motion, isolated indicating the limiting nature of the cycle with nearby trajectories converging, or diverging, from it. Limit cycles do not occur in linear systems. They represent a very important phenomenon in nonlinear systems and are common in engineering and nature. There are three kinds of limit cycles that depend on the motion patterns of the trajectories. Figure 3 illustrates the kinds of limit cycles.

1. Stable limit cycle: All trajectories in the vicinity of the limit cycle converge as time progresses.
2. Unstable limit cycles: All trajectories in the vicinity of the limit cycle diverge as time progresses.
3. Semi-stable limit cycle: Some of the trajectories in the vicinity of the limit cycle converge as time progresses.

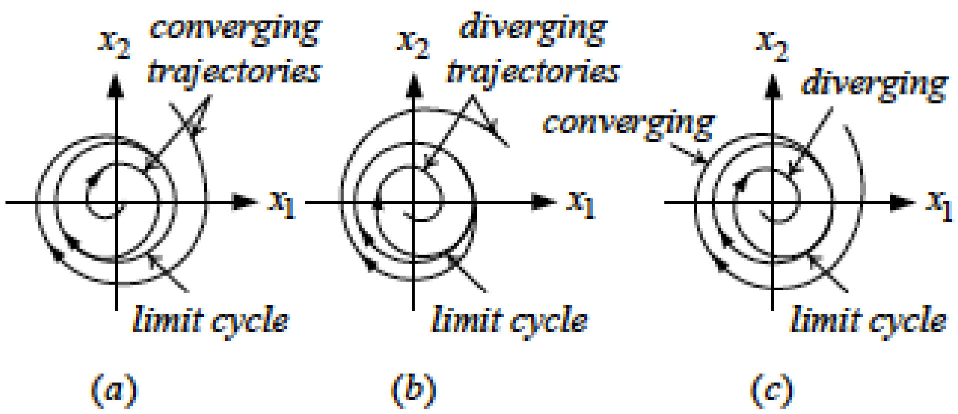


Figure 3: stable (a), unstable (b) and semi-stable (c) limit cycles. Source: Slotine J.J.E (1991).

The Van der Pol Equation

The Van der Pol oscillators are a second-order differential equation that describes many physical systems. The equation models a nonlinear system in which energy is added and subtracted from the system, resulting in a periodic motion called a limit cycle. The equation is given below (Nguyen, 2002)

$$\frac{d^2x}{dt^2} + \upsilon(x^2 - 1)\frac{dx}{dt} + x = 0, \quad \upsilon > 0 \tag{13}$$

the sign of $(x^2 - 1)\frac{dx}{dt}$ changes, depending upon whether $|x|$ is greater or less than unity. If $\upsilon = 0.2$ is used in simulation then the limit cycle can be shown that it exists because $\upsilon = 0.2$ is very small.

Chaos

This is caused by small perturbations of initial conditions of nonlinear systems, meaning that nonlinear systems are extremely sensitive to initial conditions. In a linear system, a small perturbation does not cause a huge difference in output. Chaos cannot be predicted even if there is an exact model of the nonlinear system. Atmospheric dynamics also display clear chaotic behaviour, thus making long-term weather prediction impossible (Nguyen, 2002).

Direction Fields

As more and more trajectories are added to the phase portrait it will become congested. Short arrows are used to indicate the direction and speed of the motion at each point in the phase plane. The plot that we get is called the direction field**.** A direction field is easier to plot than a phase portrait. Simulations of the differential equations must be carried out in order to plot the trajectories while the direction field can be determined directly from the differential equation model. The direction field can be constructed by selecting a mesh of points in the phase plane and at each point draw an arrow in the appropriate direction.

Nullclines

These are points in the phase portrait where the trajectories change their direction with respect to one of the axes. One of the two variables could have reached a local maximum or local minimum. These changes occur on the phase plane whenever the trajectory is directed either vertically, or horizontally, and can be determined directly from the model. The turning points are called $\dot{x}_1 - nullcline$ if

$$\dot{x}_1 = f(x_1, x_2) = 0 \tag{14}$$

and $\dot{x}_2 - nullcline$ if

$$\dot{x}_2 = g(x_1, x_2) = 0 \tag{15}$$

Points on the $\dot{x}_1 - nullcline$ have direction arrows with no horizontal component (vertically orientated) and points that are on the $\dot{x}_2 - nullcline$ have direction arrows with no vertical component (horizontally orientated). The trajectories intercept the $\dot{x}_1 - nullcline$ when they are orientated horizontally and the $\dot{x}_2 - nullcline$ when they are orientated vertically. The nullclines intersect at the steady state and can be determined directly from the model, without running actual simulations. The equations (14) and (15) are typically nonlinear and as a result may not be solvable except numerically.

3.2 Bifurcation Analysis

Bifurcation theory is the mathematical study of changes in the qualitative or topological structure of a given family, such as the integral curves of a family of vector fields, and the solutions of a family of differential equations (Afrajmovich, V. S. et al. 1994). Bifurcation means division into two. Poincare first used the term bifurcation to describe the splitting of equilibrium solutions into a family of differential equations.

If

$$\dot{x} = f_\upsilon(x)\,; \quad x \in \Re^n,\ \upsilon \in \Re^k$$

is a system of differential equations depending on the k-dimensional parameter, υ, then the equilibrium solutions are given by the solutions of the equations $f_\upsilon(x) = 0$. As υ varies, the implicit function theorem implies that these equilibria are described by smooth functions of υ, away from those points at which the Jacobian of the derivative of $f_\upsilon(x)$ with respect to x, $D_x f_\upsilon$ has a zero eigenvalue. The graph of each of these functions is a branch of equilibria of $\dot{x} = f_\upsilon(x)$ At equilibrium $(x_0; v_0)$, where $D_x f_\upsilon$ has a zero eigenvalue, several branches of equilibrium may come together and it becomes a point of bifurcation (Berkooz, G. et al 1993).

In most cases, if the model parameters are changed, then the position of a model's steady state shifts and, when the plot is constructed from the model, a continuation diagram is produced. A qualitative change in the long-term behavior of the system is caused by the variation of parameter values. Bifurcation points are where parameter values, at which such changes occur, will appear on continuation diagrams (referred to as bifurcation diagram).

Types of Bifurcations

- Transcritical bifurcation: A transcritical bifurcation is one in which a fixed point exists for all values of a parameter and is never destroyed. Such a fixed point, however, interchanges its stability with another fixed point as the parameter is varied. In other words, both before and after the bifurcation, there is one unstable and one stable fixed point. Their stability is, however, exchanged when they collide. So, the unstable fixed point becomes stable and vice versa

(Strogatz, 2001).

- Fold bifurcation: This bifurcation is also known as saddle-node or tangent bifurcation. A point υ_0 is called a fold bifurcation point for $F(\upsilon\,;\upsilon) = 0$ if there exists a solution $(\upsilon_0;\upsilon_0)$ with the property that for all sufficiently small $\partial > 0$ there exists $\gamma > 0$ such that $|\upsilon - \upsilon_0| < \gamma, F(\upsilon\,;\upsilon) = 0$ has no solutions in $B(\upsilon_0\,;\partial)$ for $\upsilon < \upsilon_0$ and two solutions in $B(\upsilon_0;\partial)$ for $\upsilon > \upsilon_0$ (Guckenheimer and Holmes, 1997). $B(\upsilon_0\,;\partial)$ is a behavioural equations and $F(\upsilon\,;\upsilon) = 0$ is a function with $(\upsilon\,;\upsilon)$ as parameters.
- Pitchfork bifurcation: It is a local type of bifurcation where the system transitions from one fixed point to three fixed points. In continuous dynamic systems pitchfork bifurcation generally occurs in systems with symmetry. This bifurcation can either be subcritical (if the bifurcating branch exists for values of the parameter υ less than the bifurcation value υ_c) or supercritical (if the bifurcating branch exists for values of the parameter υ greater than the bifurcation value υ_c).
- Hopf bifurcation: This bifurcation is also known as Poincaré-Andronov-Hopf bifurcation. The term refers to the local birth or death of a periodic solution (self-excited oscillation) from equilibrium as a parameter crosses a critical value. It is the simplest bifurcation, not just involving equilibria, and therefore belongs to what is sometimes called dynamic (as opposed to static) bifurcation theory. In a differential equation a Hopf bifurcation typically occurs when a complex conjugate pair of eigenvalues of the linearised flow at a fixed point becomes purely imaginary. This implies that a Hopf bifurcation can only occur in systems of dimension two or higher (Marsden and M. McCracken, 1976).

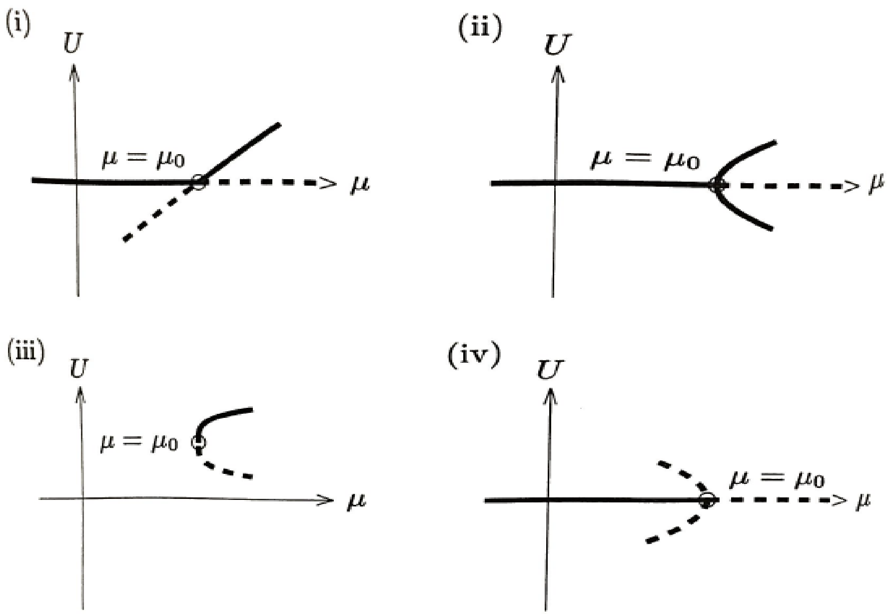


Figure 4: Types of bifurcations: (i) transcritical, (ii) supercritical pitchfork, (iii) fold, (iv) subcritical pitchfork.

Source: Stuart and Humphries (1996)

In Figure 4, the thick solid line indicates steady state and broken line indicates unstable steady. μ is the constant parameter.

3.3 Sensitivity Analysis

Sensitivity analysis is the study of how the uncertainty in the output of a mathematical model or system can be apportioned to different sources of uncertainty in its inputs (*Saltelli et al.*, 2000). It is also, the general study of the dependence of a model's behaviour illustrated by continuation and bifurcation diagrams. The parametric sensitivity analysis is divided into global sensitivity analysis (addressing wide variations in parameter values) and local sensitivity analysis (addressing small variation around a nominal operating condition). Sensitivity analysis is important to the reliability of simulation results (Ingalls, B. 2008).

Sensitivity analysis is the effect of a perturbed input on the model's output that determines how the "variation in output can be apportioned to different sources of variation" (*Saltelli et al*., 2000). Sensitivity analysis, furthermore, not only determines the effect of variations in assumed information on the model-output it also assists in developing an intuition about model structure and guides data collection efforts (Sterman 2000).

The initial step of sensitivity analysis is *uni-variate*, which is conducted according to a "*one-at-a-time approach"* (*Saltelli et al*., 2000). The changes in model output, which stem from the perturbation of each parameter, are analysed separately and the most influential parameters are estimated roughly. On the other hand, in nonlinear and complex models, *uni-variate* sensitivity analysis is insufficient for a comprehensive study of the model. Simultaneous changes in more than one parameters' values may create an unexpected output change because of the nonlinear relationships among different model components (Sterman, 2000). Therefore, a uni-variate sensitivity analysis should be succeeded by a *multi-variate sensitivity* analysis.

Sensitivity analysis may reveal important information to the researcher. The results of sensitivity analysis may allow the modeler to identify which of the model parameters are most significant to the simulation's output. The parameters, to which model output is sensitive, require more intensive data analysis in order to decrease the uncertainty in the parameter value.

As a first step in sensitivity analysis, the distribution function and range of each parameter are determined by using the information and sampled data obtained from the real system. Typically, ± 20% of the parameter value is used as the distribution range (Sterman, 2000). These parameter ranges and distributions can be entered to Vensim's

Sensitivity Simulation module, which is explained in detail in the study by Ford and Flynn (2005). The local sensitivity coefficients can be determined by numerical approximation or implicit differentiation.

- Numerical approximation involves determining the coefficient by simulation. The coefficient at $p = p_0$ can be determined by simulating the model at $p = p_0$ and at another nearby value $p = p_0 + \Delta p_0$, where Δp_0 should be normally be chosen less than a 5% deviation from p_0 $(Saltelli\ et\ al., 2000)$.
- If the explicit formula for steady state is available, then the coefficients will be determined by direct differentiation. If the formula is not available, then the coefficients will be determined by implicit differentiation of the differential equation model.

3.4 Stability Analysis

The long term behaviour of biochemical and genetic networks will be either

- Convergence to a steady state; or
- Convergence to a sustained periodic oscillation (limit cycle oscillations) (Ingalls, 2012).

In systems biology, models do not have divergence. In phase plane analysis all trajectories approach a unique steady state. Figure 5 shows symmetric biochemical network.

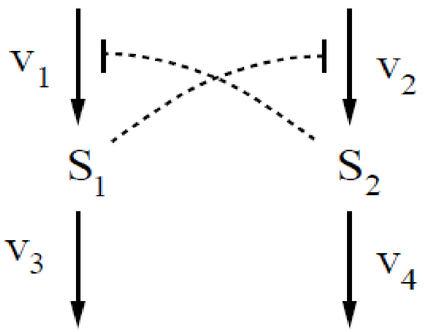


Figure 5: Symmetric biochemical network. **Source: Ingalls (2012)**

This reaction scheme is symmetric because each species allosterically inhibits production of the other, resulting in mutual antagonism. With cooperative inhibition and first-order consumption rates, the model is

$$\frac{d}{dt}s_1(t) = \frac{k_1}{1+\left(\frac{s_2(t)}{K_2}\right)^{n_1}} - k_3 s_1(t)$$

$$\frac{d}{dt}s_2(t) = \frac{k_2}{1+\left(\frac{s_1(t)}{K_1}\right)^{n_2}} - k_4 s_2(t). \tag{16}$$

Where s_1 *and* s_2 are two types of species, n is the number of molecules, k_i is the reaction rate and K is the concentration. Considering an asymmetric model parametrisation in which $n_1 > n_2$, the inhibition by s_2 is more effective than the inhibition by s_1. If the other parameters are symmetric, the model will exhibit a steady state.

Bistability

This is when a system exhibits two distinct steady states. If it exhibits one steady state it is referred to as monostable. Bistability provides a system with a type of memory – the system's long-term behaviour reflects its past condition. There are two essential ingredients to bistability: positive feedback and nonlinearity. Positive feedback is implemented in a double negative feedback loop (each species inhibits production of the other and thus inhibits the inhibition of itself). Nonlinearity is provided by the cooperative inhibition mechanism. These two ingredients are necessary for stability, but they do not guarantee it: the model structure and parameter values must also be properly aligned (Ingalls, 2012).

Stable and Unstable Steady States

The points where nullclines intersect in the system are called steady states. If the system attracts nearby trajectories, the steady state will be stable, but if it repels the trajectories from it, the steady state will be unstable. In theory, the unstable steady state can be maintained by perfectly balanced initial conditions. If there is a deviation from the balance, it will cause the trajectory to tend toward a stable steady state. In phase plane analysis, stability analysis relied on graphical representations and is restricted to two-species networks. The researcher is going to look at a technique for stability analysis that does not rely on graphical representations and is not restricted to two species networks linearised stability analysis. Linearised stability analysis approximates any nonlinear system by a linear system and can be used to test for stability of steady states (Ingalls, 2012).

A function $f(s)$ near a particular point $s = \bar{s}$ by the tangent line centered at $\bar{s}$, as illustrated in Figure 6:

$$f(s) = f(\bar{s}) + \frac{df}{ds}(\bar{s}).(s - \bar{s}). \tag{18}$$

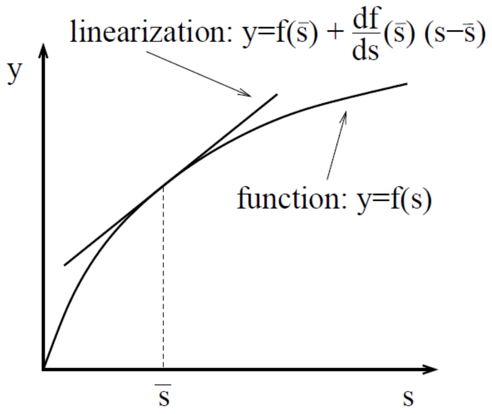


Figure 6: Linear approximation of a function of a single variable. Source: Ingalls (2012)

The tangent line is called the linearization (or linear approximation) of $f(s)$ at $s = \bar{s}$.

Stability Analysis for Linear Systems

The general form of a two-state linear system is

$$\frac{d}{dt}x_1(t) = ax_1(t) + bx_2(t)$$
$$\frac{d}{dt}x_2(t) = cx_1(t) + dx_2(t). \qquad (19)$$

This system can be solved explicitly. Solutions take the form

$$\begin{aligned} x_1(t) &= c_{11}e^{\lambda_1 t} + c_{12}e^{\lambda_2 t} \\ x_2(t) &= c_{21}e^{\lambda_1 t} + c_{22}e^{\lambda_2 t}. \end{aligned} \qquad (20)$$

The constants c_{ij} depend on the initial conditions, but the values λ_1 and λ_2 are inherent to the system. The λ_1 and λ_2 are the eigenvalues of the system's Jacobian (10).

The Jacobian is constructed from (19).

The roots λ_1 and λ_2 can be explicitly represented as

$$\lambda^2 - (a+d)\lambda + (ad - bc) = 0 \qquad (21)$$

Applying the quadratic formula gives

$$\lambda_1 = \frac{(a+d)+\sqrt{(a+d)^2-4(ad-bc)}}{2}$$
$$\lambda_2 = \frac{(a+d)-\sqrt{(a+d)^2-4(ad-bc)}}{2}. \tag{22}$$

Depending on the sign of the discriminant $(a+d)^2-4(ad-bc)$, these two eigenvalues may be real-valued or complex-valued. The general behaviour of the solutions to (21) depends on the nature of the exponential functions $e^{\lambda_1 t}$ and $e^{\lambda_2 t}$. To classify the behaviour of these functions, there are two cases to consider;

Case 1. The discriminant is positive, so that λ_1 and λ_2 are real numbers. Then if,

a) both eigenvalues are negative, then both solutions tend to zero and the steady state is a stable node.

b) either eigenvalue is positive, then most of the solutions diverge and the steady state is unstable

c) both eigenvalues are positive, then all trajectories diverge and the steady state is an unstable node

d) one eigenvalue is positive and the other is negative, then the steady state a saddle point (unstable).

Case 2. The discriminant is negative, so the eigenvalues are complex-valued. Then the solutions of the eigenvalues will be

$$\lambda_1 = \alpha + \beta i$$
$$\lambda_2 = \alpha - \beta i. \tag{23}$$

Since the solutions involve the terms $e^{\lambda_1 t}$ and $e^{\lambda_2 t}$, there is need to evaluate the exponential of complex numbers. Substituting into *Euler's formula,* the following is obtained

$$x_1(t) = c_{11}e^{\alpha t}(\cos(\beta t)+i\sin(\beta t))+c_{12}e^{\alpha t}(\cos(\beta t)-i\sin(\beta t))$$
$$x_2(t) = c_{21}e^{\alpha t}(\cos(\beta t)+i\sin(\beta t))+c_{22}e^{\alpha t}(\cos(\beta t)-i\sin(\beta t)). \tag{24}$$

The long-term behaviour is determined solely by the exponential term $e^{\alpha t}$. Then if

a) α, the real part of the eigenvalues, is negative, then the solutions converge to zero. In this case the steady state is stable and it is called a stable spiral point, or focus. The solutions will exhibit damped oscillations as they converge.

b) α , the real part of the eigenvalues, is positive, then the solutions diverge. The steady state is unstable, and is called an unstable spiral point

There is a linearised stability criterion

1. If both eigenvalues of the Jacobian have negative real part, then the steady state is stable.
2. If either eigenvalues have positive real part, then the steady state is unstable.

In summary, to apply the linearised stability criterion to a nonlinear model:

1. Determine a steady state of interest.
2. Develop the system Jacobian at that point (by taking the appropriate partial derivatives).
3. Calculate the eigenvalues of the Jacobian.
4. Test the sign of their real part.

Summary

The four types of analysis were discussed fully. All the steps to be followed have been detailed down. The Jacobian is very important in determining the eigenvalues that will be used in determining the stable points. There are other methods that could be used as well that the author did not mention such as Gauss Siedel and relaxation methods. The author would wish to take up a study to investigate the three different methods and their applicability to different modeling situations. Another area of interest will be the Van del bel equation, the way it is used to study physical systems will help a great deal. In summary it has been seen that there are different analysis methods that can be used depending on what one wants to do with the results. The next chapter will discuss and solve mathematical problems.

Chapter 4 Discussion of Mathematical Models

Introduction

In this chapter, the author will solve mathematical modeling questions dealing with limit cycle stability, bifurcation, phase plane analysis of linear and nonlinear system. With nonlinear system, a model on chemostat will be solved.

Example of Limit Cycle Stability

To check for stability, we need to transform the rectangular coordinates to polar coordinates (r,θ). Then we find an expression for the derivative of r.

- If $\dot{r} = 0$, then the system is on the limit cycle.
- The system will be stable if $\dot{r} > 0$ inside the limit cycle and if $\dot{r} < 0$ outside the limit cycle.

- It will be unstable if $\dot{r} < 0$ inside the limit cycle and if $\dot{r} > 0$ outside the limit cycle.
- Lastly the system will be semi-stable $\dot{r} > 0$ inside and outside limit cycle or $\dot{r} < 0$ inside and outside the limit cycle.

The following polar equations will be used for (r, θ).

$$r^2 = x_1^2 + x_2^2$$

$$tan(\theta) = \frac{x_2}{x_1}$$

$$\dot{r} = \frac{x_1\dot{x}_1 + x_2\dot{x}_2}{r}$$

$$\dot{\theta} = \frac{x_1\dot{x}_2 - x_2\dot{x}_1}{r^2}. \quad (25)$$

Consider the differential equations

$$\dot{x}_1 = x_2 - x_1\left(x_1^2 + x_2^2 - 1\right)$$
$$\dot{x}_2 = -x_1 - x_2\left(x_1^2 + x_2^2 - 1\right), \tag{26}$$

with initial conditions

$$r_0 = \sqrt{\frac{1}{c_0 + 1}},\ \theta(0) = \theta_0,$$

then substituting for $\dot{r}$ and $\dot{\theta}$ we get

$$\dot{r} = \frac{x_1\dot{x}_1 + x_2\dot{x}_2}{r}$$

$$= -\frac{(x_1^2 + x_2^2)(x_1^2 + x_2^2 - 1)}{r}$$

$$= -\frac{r^2(r^2 - 1)}{r}$$

$$= -r(r^2 - 1)$$

$$\dot{\theta} = \frac{x_1\dot{x}_2 - x_2\dot{x}_1}{r^2}$$

$$= -\frac{x_1^2 + x_2^2}{r^2}$$

$$= -1$$

r increases inside the unit circle and decreases outside it. So, there is a stable limit cycle

when

$$r = 1\ (unit\ circle)$$

$$\dot{\theta} = -1.$$

Solution: $r = (1 + c_0 e^{-2t})^{\frac{-1}{2}}, c_0 = r^{-2} - 1$

$\theta = \theta_0 - t.$

Limit as $t \to \infty$ of r is unity.

Example of Bifurcation Analysis

Given the differential equation

$$\dot{x}(t) = (a-1)x(t). \tag{27}$$

The steady state is when $x = 0$. The parameter value $a = 1$ is a bifurcation point in the system.

Look at the case when $a < 1$.

- Then for $x < 0$ there is $\dot{x} > 0$ and for $x > 0$ there is $\dot{x} < 0$.
- The steady state when $x = 0$ is stable, trajectories converge to the point $x = 0$.

Next, look at the case for which $a > 1$.

- Then, for $x < 0$ there is $\dot{x} < 0$ and for $x > 0$ there is $\dot{x} > 0$.

The steady state at $x = 0$ is thus unstable, as trajectories are repelled from this point.

Example of Phase Plane Analysis

Consider the biochemical network, which involves two species, S_1 and S_2. To simplify the analysis, we suppose that all reaction rates follow mass action (or equivalently, Michaelis – Menten kinetics with all enzymes operating in their first-order regime). The first kinetic model that successfully explained this situation was started by Leonor Michaelis and Maud Menten (Ingalls, 2012). They assumed that the enzyme directly interacts with substrate in a stoichiometric manner, the interaction results in a well-defined intermediate complex, and the interaction leads to thermodynamic equilibrium.

The allosteric inhibition of v_1 will be modeled by presuming strong cooperative binding of n molecules of S_2. We can then write

$$v_1 = \frac{k_1}{1 + \left(\frac{S_2}{K}\right)^n}$$

$$v_2 = k_2$$

$$v_3 = k_3 s_1$$

$$v_4 = k_4 s_2$$

$$v_5 = k_5 s_1$$

where, $k_i\ is\ the\ concentration, v_i\ are\ reaction\ rates\ (i = \{1,2..5\})$

$and\ are\ modeled\ by\ presuming\ a\ strong\ cooperative\ binding\ of\ n\ molecules\ of\ S_2,$

$s_1 = [S_1]$ and $s_2 = [S_2]$ so that the model is,

$$\frac{d}{dt}s_1(t) = \frac{k_1}{1 + \left(\frac{s_2(t)}{K}\right)^n} - k_3 s_1(t) - k_5 s_1(t)$$

$$\frac{d}{dt}s_2(t) = k_2 + k_5 s_1(t) - k_4 s_2(t). \tag{28}$$

The nullclines can be determined analytically.

The $s_1 - nullcline$ is defined by,

$$0 = \frac{k_1}{1+\left(\frac{s_2(t)}{K}\right)^n} - k_3 s_1(t) - k_5 s_1(t) \tag{29}$$

which can be simplified to,

$$s_1 = \frac{k_1}{\left(1 + \left(\frac{s_2(t)}{K}\right)^n\right)(k_3 + k_5)}$$

The $s_2 - nullcline$ is defined by,

$$0 = k_2 + k_5 s_1(t) - k_4 s_2(t).$$

which can be written as,

$$s_2 = \frac{k_1 + k_5 s_1}{k_4}.$$

Example of Stability Analysis for Nonlinear Systems (Chemostat)

A chemostat is a growth vessel into which fresh medium is delivered at a constant rate and cells and spent medium overflow at that same rate.

Consider the model,

$$\frac{dx}{dt} = k(c) - Dx, \quad \frac{dc}{dt} = D(c_0 - c) - \frac{1}{y}k(c)x, \tag{30}$$

where $k(c)$ is the growth-rate function D is the dilution rate and c is the nutrient concentration. The typical graph of $k(c)$ is shown in Figure 7.

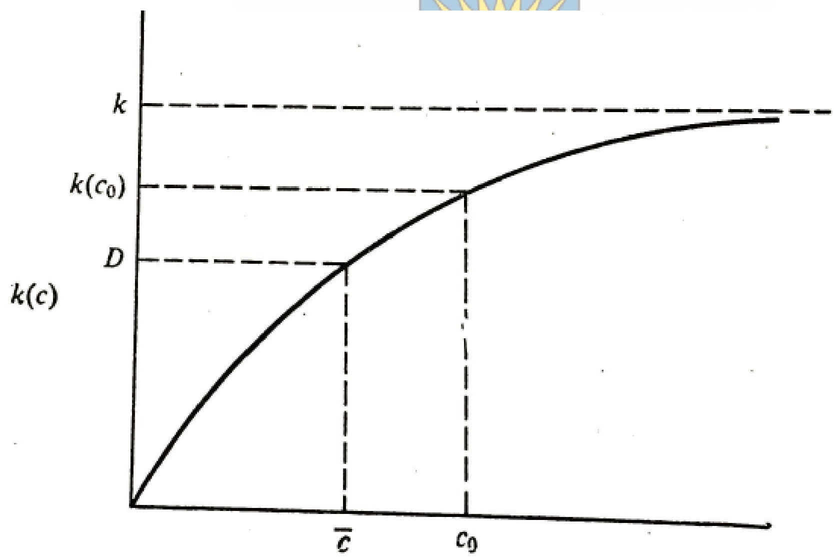


Figure 7: Typical graph of specific growth-rate function. **Source: Kapur (1992)**

The system has the following two possible steady states:

$$\bar{x} = 0,\ \bar{c} = c_0;$$

$$k(c) = D,\ \bar{x} = y(c_0 - \bar{c}) \tag{31}$$

The first state is called the washed-out steady state because, in this state no microorganisms are produced. The second state, when it exists, is called the normal steady state and is of greater interest. The first state can arise when $D > k(c_0)$ so that $\frac{dx}{dt}$ is always negative and $x \to 0,\ c \to c_0$. To discuss the stability of this steady state, we consider slight deviations $u(t)$ and $v(t)$ from the steady state, and write

$$x(t) = u(t),\ \ c(t) = c_0 + v(t). \tag{32}$$

Substituting in (30) and neglecting products, squares and higher powers of $u(t)$ and $v(t)$ we get

$$\frac{du}{dt} = [k(c_0) - D]u,\ \ \frac{dv}{dt} = -D_v - \frac{1}{y}k(c_0)u. \tag{33}$$

We try the solution

$$u(t) = Ae^{\lambda t},\ \ v(t) = Be^{\lambda t} \tag{34}$$

to have

$$\begin{aligned} &[\lambda + D - k(c_0)]A = 0, \\ &\frac{1}{y}k(c_0)A + (\lambda + D)B = 0 \end{aligned} \tag{35}$$

Eliminating A and B, we obtain the equation for determining λ

$$[\lambda + D - k(c_0)](\lambda + D) = 0. \tag{36}$$

Both the roots are real, and both are negative if $D > k(c_0)$ and if this is satisfied then $u(t)$ and $v(t)$ approach zero as $t \to \infty$ so that $x(t) \to 0$ and $c(t) \to c_0$. Consequently, the equilibrium position is stable and is in fact a node. Then if $D < k(c_0)$, one of the values of λ is positive, $u(t)$ and $v(t)$ can increase so that the equilibrium position is unstable.

Biologically, the discussion gives the following: if $D > k(c_0)$, and some microorganisms are introduced in the chemostat, they will be ultimately washed out; however, if $D < k(c_0)$, the populations of the microorganisms will increase.

We now discuss the normal steady state position. The second set of equations (35) will give a positive real value of $\bar{c}$ only if $D < k$, and then $\bar{x} > 0$ only if

$$\bar{c} < c_0, \text{ or } k(\bar{c}) < k(c_0) \text{ or } D < k(c_0). \tag{37}$$

Thus, a necessary and sufficient condition for the existence of the normal steady state position is $D < k(c_0)$.

Now, to discuss the stability of the normal state, we substitute

$$x(t) = \bar{x} + u(t), \quad c(t) = \bar{c} + v(t) \tag{38}$$

in (32) and get

$$\frac{du}{dt} = [(k(\bar{c}) + v(t)k \cdot (\bar{c}) + \ldots) - D][\bar{x} + u(t)],$$

$$\frac{dv}{dt} = D[c_0 - \bar{c} - v(t)] - \frac{1}{y}[k(\bar{c}) + v(t)k \cdot (\bar{c}) + \ldots][\bar{x} + u(t)] \tag{39}$$

Neglecting products, squares, and higher powers of $u(t)$ and $v(t)$ we obtain

$$\frac{du}{dt} = k(\bar{c})\bar{x}v(t), \qquad \frac{dv}{dt} = -Dv - [v(t)k \cdot (\bar{c})\bar{x} + k(\bar{c})u(t)] \tag{40}$$

using solution (34) we get

$$\lambda A - k \cdot (\bar{c})\bar{x}B = 0,$$

$$\frac{1}{y}k(\bar{c})A + \left[\lambda + D + \frac{1}{y}k \cdot (\bar{c})\bar{x}\right] B = 0. \tag{41}$$

Eliminating A and B, we get

$$\lambda^2 + \lambda\left[D + \frac{1}{y}k \cdot (\bar{c})\bar{x}\right] + \frac{1}{y}k(\bar{c})k \cdot (\bar{c})\bar{x} = 0 \tag{42}$$

Since $D, y, \bar{x}, k(\bar{c})$ and $k(\bar{c})$are all positive, both the roots of this equation are real and negative or both its roots are complex but with negative real parts. In either case $u(t)$ and $v(t)$ approach zero as $t \to \infty$ and the normal steady state is asymptotically stable;

in fact, it is a node. Therefore, the result we get is as shown in Table 2:

Steady state	$D > k(c_0)$	$D < k(c_0)$
Washed-out state	Asymptotically stable; node	Unstable; saddle point
Normal state	Does not exist	Asymptotically stable; node

Table 2: Steady state results for Chemostat

We also get the operating diagram shown in Figure 8.

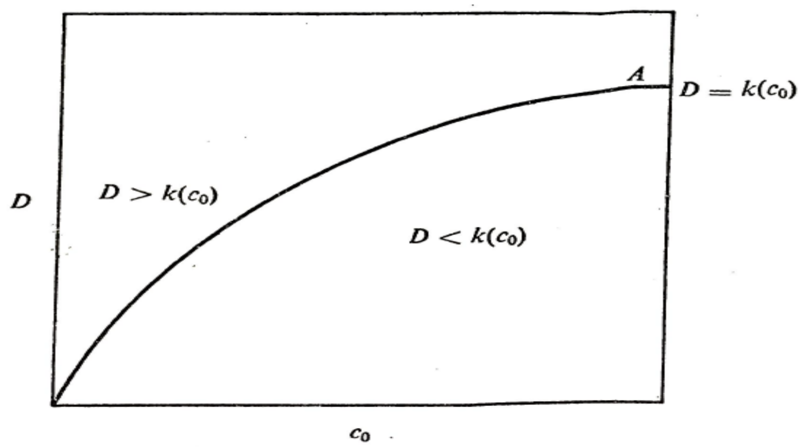


Figure 8: Operating diagram for the stability of the two states **Source: Kapur (1992)**

If the point $(D; c_0)$ of the operating conditions lies below curve A, the normal steady state $(\bar{x}\,; \bar{c})$is the only stable steady state. This means that we should expect that, whatever be the non-zero initial values of $(x\,; c)$in the chemostat, ultimately, they will converge to $(\bar{x}\,; \bar{c})$. Similarly, if the point $(D; c_0)$ lies above the curve A, the washed-out steady state is the only stable equilibrium state. Thus, whatever be the initial values of $(x\,; c)$ in the chemostat, these should always converge to $(0; c_0)$. These results are based on the local stability analysis, which have been discussed above. To see whether these are true for large deviations from steady state positions, numerical integrations of the basic equations is carried out. We do this for Monod's model for which our original model becomes

$$\frac{dx}{dt} = \left(\frac{kc}{K+c} - D\right)x, \quad \frac{dc}{dt} = D(c_0 - c) - \frac{1}{y}\frac{kc}{K+c}x. \tag{43}$$

We now use the non-dimensional variables and parameters

$$X = \frac{x}{yc_0}, \tau = kt, C = \frac{c}{c_0}, \overline{K} = \frac{K}{c_0}, \overline{D} = \frac{D}{k} \tag{44}$$

to get

$$\frac{dX}{d\tau} = \left(\frac{C}{\overline{K}+C} - \overline{D}\right)X, \quad \frac{dC}{d\tau} = \overline{D}(1 - C) - \frac{C}{\overline{K}+C}X. \tag{45}$$

The curve A now becomes

$$\bar{D} = \frac{1}{\bar{K}+1}. \tag{46}$$

We now take two operating conditions, one above the curve, namely $\bar{K} = 1,\ \bar{D} = 1$ and the other below the curve $\bar{K} = 1,\ \bar{D} = \frac{1}{3}$. The differential equations and the equilibrium points for the two cases are as follows:

$$\frac{dX}{d\tau} = -\frac{1}{1+C}X, \quad \frac{dC}{d\tau} = (1 - C) - \frac{CX}{1+C}, \quad (0\,;1) \tag{47}$$

$$\frac{dX}{d\tau} = \frac{2C-1}{3(1+C)}X, \quad \frac{dC}{d\tau} = \frac{1}{3}(1 - C) - \frac{CX}{1+C}, \quad (0\,;1),\ \left(\frac{1}{2};\frac{1}{2}\right). \tag{48}$$

The trajectories on the XC-plane for the above equations are shown below in Figure 9 and Figure 10 respectively.

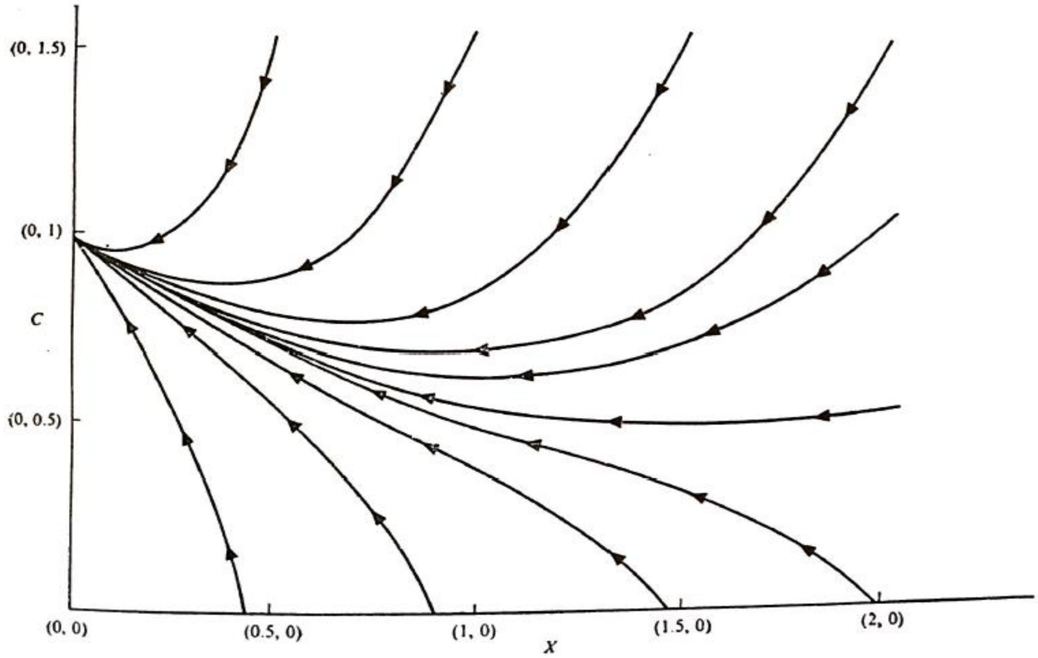


Figure 9: Trajectories for the first solution (47) **Source: Kapur (1992)**

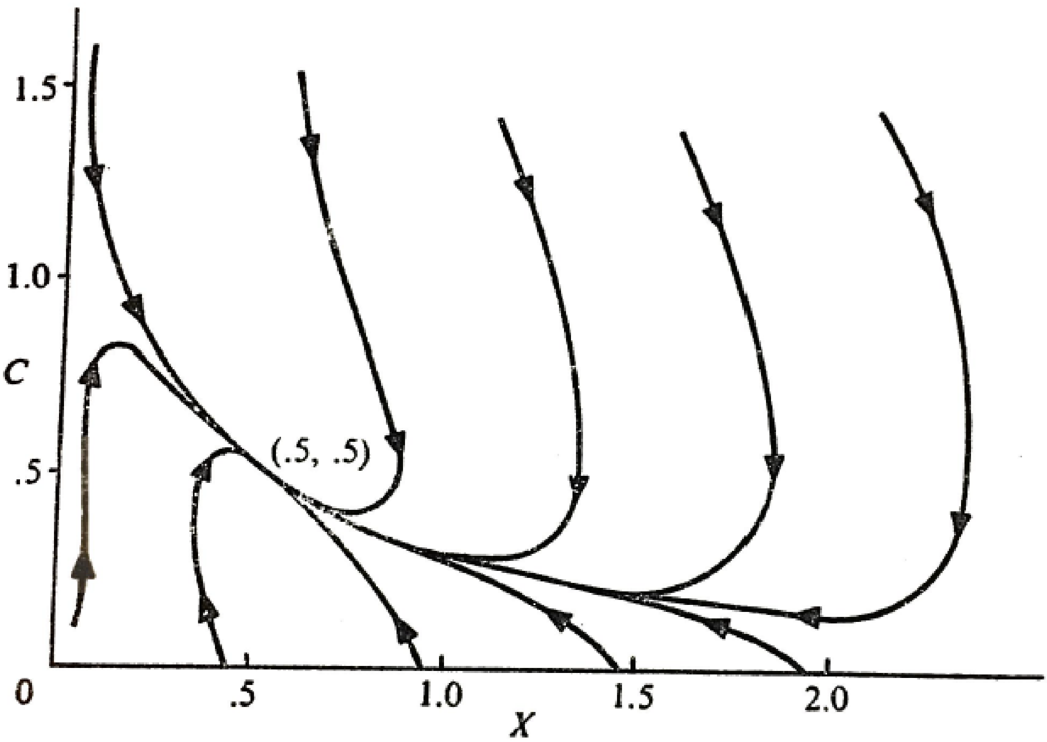


Figure 10: Trajectories for the second solution (48) **Source: Kapur (1992)**

Summary

The author managed to solve different types of questions on phase plane of linear systems and nonlinear systems. Bifurcation analysis problem was also solved. Unfortunately, computer programs could not be run to solve more problems. The next chapter gives an outline of the computer programs that the author could have done.

Chapter 5 Computational Software

Introduction

The mathematical approaches covered in this research can be executed in a number of computational software packages. This chapter offer two such programs: MATLAB (Matrix Laboratory) and XPPAUT (X-windows Phase Plane Auto). Many researchers subscribe to MATLAB to be the standard tool for analysis, but it is a commercial product, which may be too expensive to many. XPPAUT is then suggested for users who have confined experience with computational software and it is freely available. There are many other software packages that can be used as well.

MATLAB

MATLAB software can be bought directly from the company website (www.mathworks.com/matlab) or may be accessed from institutional license. It is well suited for matrix calculations. The tutorials are available online and documentation provided by company. User-coded scripts is used in most analysis and the interface is command-line driven (Gilat, A. 2008).

The command 'plot' is used to plot trajectories in the phase plane analysis. Running multiple simulations and plotting them together can plot a collection of trajectories. A command 'quiver' is used to produce direction field. The command *mesh grid* generates a mesh of point at which the direction arrows can be placed. The length of the arrows in the x and y directions can then be assigned by calculating the right-hand-side of the differential equations. Dividing each arrow by its length will result in a scaled direction field.

The command *ezplot* will generate nullclines. Although the nullclines in chain1.m can be solved explicitly, we nevertheless use this model to illustrate the general procedure. The ezplot command is also used to plot the solution to implicit equations. The program PPLANE, by John Polking, provides a GUI for phase plane analysis in MATLAB (Gilat, A. 2008). The interface allows the user to specify model equations and display a direction field or nullclines.

MATLAB can be used to numerically approximate parametric sensitivity. A template script is:

```
nom par=5;                                        % set nominal parameter value
par=nom par;                                      % assign nominal parameter value
[t nom, s nom]=ode45(ODEFUN,[0,Tend],s0);         % nominal trajectory
s nom ss = s nom(length(t nom));                  % steady-state concentration
delta=0.05;                                       % set deviation (5 percent)
par=par*(1+delta);                                % perturbed parameter value
[t pert,s pert]=ode45(ODEFUN,[0,Tend],s0);        % perturbed trajectory
s pert ss=s pert(length(t pert));                 % steady-state concentration
abs sens=(s pert ss-s nom ss)/(delta*nom par);    % absolute sensitivity
rel sens=abs sens*(nom par value/s nom ss);       % relative sensitivity
```

Source: Gilat, A. (2008)

XPPAUT

G. Bard Ermentrout created XPPAUT and is maintaining it. The name of the program incorporates three key features: it runs in the X-windows environment; Phase Plane analysis is one of its primary uses; and it employs a program called AUTO for bifurcation analysis. (E. Doedel created AUTO.) Ermentrout, B. (2002). The XPPAUT software and documentation are available online.

Summary

The computer programs mentioned in this chapter are so far leading in the analysis of models, each has got its own advantages that outweigh the other package. So, it depends really on what one hopes to achieve that will decide which package to use.

Chapter 6 Conclusions and Recommendations

Research assisted in providing a deeper understanding of different ways of analysing dynamic mathematical models. Intimate knowledge of the physical processes is required in the modeling of any physical system. The modeler must decide what processes are to be modeled and how detailed an analysis is required. The modeling process can be greatly altered by approximations in the calculated dynamic behavior. Therefore, each simplifying assumption must be justified.

The modeling process is verbose in that one repeatedly refines the models to show the current level of understanding. Therefore, there is a need to use top of the range computational software.

As mathematics students at University of Fort Hare, we have been exposed to many subjects such as Ordinary Differential Equations, Calculus of Variations, Numerical Analysis and Mathematical Modeling. Various similarities and connections were noticed among these subjects. That is in fact the motivation behind the idea of presenting the analysis of Dynamic Mathematical Modeling. Hopefully, I will continue to research on different analysis that can be used to understand mathematical systems better.

If in any system, there are problems arising, then action must be taken to solve such problems. However, making the wrong decision could propagate the problem, and ultimately collapse the system. Therefore, understanding the behaviours and structures of systems is essential for problem solving. In general, systems contain many complex relationships, which might cause them to be nonlinear, and make it difficult for the human mind to think through the problem. Therefore, many graphical and mathematical modeling methods have been developed as potential tools to understand a system.

To this end it is highly recommended to familiarise with a lot of different ways of analysing systems so that one is able to understand models that will make life easier. Also the researcher is recommending to research on different computational software that will assist in more analysis of systems.

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