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**BIFURCATION ANALYSIS
IN CHEMICAL ENGINEERING**

Evrin YAVUZ

Chemical Engineering Department

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Supervisor: Prof. Dr. Beno KURYEL

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III

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Jüri Üyeleri:

İmza:

Jüri Başkanı : Prof. Dr. Beno KURYEL

.....

Üye : Prof. Dr. Süheyda ATALAY

.....

Üye : Prof. Dr. Turgut ÖZİŞ

.....

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1.0 INTRODUCTION

Exploring nonlinear phenomena in the nature has become a major subject in many fields during the last decades, from physics, chemistry, biology, engineering and social science to daily life.

The approach pursued in this study is directed toward nonlinear systems which undergo bifurcations, and possibly chaotic motion, as a parameter is varied.

Such systems naturally possess several, and possibly infinitely many, equilibria and periodic orbits. The approach is of particular relevance to systems for which the model possesses a high degree of uncertainty. Often, an engineering system is designed to perform well, and to be stable, for a large range of parameter values. However, technological demands are pushing systems to the limits of their performance, and many engineering systems are being operated under conditions which may be viewed as 'stressed'. It is this stressed operation which gives rise to nonlinear dynamic phenomena, such as bifurcations leading, in some cases, to chaos [Wang et al, 1992].

Behaviour in a nonlinearly complex system that appears irregular or unpredictable actually is determinate. The apparently unpredictable behaviour in systems governed by complicated, so nonlinear deterministic laws is the result of high sensitivity to initial conditions. For example, Edward Lorenz discovered that a simple model of heat

convection exhibits chaotic behaviour. In a now-classic example of such sensitivity to initial conditions, he suggested that the mere flapping of a butterfly's wings could eventually result in large-scale changes in the weather (the “butterfly effect”).

In mathematics and physics, chaos theory describes the behaviour of certain nonlinear dynamical systems that under certain conditions exhibit a phenomenon known as chaos. Among the characteristics of chaotic systems, described below, is the sensitivity to initial conditions (popularly referred to as the “butterfly effect”). As a result of this sensitivity, the behaviour of systems that exhibit chaos appears to be unpredictable, even though the system is deterministic in the sense that it is well defined and contains no random parameters. Examples of such systems include the atmosphere, the solar system, plate tectonics, turbulent fluids, economics, and population growth [http://en.wikipedia.org/wiki/Chaos_theory].

The word chaos originates from a Greek word *Χάος* and its everyday meaning is ‘a state without order’. This word reminds one of a totally disorganized state, in contrast with cosmos, an ordered state, it indicates a phenomenon which is not totally disordered but disordered moderately and shows a temporarily irregular motion. Moreover, it refers to

‘an irregular oscillation governed by a relatively simple rule’.

Here ‘oscillation’ simply represents a variation of certain quantities.

Figure 1.1 serves as evidence for an irregular oscillation or a nonperiodic oscillation governed by a simple rule at all. This is a graph of an irregular series $\{x_n\}$ as a function of n . Where on earth is a simple rule hiding behind this irregular series? Let us discover the regularity of this series as follows.

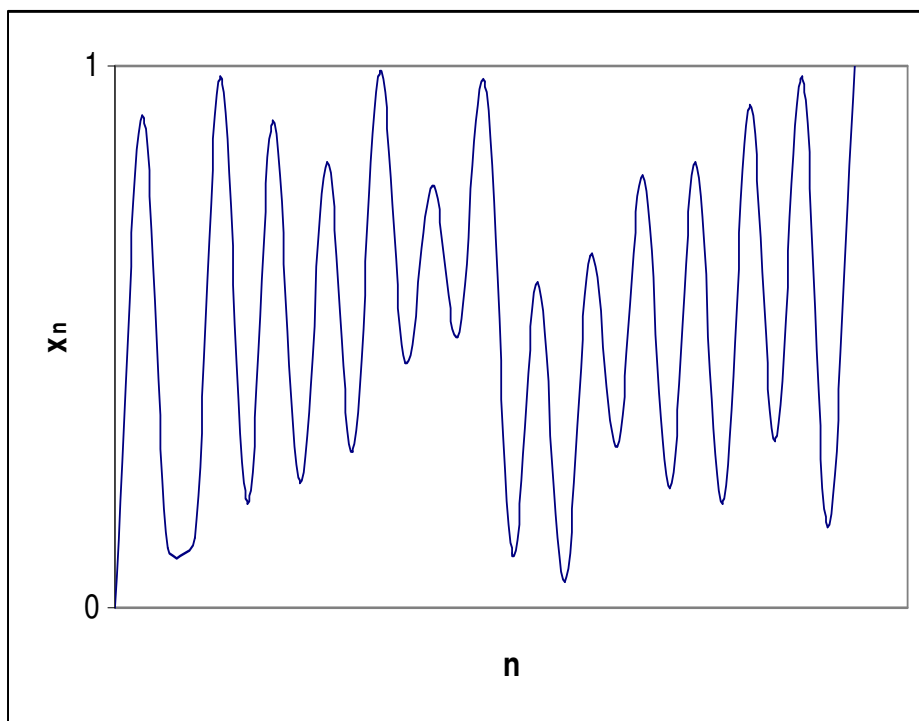


Figure 1.1 An irregular series.

Suppose, first of all, that the $(n+1)^{th}$ term x_{n+1} depends only on the n^{th} term x_n . This may be written as the Ansatz

$$x_{n+1} = f(x_n) \quad (1.1)$$

So as to visualize this relation concretely, let us consider a plane whose Cartesian coordinates are x_n (abscissa) and x_{n+1} (ordinate). That is, the points (x_n, x_{n+1}) ($n=1,2,3,\dots$) are plotted in order. This plot reveals a parabola, which is convex upward, as shown in Figure 1.2.

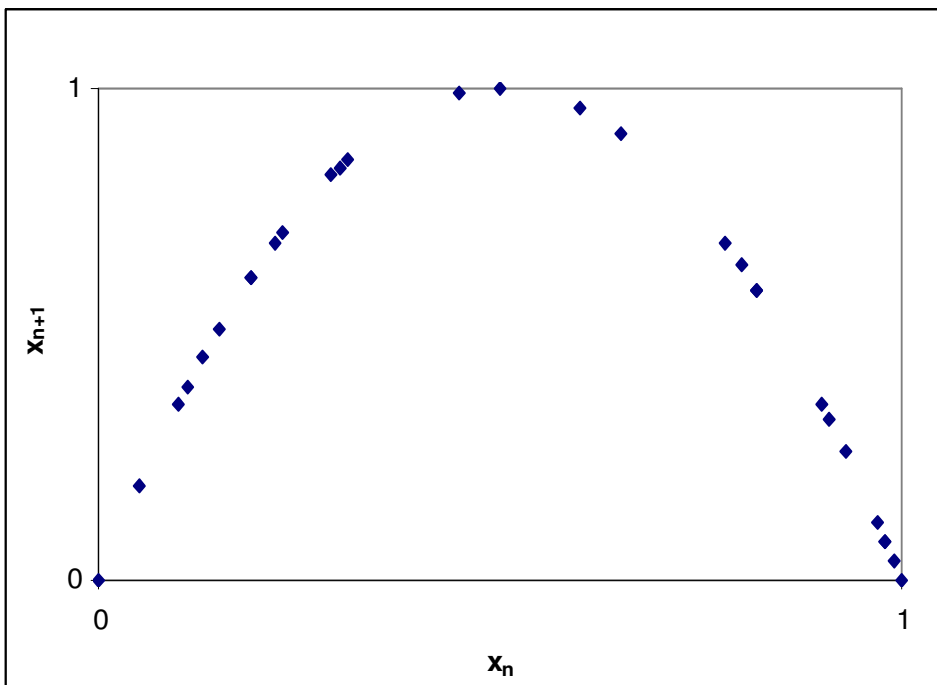


Figure 1.2 The plot of (x_n, x_{n+1}) ($n=1, 2, 3, \dots$) for the series shown in

Figure 1.1.

This plot defines the logistic map. This relation is called a map from x_n to x_{n+1} . The map in our case is

$$x_{n+1} = L(x_n) = 4x_n(1 - x_n) \quad (1.2)$$

In other words, the function $f(x)$ in equation (1.1) is given by $f(x) = 4x(1 - x)$. The relation where the value of x_{n+1} is determined only by x_n is called traditionally a one-dimensional map. The map defined by equation (1.2) is called the *logistic map*. It is surprising that a series generated by such a simple rule looks apparently irregular. The irregularity of this series is better seen if it is plotted to larger n . The series then behaves as if it takes any value in the interval $[0,1]$. It is phenomenological peculiarity of chaos that it behaves irregularly even though it is generated by such a simple rule as equation (1.2) [Nagashima et al, 1999].

Phase space is a very nice way of seeing all the dynamics of a system at once. Very simply it is a plot that has every aspect of the dynamics as an axis. Very often this produces a picture with more than three dimensions, but in many simple cases two or three dimensions are all that are required. For a simple physical system where x represents position, the derivative of x would represent velocity. If the system is a second order differential equation, such as the pendulum, then at any time the state of the pendulum could be completely given by the position and the velocity. Note that position is not sufficient to uniquely

determine the system's state. A pendulum hanging straight down and still is very different from a pendulum that is swinging but at this very instant is hanging straight down as it swings past the resting pendulum.

This setup makes it very easy to see fixed points. This is where the curve crosses the x axis, when velocity is zero. When the curve is below the x axis, (when the velocity is negative), then the particle is moving to the left, (in the negative direction). When the curve is above the x axis the particle moves to the right, (the positive direction). Together these can be put together to analyze the stability of the fixed point. If the particle moves to the fixed point from both sides, then it is stable. If the particle moves away from the fixed point on both sides then it is unstable. Here is a typical phase portrait for the system:

$$\frac{dx}{dt} = x^2 - 1$$

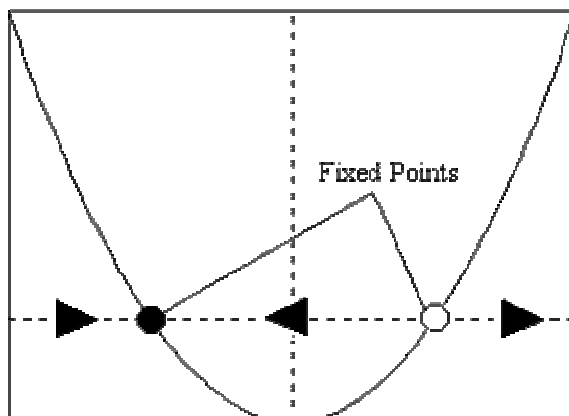


Figure 1.3 Phase portrait of the system.

In this diagram, the arrows on the x axis indicate the direction of the flow. The dots marked fixed points indicate points where the flow is zero. The open dot indicates an unstable fixed point, while the filled dot indicates a stable fixed point [Strogatz, 1994].

A central problem in the study of nonlinear dynamical systems is to understand how the asymptotic behaviour alters as a system parameter changes. Qualitative changes in the system's asymptotic behaviour are called *bifurcations*, whereas the critical parameter values at which the bifurcations occur are the *bifurcation points*. The phenomenon of bifurcation is extremely common in nonlinear systems. For instance, chaos typically arises from a nonchaotic state through a series of bifurcations and the number of bifurcations involved in the creation of chaos can be as few as one or can be as many as infinite.

Understanding various types of the bifurcations has been one of the focuses in the study of nonlinear physical systems. Since almost all qualitative changes in the system's behaviour are due to bifurcations, it is of paramount physical interest to characterize bifurcations in terms of fundamental quantities of the system. It is fundamental to characterize a bifurcation in terms of the periodic orbits embedded in the natural dynamics of the system. Thus the knowledge of periodic orbits is the key to understand the bifurcation and, consequently, the key to understand the dynamics of the system [Nagai, 1997].

By the help of examples in this study it should be clear that the term bifurcation refers to the phenomenon of a system exhibiting qualitatively new dynamical behaviour as parameters are varied. However, the phrase “as parameters are varied” deserves careful consideration.

If such a situation is imagined that wind blowing through blinds hanging in an open window. The “parameter” in this system will be the wind speed. From experience, most people have observed that nothing much happens when the wind speed is low enough, but, for high enough wind speeds, the blinds begin to oscillate or “flutter”. Thus, at some critical parameter value, a Hopf bifurcation occurs. Let us assume the wind speed constant. At low constant speeds, the blinds lie flat; at constant speeds above a certain critical value, the blinds oscillate. But the wind speed increases over time, even though this is what happens in practice. Dynamical systems having parameters that change in time (no matter how slowly) and that pass through bifurcation values often exhibit behaviour that is very different from the analogous situation where the parameters are constant [Wiggins, 2003].

In this study, nonlinear systems depending, for simplicity, on a single bifurcation parameter was firstly considered. For the usual values of the parameter, the system operates at a stable equilibrium, and perturbations away from this mode of operation tend to be attenuated (stability). As the parameter is varied, the equilibrium loses stability at a bifurcation point, giving rise to new equilibria or periodic orbits, perhaps.

If any of the bifurcated solutions is stable, the system may operate at such a solution. For the variations of the parameter, these bifurcated solutions may also lose stability, and so on.

The basics of the bifurcation and one dimensional bifurcation were firstly discussed. While moving up from one dimensional systems to two dimensional systems, it was still found that fixed points can be created and destroyed or destabilized as parameters varied –but now the same is true for closed orbits as well. Thus the ways in which oscillations can be turned on or off were described. If the phase portrait changes its structure as a parameter is varied, it can be said that a *bifurcation* has occurred. Examples include changes in the number or stability of fixed points, closed orbits, or saddle connections as a parameter is varied.

It was concentrated on the computation of equilibrium states (steady states) in various physical system models, and on the computation of bifurcations of equilibria. A bifurcation is a sudden, macroscopic change in the qualitative behaviour of a system as some parameter is varied. These changes include the appearance and disappearance of equilibrium states (fold or saddle-node bifurcation), the exchange of stability of two equilibria (transcritical bifurcation), and the change of stability of an equilibrium point (hopf bifurcation).

Reaction-diffusion equations are important to a wide range of applied areas such as cell processes, drug release, ecology, spread of diseases, industrial catalytic processes, transport of contaminants in the

environment, chemistry in interstellar media, to mention a few. Some of these applications, particularly in chemistry and biology, will be considered. In chemical systems which are not well mixed, it has taken into account the fact that chemicals move through space due to diffusion. The dynamics of reaction-diffusion has been subject of intense research activity over the last decades. The reason is that these systems exhibit very rich dynamic behaviour including periodic solutions and chaos.

The applications of bifurcation with a short account of the laws of diffusion were begun. It was aimed to show the diffusion effect to reaction mechanism by bifurcation. A reaction-diffusion model of a chemical reaction, Gray-Scott model by Pearson is studied. In this study, a bifurcation and stability analysis of the coupled nonlinear system of PDE's were performed [Lin et al, 1999].

Another reaction mechanism to be studied, commonly called the Brusselator, is an example of an autocatalytic, oscillating chemical reaction. An autocatalytic reaction is one in which a species acts to increase the rate of its producing reaction. In many autocatalytic systems complex dynamics are seen, including multiple steady-states and periodic orbits. The dynamics and chemistry of oscillating reactions has only been the subject of study for the last 50 years, starting with the work of Boris Belousov. Belousov was studying the Krebs's cycle when he stumbled upon an oscillating system. He witnessed a mixture of citric acid, bromate, and cerium catalyst in a sulphuric acid solution undergoing periodic colour changes. These changes indicated the cyclic formation

and depletion of differently oxidized cerium species. The scientific community of the time believed that oscillations in a chemical system were disallowed by thermodynamic laws, so Belousov's work remained unpublished for years.

Dynamics of the Brusselator ODEs were studied in this thesis both with diffusion terms [Roussel, 2005] and without taking account the fact that chemicals move through space due to diffusion. Initially, the process model is presented and the bifurcation studies of the Brusselator model showed that the system exhibits very rich dynamical behaviour for different regions in the bifurcation parameter space [Ault et al, 2003].

In the early 19th century, Pierre François Verhulst examined a model that describes how a population of animals (e.g. insects, hares, or something like that) grows from one generation to the next. Graphs of this model were made using different control parameters and initial conditions. By changing parameters, the stability of solutions, bifurcations, and chaos were investigated [<http://www.chaospro.de/bifurcation.php>].

The dynamics of nonlinear prey-predator model given by Lotka (1925) and Volterra (1926) is also investigated. In the 1920s, the Italian mathematician Vito Volterra proposed a differential equation model to describe the population dynamics of two interacting species, a predator and its prey. He hoped to explain the observed increase in predator fish (and corresponding decrease in prey fish) in the Adriatic Sea during

World War I. Such mathematical models have long proven useful in describing how populations vary over time. Data about the various rates of growth, death, and interaction of species naturally lead to models involving differential equations. Independently, in the United States, the very equations studied by Volterra were derived by Alfred Lotka to describe a hypothetical chemical reaction in which chemical concentrations oscillate.

This model consists of a system of ordinary differential equations for the rate of population growth of n interacting species depending on the current population [Chauvet et al, 2002].

For chemical engineering processes, a bifurcation analysis often provides information on the nonlinear dynamics of the process which turns out to be crucial for a safe and optimal process design. Based on the bifurcation analysis a designer may, for example, decide which regions of the parameter space to avoid in order avoiding undesirable behaviour such as loss of stability or occurrence of hysteresis. However, even if a designer can rely on a thorough bifurcation analysis of the process of interest, the process design step often lacks rigor, e.g. because regions of the parameter space to be avoided are largely overestimated in order to over-design safety margins.

More rigorous design approaches based on process optimization have so far not taken requirements on the nonlinear dynamic behaviour of the process into account and therefore often result in process designs

which are optimal but unstable or parametrically unacceptably close to saddle-node, Hopf or another type of bifurcations. For example, the closest distance of a stable equilibrium to the manifold of Hopf- and saddle node bifurcations can obviously be used as a measure of the parametric robustness against loss of stability.

The use of bifurcation analysis for physical, chemical and biological system design is discussed, proposing that bifurcation analysis could be used to assess and understand the structural stability of engineering systems of interest.

A new approach for computing equilibrium states and bifurcations of equilibria in a few physical, chemical and biological models were proposed, the feasibility of using this approach was considered. This technique provides a mathematical and computational guarantee that all equilibrium states and bifurcations of equilibria will be located (or, more precisely, enclosed within a very narrow interval). There are other dynamical features of interest, such as limit cycles (and their bifurcations); however, our attention here will be limited to equilibrium states and their bifurcations. While the focus here is these models, there are clearly applications of this technique in the analysis of other dynamical systems of interest in chemical engineering.

In mathematics particularly in dynamical systems, a bifurcation diagram shows the possible long-term values (equilibria/fixed points or periodic orbits) of a system as a function of a bifurcation parameter in the

system. Bifurcation diagrams are one way of demonstrating the nature of chaos. They show how an iterative function may, for certain values of a constant, converge to a steady state over time, while for other values it may oscillate between a number of different states, and for yet others, vary chaotically without ever settling into a pattern. The bifurcation diagrams were drawn for all our applications in 2-dimensional and also 3-dimensional by the help of Excel, Graphis and Gnuplot. The system behaviour by the help of these graphs is also determined.

2.0 BASICS OF BIFURCATION ANALYSIS

2.1 Nonmathematical Introduction

Every day of our lives we experience changes that occur either gradually or suddenly. We often characterize these changes as quantitative or qualitative, respectively. For example, consider the following simple experiment (Figure 2.1). Imagine a board supported at both ends, with a load on top. If the load λ is small enough, the board will take a bent shape with a deformation depending on the magnitude of λ and on the board's material properties (such as stiffness, K). This state of the board will remain *stable* in the sense that a small variation in the load λ (or in the stiffness K) leads to a state that is only slightly perturbed. Such a variation (described by Hooke's law) would be referred to as a quantitative change. The board is deformed within its elastic regime and will return to its original shape when the perturbation in λ is removed.

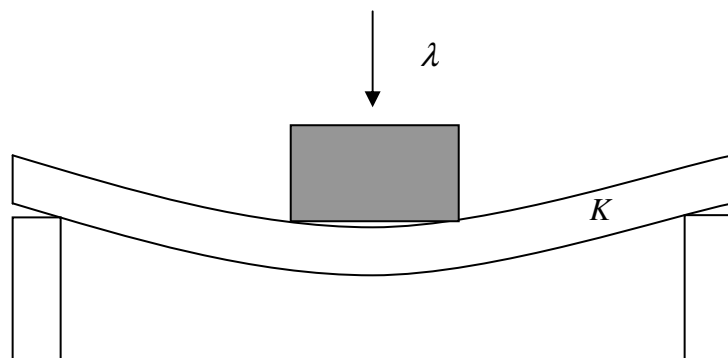


Figure 2.1 Bending of a board.

The situation changes abruptly when the load λ is increased beyond certain *critical level* λ_0 at which the board breaks. This sudden action is an example of a qualitative change; it will also take place when the material properties are changed beyond a certain limit. Suppose the shape of the board is modelled by some function (solution of an equation). Loosely speaking, we may say that there is a solution for load values $\lambda < \lambda_0$ and that this solution ceases to exist for. The load $\lambda > \lambda_0$ and stiffness K are examples of *parameters*.

The outcome of any experiment, any event, and any construction is controlled by parameters. The practical problem is to *control the state* of a system--that is, to find parameters such that the state fulfils our requirements. This role of parameters is occasionally emphasized by terms such as *control parameter*, or *design parameter*. Varying a parameter can result in a transition from a quantitative change to a qualitative change. The following pairs of verbs may serve as illustrations:

bend $\rightarrow$ break
incline $\rightarrow$ tilt over
stretch $\rightarrow$ tear
inflate $\rightarrow$ burst.

The verbs on the left side stand for states that are stable under small *perturbations*; the response of each system is a quantitative one.

This behaviour ends abruptly at certain critical values of underlying parameters. The related drastic and irreversible change is reflected by the verbs on the right side. Close to a critical threshold the system becomes most sensitive; tiny perturbations may trigger drastic changes. To control a system may mean to find parameters such that the state of the system is safe from being close to a critical threshold.

The above-mentioned problems are much too limited to cover phenomena that we will later want to denote with the term *bifurcation*. The extended range of phenomena we have in mind is indicated by the pair

stationary state $\leftrightarrow$ motion.

Let us mention a few examples. The electric membrane potential of nerves is stationary as long as the stimulating current remains below a critical threshold; if this critical value is passed, the membrane potential begins to oscillate, resulting in nerve impulses. The motion of a semi-trailer is straight for moderate speeds (assuming the rig is steered straight); if the speed exceeds a certain critical value, the vehicle tends to sway. Or take the fluttering of a flag, which will occur only if the moving air passes fast enough. Similarly, the vibration of tubes depends on the speed of the internal fluid flow and on the speed of an outer flow. This type of oscillation also occurs when obstacles, such as bridges and other high structures, are exposed to strong winds. Many other examples--too complex to be listed here--occur in combustion, fluid dynamics, and geophysics.

The transition from a stationary state to motion, and vice versa, is also a qualitative change. Here, speaking again in terms of *solutions* –of governing equations –we have a different quality of solution on either “side” of a critical parameter. Let the parameter in question again be denoted by λ , with critical value λ_0 . Thinking, for instance, in terms of wind speed, the state (e.g., of a flag or bridge) is stationary for $\lambda < \lambda_0$ and oscillatory for $\lambda > \lambda_0$. Qualitative changes may come in several steps, as indicated by the sequence

stationary state
regular motion
irregular motion.

The transition from regular to irregular motion is related to the onset of turbulence, or “chaos”. As a first tentative definition, we will denote a qualitative change caused by the variation of some physical (or chemical or biological, etc.) parameter λ as *branching* or *bifurcation*. We will use the same symbol λ for various kinds of parameters. Some examples of parameters are listed in the Table 2.1.

Table 2.1 Examples of parameters.

Phenomenon	Controlled by a typical parameter
Bending of road	Load
Vibration of an engine	Frequency or imbalance
Combustion	Temperature
Nerve impulse	Generating potential
Superheating	Strength of external magnetic field
Oscillation of an airfoil	Speed of plane relative to air
Climatic changes	Solar radiation

Some important features that may change at bifurcations have already been mentioned. The following list summarizes various kinds of qualitative changes:

stable $\leftrightarrow$ unstable

symmetric $\leftrightarrow$ asymmetric

stationary $\leftrightarrow$ periodic (regular) motion

regular $\leftrightarrow$ irregular

order $\leftrightarrow$ chaos.

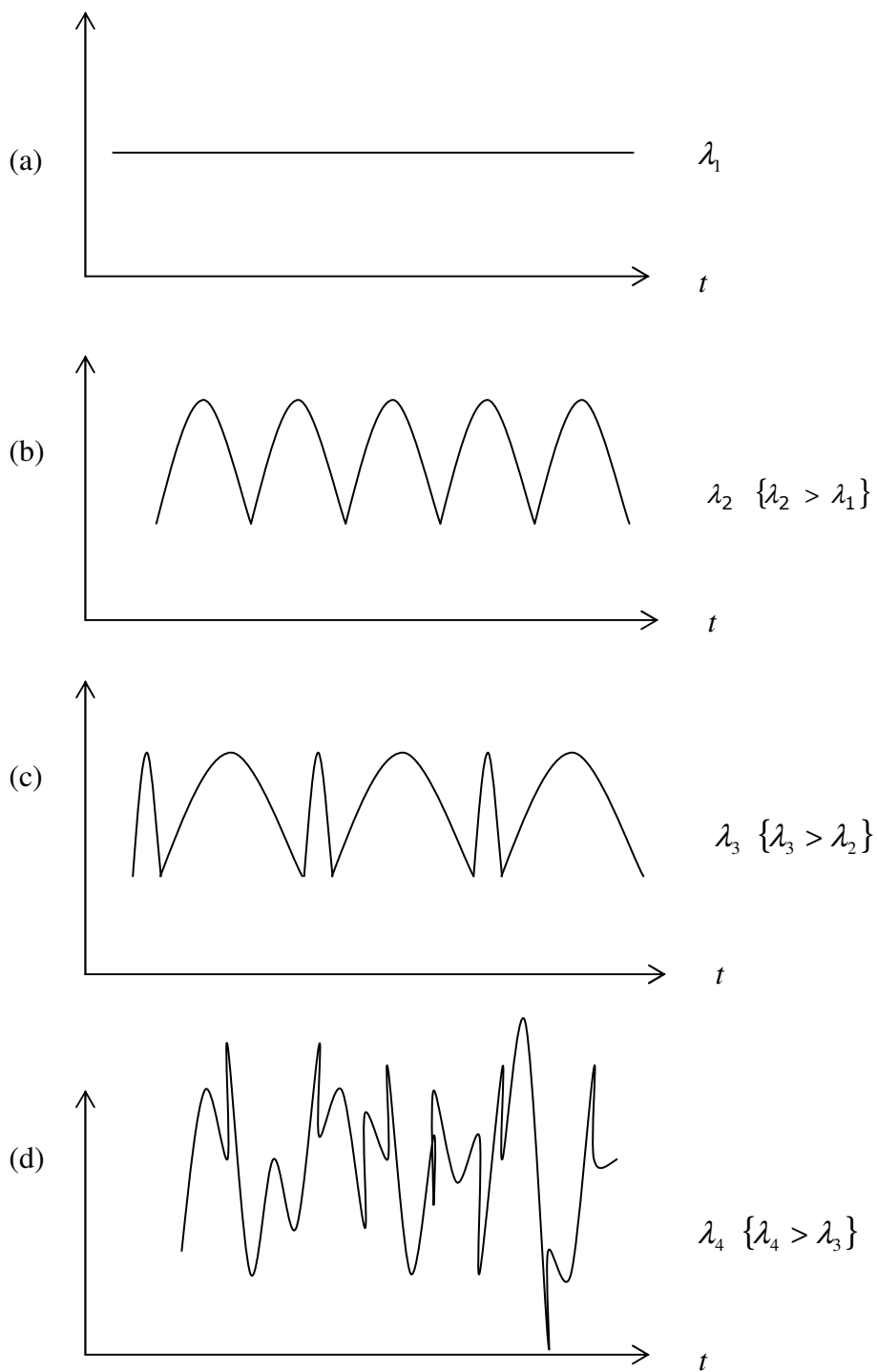


Figure 2.2 Velocity of a combustion front.

Several of these changes may take place simultaneously in complicated ways.

The quality of solutions or states is also distinguished by their geometrical shape –that is, by their *pattern*. For example, the four patterns in Figure 2.2 characterize four possibilities of how the velocity of a specific combustion front varies with time [Seydel, 1994].

The manner of combustion front propagation is strongly dependent on the process of heat dispersion (by heat transfer and heat loss) and heat generation (by chemical reaction). Any change in the processing conditions may give rise to a variation in the velocity and temperature of the combustion propagation front and further influence the instability of the combustion front. It has been shown that when the exothermic heat is reduced or the thermal conductivity is significantly enhanced, it may convert the propagation mode from stable to unstable combustion. A further decrease in the combustion temperature, the unstable combustion front may stop propagating. It has also been reported that if the difference of thermal activity (C_p)(heat capacity) between the reactants and product is increased, stable combustion also changes to the unstable mode. In unstable combustion, the combustion temperature and propagation velocity are not uniform with time, and the combustion front propagates in an oscillatory or spin manner. These temperature alterations along the specimen influence the homogeneity of microstructures. In turn, the microstructure distribution affects other physical properties of the synthesized products. For structural applications it is often important to obtain reliable products with

homogeneous structures and properties. Therefore it is necessary to investigate the temperature and propagation velocity variation during unstable combustion and explore the processing conditions when unstable combustion may occur [Li, 2002].

The solution profile of Figure 2.2a is “flat” or stationary; this pattern stands for a uniformly propagating reaction front. Figure 2.2b shows a wavy pattern, representing a regularly pulsating velocity of the combustion front. The pattern of Figure 2.2c is again wavy but less regular, and the pattern of Figure 2.2d appears to be irregular (chaotic). The four different patterns of Figure 2.2 arise for different values of a parameter λ ; new patterns form when the parameter passes critical values. This example illustrates why such bifurcation phenomena are also called *pattern formation* [Seydel, 1994].

2.2 Stationary Points and Stability (ODEs)

2.2.1 Trajectories and equilibria

Many kinds of qualitative changes can be described by systems of ordinary differential equations (ODEs). Suppose the state of the system is described by functions $y_1(t)$ and $y_2(t)$. These state variables may represent, for example, the position and velocity of a particle, concentrations of two substances, or electric potentials. The independent variable t is often “time”. Let the physical (or chemical, etc.) law that

governs $y_1(t)$ and $y_2(t)$ be represented by two ordinary differential equations

$$\begin{aligned}y_1' &= f_1(y_1, y_2), \\y_2' &= f_2(y_1, y_2)\end{aligned}\tag{2.1}$$

In vector notation equation (2.1) can be written as $\mathbf{y}' = \mathbf{f}(\mathbf{y})$. This system is called *autonomous*, because the functions f_1 and f_2 do not depend explicitly on the independent variable t . As illustrated in Figure 2.4, solutions $y_1(t), y_2(t)$ of this two dimensional system form a set of trajectories (flow lines, orbits) densely covering part or all of the y_1, y_2 plane. A figure like Figure 2.4 depicting selected trajectories is called a *phase diagram*; the (y_1, y_2) plane is the phase plane. A specific trajectory is selected by requesting that it pass through a prescribed point (z_1, z_2) of *initial values*

$$y_1(t_0) = z_1, \quad y_2(t_0) = z_2.$$

Because the system is autonomous, we can take $t_0 = 0$. Imagine a tiny particle floating over the (y_1, y_2) plane, the tangent of its path being given by the differential equations. After time t_1 has elapsed, the particle will be at the point

$$((y_1(t_1), y_2(t_1)))$$

The set of all trajectories that start from some part of the y plane is called the *flow* from that part.

Of special interest are equilibrium points (y_1^*, y_2^*) , which are defined by

$$y_1' = 0, \quad y_2' = 0.$$

In equilibrium points, the system is at rest; equilibrium solutions are constant solutions these points (y_1^*, y_2^*) are also called stationary solutions, and seldom singular points, critical points, rest points, or fixed points. Stationary points are solutions of the system of equations given by the *right-hand side* $\mathbf{f}$ of the differential equation,

$$\begin{aligned} f_1(y^*, y^*) &= 0 \\ f_2(y^*, y^*) &= 0. \end{aligned}$$

In vector notation, this system of equations is written as $\mathbf{f}(\mathbf{y}^*) = \mathbf{0}$, which defines stationary solutions $\mathbf{y}^*$. For a practical evaluation of stationary points in two dimensions, we observe that each of these two equations defines a curve named null cline. Hence, stationary solutions are intersections of null clines. This suggests starting with drawing the null clines in phase plane. In this way, not only the equilibria are obtained, but also some information on the global behaviour of the trajectories intersect the null cline defined by $f_1(y_1, y_2) = 0$ vertically and intersect the null cline of $f_2(y_1, y_2) = 0$ horizontally.

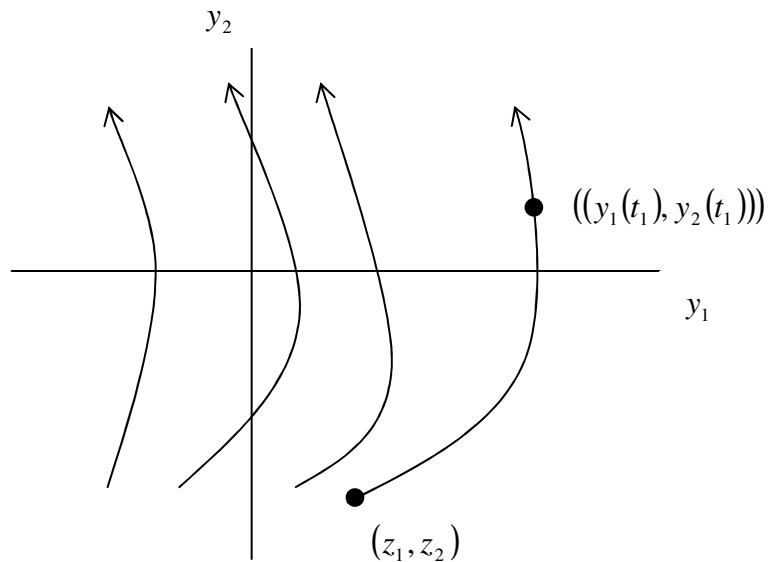


Figure 2.3 Trajectories in a phase plane.

2.2.2 Deviations

Every differential equation and every solution thereof is affected by certain “deviations”. Deviations can influence a final “solution” in several ways. First, there may be *fluctuations* of the model. Physical laws [represented by the right-hand side $\mathbf{f}$ in equation (2.1)] are formulated in terms of a few macro variables, such as number of micro-organisms, concentration, pressure, or temperature. Macroscopic variables simplify and average the physics of countless microscopic particles. The individual behaviour of these particles is subject to molecular interaction and infinitesimal random perturbations (noise), causing variations in the

function $\mathbf{f}$ that represents the average dynamics. More significant are the deviations caused by inadequacies in the measurements upon which $\mathbf{f}$ is based. The assumptions and the model that has led to $\mathbf{f}$ may be inadequate. That is, coefficients involved in $\mathbf{f}$ must be regarded as being subject to ever-present deviations. The class of deviations acting on $\mathbf{f}$ may be called “interior” perturbations.

A second type of deviation occurs when $\mathbf{y}$ is affected by an “external” force, which is not represented by the differential equation. As an example, think about touching an oscillating pendulum, thereby causing momentarily a sudden change in the dynamic behaviour. Mathematically speaking, such “outer” perturbations can be described as a jump in the trajectory at some instant t_1 ,

$$(y_1(t_1), y_2(t_1)) \rightarrow (z_1, z_2).$$

When the perturbation ends at $t_2 > t_1$, the system (e.g., pendulum, chemical reaction) is again governed by the differential equation (2.1) starting from the initial values

$$y_1(t_2) = z_1, \quad y_2(t_2) = z_2$$

and travelling along a neighbouring trajectory.

Further deviations occur when the differential equation is integrated numerically. Discretization errors of a numerical

approximation scheme and rounding errors are encountered. These inevitable errors can be seen as a kind of noise affecting the calculated trajectory or interpreted as a great number of small perturbations of the kind illustrated in Figure 2.4.

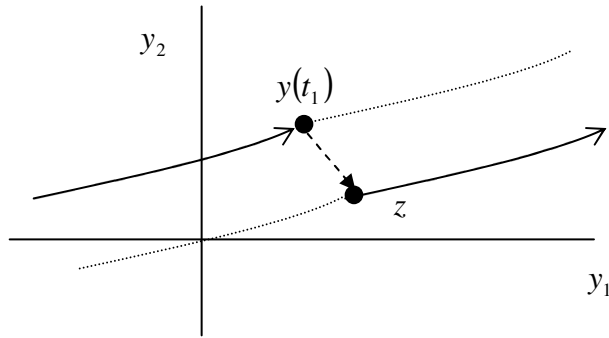


Figure 2.4 Perturbation of a trajectory.

Now assume that our travelling particle $\mathbf{y}$, its itinerary given by differential equation (2.1), is in a stationary state, $(z_1, z_2) = (y_1^*, y_2^*)$. Theoretically, the particle would remain there forever, but in practice there is rarely such a thing as “exactness”. Due to perturbations, either the position (z_1, z_2) of the particle or the location of the equilibrium (y_1^*, y_2^*) varies slightly. This results in a deviation a , say, time $t_0 = 0$,

$$(z_1, z_2) \neq (y_1^*, y_2^*).$$

For simplicity, we assume that for $t > 0$ no further perturbations or fluctuations arise. Then it is the differential equation that decides

whether trajectories starting from $\mathbf{z}$ remain near the equilibrium or depart from it the question is how solutions $\mathbf{y}(t)$ of the initial-value problem (in vector notation)

$$\mathbf{y}' = \mathbf{f}(\mathbf{y}), \quad \mathbf{y}(0) = \mathbf{z}$$

behave for $t > 0$.

2.2.3 Stability

Definition 2.1: A stationary solution $\mathbf{y}^*$ is said to be **asymptotically stable** if the response to a small perturbation approaches zero as the time approaches infinity. An asymptotically stable equilibrium is also called **sink**.

More formally, this means that

$$\mathbf{y}(t) \xrightarrow{t \rightarrow \infty} \mathbf{y}^*$$

for $\mathbf{y}(t)$ starting from initial values that are sufficiently close to equilibrium. Asymptotically stable equilibria are examples of *attractors*. The set of all initial values $\mathbf{z}$ from which trajectories converge to the attractor is called *domain of attraction*.

Definition 2.2: The stationary solution $\mathbf{y}^*$ is said to be **stable** if the response to a small perturbation remains small as the time approaches infinity. Otherwise the stationary solution is called **unstable** (the deviation grows). An unstable equilibrium is also called **source** and is an example for repeller.

As we see, asymptotic stability implies stability. The above classical definitions apply to general systems of ODEs, including the simplest “system” of one scalar differential equation. Let us illustrate stability with some scalar examples; the simplest is as follows:

$$y' = \lambda y;$$

solution: $y(t) = \exp(\lambda t)$

equilibrium: $y^*(t) \equiv 0$

y^* is stable for $\lambda \leq 0$, asymptotically stable for $\lambda < 0$, and unstable for $\lambda > 0$.

Since the distinction between stability and asymptotic stability is mostly artificial, we shall often use the term “stable” in the sense “asymptotically stable”.

2.2.4 Linear stability

A Taylor series expansion of f_1 about (y_1^*, y_2^*) gives

$$y_1' = f_1(y_1, y_2) = f_1(y_1^*, y_2^*) + \frac{\partial f_1}{\partial y_1}(y_1^*, y_2^*)(y_1 - y_1^*) + \frac{\partial f_1}{\partial y_2}(y_1^*, y_2^*)(y_2 - y_2^*)$$

+ terms of higher order

The terms of higher order are at least of order 2; they are denoted $O(|\mathbf{y} - \mathbf{y}^*|^2)$. Expanding also the f_2 of the second differential equation, observing that $f_1(y_1^*, y_2^*) = f_2(y_1^*, y_2^*) = 0$, and dropping the high-order terms give two differential equations that are linear in $y_1 - y_1^*$ and $y_2 - y_2^*$. This system of equations is easily written down using the notation of the *Jacobian Matrix* $\mathbf{f}_y$ of the first-order partial derivatives. Evaluated at the equilibrium, the Jacobean is

$$\frac{\partial \mathbf{f}}{\partial \mathbf{y}}(\mathbf{y}^*) = \begin{pmatrix} \frac{\partial f_1}{\partial y_1}(y_1^*, y_2^*) & \frac{\partial f_1}{\partial y_2}(y_1^*, y_2^*) \\ \frac{\partial f_2}{\partial y_1}(y_1^*, y_2^*) & \frac{\partial f_2}{\partial y_2}(y_1^*, y_2^*) \end{pmatrix}.$$

This matrix, evaluated at the stationary solution $\mathbf{y}^*$, will be denoted $\mathbf{f}_y^*$. Now the linearised system in vector notation reads

$$\mathbf{h}' = \mathbf{f}_y^* \mathbf{h} \quad (2.2)$$

The vector $\mathbf{h}$ represents first-order approximations

$$h_1(t) \approx y_1(t) - y_1^*$$

$$h_2(t) \approx y_2(t) - y_2^*$$

of small distances between the points $\mathbf{y}(t)$ on the trajectories and the stationary point $\mathbf{y}^*$. The smaller distance $\mathbf{y} - \mathbf{y}^*$, the better the approximation $\mathbf{h}$. That is, under certain assumptions $\mathbf{h}(t)$ describes the

local behaviour of the solution. The approximation $\mathbf{h}(t)$ indicates how the process evolves when the initial state deviates slightly from its equilibrium values. Thus, the question of local stability is reduced to a discussion of the linear system equation (2.2). The standard procedure is to insert the ansatz (hypothesis) $\mathbf{h}(t) = e^{\mu t} \mathbf{w}$,

$$\begin{aligned} h_1(t) &= e^{\mu t} w_1 \\ h_2(t) &= e^{\mu t} w_2 \end{aligned} \tag{2.3}$$

into equation (2.2). A straightforward calculation shows that the *eigenvalue problem*

$$(\mathbf{f}_y^* - \mu \mathbf{I}) \mathbf{w} = 0 \tag{2.4}$$

results, with eigenvalue μ , constant eigenvector $\mathbf{w}$, and identity matrix

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

First, the eigenvalues μ_1 and μ_2 are calculated. The existence of a nontrivial solution $\mathbf{w} \neq 0$ of equation (2.4) requires μ_1 and μ_2 to be the roots of the *characteristic equation*

$$\det(\mathbf{f}_y^* - \mu \mathbf{I}) = 0$$

In the two-dimensional situation, this is a quadratic equation; its roots μ_1 and μ_2 are easily obtained. Then eigenvectors $\mathbf{w}$ can be calculated as solutions of the specific system of linear equations that results from intersecting μ_1 and μ_2 into equation (2.4).

2.2.4.1 Duffing Equation (without external forcing)

Consider the second-order differential equation

$$u'' + u' - u + u^3 = 0, \quad (2.5)$$

which is a special case of Duffing equation

$$u'' + au' + bu + cu^3 = d \cos \omega t.$$

Duffing equations are used to describe oscillations in series-resonance circuit, where a nonlinear inductor or capacitor is modelled by a cubic polynomial. For our purpose of illustrating some calculus, we choose in equation (2.5) simple coefficients and omit the excitation ($d = 0$).

We need to convert this equation into a first-order system. We introduce a vector $\mathbf{y}$ via $y_1 = u$, $y_2 = u'$. Then the equation (2.5) is written as a first-order system of ODEs,

$$\begin{aligned}y_1' &= y_2 =: f_1(y_1, y_2), \\y_2' &= y_1 - y_1^3 - y_2 =: f_2(y_1, y_2).\end{aligned}$$

The phase plane associated with the scalar second-order equation (2.5) displays u and u' . Calculating stationary points, one finds that $y_2^* = 0$ and that y_1^* is a solution of

$$0 = y_1(1 - y_1^2).$$

This equation has three distinct roots, and above system thus has three distinct stationary points (y_1^*, y_2^*) ,

$$(0,0), \qquad (1,0), \qquad (-1,0).$$

The Jacobean matrix of the first-order partial derivatives is

$$\mathbf{f}_y = \begin{pmatrix} 0 & 1 \\ 1 - 3y_1^2 & -1 \end{pmatrix}.$$

The three equilibrium points (y_1^*, y_2^*) produce three eigenvalue problems; see equation (2.4). In this particular example, the analysis is simple because the Jacobean $\mathbf{f}_y$ and therefore equation (2.4) are identical for the two equilibria $(\pm 1, 0)$. Pursuing the analysis in more detail, we obtain the following results:

$$(y_1^*, y_2^*) = (0, 0):$$

$$\mathbf{f}_y^* = \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix},$$

$$\text{characteristic equation:} \quad 0 = \mu^2 + \mu - 1,$$

$$\text{roots:} \quad \mu_{1,2} = \frac{1}{2}(-1 \pm \sqrt{5}).$$

Two distinct roots imply the existence of two eigenvectors, which are obtained by equation (2.4),

$$\begin{pmatrix} -\mu & 1 \\ 1 & -1 - \mu \end{pmatrix} \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The first component of this system of linear equations is

$$-\mu\omega_1 + \omega_2 = 0,$$

which suggest choosing $\omega_1 = 1$. This implies that $\omega_2 = \mu$ and generates two eigenvectors:

$$\mathbf{w} = \begin{pmatrix} 1 \\ \mu \end{pmatrix}, \quad \mu = \mu_1, \mu_2.$$

$$(y_1^*, y_2^*) = (\pm 1, 0):$$

$$\mathbf{f}_y^* = \begin{pmatrix} 0 & 1 \\ -2 & -1 \end{pmatrix},$$

characteristic equation: $0 = \mu^2 + \mu + 2,$

roots: $\mu_{1,2} = \frac{1}{2}(-1 \pm \sqrt{-7}).$ (Complex conjugates).

We omit calculation of the complex eigenvectors because we do not need them. In the meantime, we will discuss important types of qualitative behaviour of trajectories close to equilibrium. What follows is based on the ansatz $\mathbf{h}(t) = e^{\mu t} \mathbf{w}$ in equation (2.3) with the associated eigenvalue problem equation (2.4).

2.2.4.2 Nodes

μ_1, μ_2 **real**, $\mu_1 \cdot \mu_2 > 0$, $\mu_1 \neq \mu_2$.

In this case, where both eigenvalues are real and have the same sign, the stationary point $\mathbf{y}^*$ is called a *node*. This case splits into two subcases:

a) $\mu < 0$ implies $\lim_{t \rightarrow 0} e^{\mu t} = 0$.

Therefore, $\mathbf{h}(t)$ tends to zero and $\mathbf{y}(t)$ converges to $\mathbf{y}^*$ in a sufficiently small neighbourhood of the node. This type of node is called a *stable node*. Small perturbations die out at stable nodes.

b) $\mu > 0$ implies $\lim_{t \rightarrow 0} e^{\mu t} = \infty$.

As a consequence, $\mathbf{h}(t)$ explodes which means locally that the trajectories $\mathbf{y}(t)$ leave the neighbourhood of the node. This type of node is an *unstable node*.

2.2.4.3 Saddles

μ_1, μ_2 **real**, $\mu_1 \cdot \mu_2 < 0$.

When the real eigenvalues have different signs, the stationary point is called a *saddle point*. Because one of the eigenvalues is positive, two of the four trajectories associated with the eigenspaces leave the equilibrium. A saddle point, therefore, is always unstable.

2.2.4.4 Foci

μ_1, μ_2 **complex conjugates with nonzero real part**.

Set $\mu_1 = \alpha + i\beta$, $\mu_2 = \alpha - i\beta$

(i : imaginary unit), where α and $\pm\beta$ denote the real and imaginary parts, respectively. Going back to ansatz equation (2.3), the time-dependent part of $\mathbf{h}(t)$ is

$$e^{(\alpha+i\beta)t} = e^{\alpha t} e^{i\beta t}.$$

The factor $e^{i\beta t} = \cos \beta t + i \sin \beta t$ represents a rotation counter clockwise through β radians if $\beta > 0$, and clockwise through $-\beta$ radians if $\beta < 0$.

The factor $\exp(\alpha t)$ is a radius which is increasing if $\alpha > 0$ and decreasing if $\alpha < 0$. Any trajectory close to the equilibrium thus resembles a *spiral*. The corresponding equilibrium is called an *unstable focus* $\alpha > 0$ or a *stable focus* $\alpha < 0$.

2.2.5 Degenerate cases; parameter dependence

As seen above, the eigenvalues of the Jacobean matrix evaluate at an equilibrium point determine the dynamic behaviour in the neighbourhood of the equilibrium. This holds for all three types of equilibrium point (nodal points, saddle points, and focal points). These type of points are generic in that assumptions ($\mu_1 \neq \mu_2$, $\mu_1 \cdot \mu_2 \neq 0$ or $\alpha = \text{Re}(\mu) \neq 0$ almost always apply. For an analysis of the exceptional cases

$$\begin{array}{ll} \mu_1 = \mu_2 & \text{(a special node),} \\ \mu_1 \cdot \mu_2 = 0 & \text{(require nonlinear terms),} \\ \mu_{1,2} = \pm \beta i & \text{(a center of concentric cycles).} \end{array}$$

Definition 2.3: The equilibrium is called *hyperbolic* or *nondegenerate* when the Jacobean $\mathbf{f}_y$ has no eigenvalue with zero real part.

The exceptional cases $\mu_1 \cdot \mu_2 = 0$ and $\mu_{1,2} = \pm \beta i$ are called *nonhyperbolic* or *degenerate*.

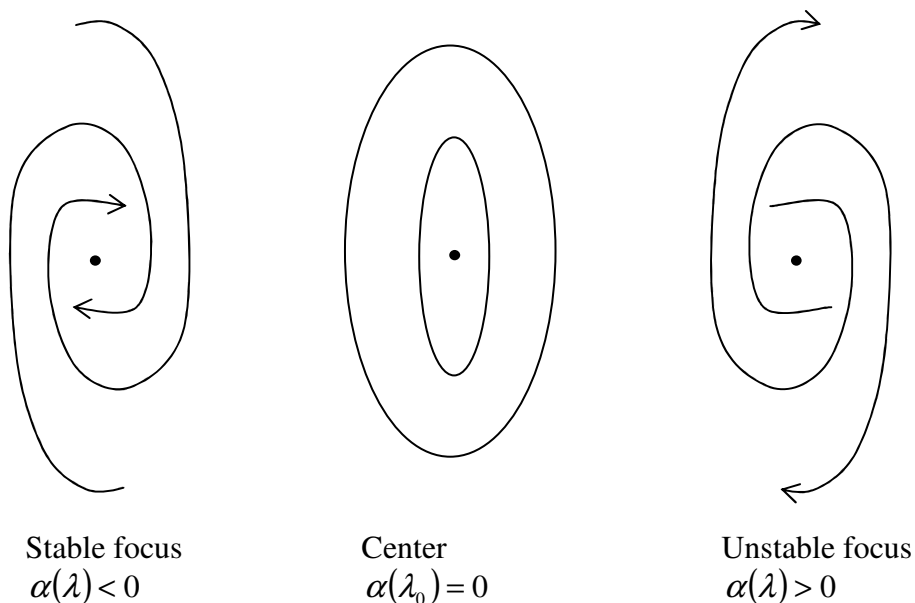


Figure 2.5 A focus changes its stability for λ passing λ_0 .

In any given case, it is unlikely that there will be a degenerate equilibrium point. Therefore, one might forget about the exceptional degenerate cases, but that would oversimplify matters. Usually a differential equation describing a real-life problem involves one or more

parameters. Denoting one such parameter by λ , the differential equation reads

$$\begin{aligned}y_1' &= f_1(y_1, y_2, \lambda), \\ y_2' &= f_2(y_1, y_2, \lambda).\end{aligned}$$

Because the systems $\mathbf{y}' = \mathbf{f}(\mathbf{y}, \lambda)$ depend on λ , we speak of a family of differential equations. Solutions now depend on both the independent variable t and the parameter λ ,

$$\mathbf{y}(t, \lambda).$$

Consequently, stationary points, Jacobean matrices, and the eigenvalues μ depend on λ ,

$$\mu(\lambda) = \alpha(\lambda) + i\beta(\lambda).$$

Upon varying the parameter λ , the position and the qualitative features of stationary point can vary problems [Seydel, 1994].

2.3 Limit Cycles

We again consider the system of ODEs, equation (2.1), $\mathbf{y}' = \mathbf{f}(\mathbf{y})$. As emphasized before, stability and instability results are of local nature. Even if one is able to find all the equilibria of a particular problem, it is

not likely that putting all the local pieces together will give a complete global picture. There are other attractors that are not easy to obtain as equilibria. One such attractor is the *limit cycle*. Limit cycles represent regular motions. Examples are nerve impulses, currents in electric circuits, vibrations of violin strings, the flutter of panels, and laser light.

One method of studying global behaviour of trajectories is a *numerical simulation*. Such a simulation may proceed as follows. Starting from various initial points $\mathbf{z}$, a numerical integration method is applied to calculate trajectories for finite time intervals $0 \leq t \leq t_f$.

2.3.1 Simulation Algorithm

- Choose $\mathbf{z}$ and t_f .
- Integrate equation (2.1), starting from $\mathbf{y}(0) = \mathbf{z}$ and terminating at $t = t_f$.

The choice of $\mathbf{z}$ and t_f strongly affects the amount of information provided by the numerical simulation. It makes sense to analyze possible stationary points first.

2.3.2 Van der Pol equation

Many electrical and biological oscillations can be modelled by the van der Pol equation (2.6). This equation is a differential equation of second order where the nonlinearity results from damping,

$$u'' - \lambda(1 - u^2)u' + u = 0 \quad (2.6)$$

The van der Pol equation (2.6) can be transformed into a system by means of, for instance, $y_1 = u$, $y_2 = u'$, leading to

$$\begin{aligned} y_1' &= y_2, \\ y_2' &= \lambda(1 - y_1^2)y_2 - y_1. \end{aligned}$$

This system has one stationary solution at $(y_1^*, y_2^*) = (0, 0)$. For $0 < \lambda < 2$, this point is unstable focus. To discuss the dynamics of the system for small positive values of λ , one tests by means of simulation where trajectories tend as $t \rightarrow \infty$. The unstable focus at $(0, 0)$ of the van der Pol equation suggests starting simulations near $(0, 0)$. The trajectory for the data

$$z_1 = 0.1, z_2 = 0, \lambda = 0.5, t_f = 75$$

is plotted in Figure 2.6. As seen in figure, the trajectory approaches a closed curve and remains there. The spiral in the core part of figure represents the transient phase; the final steady state is the closed curve.

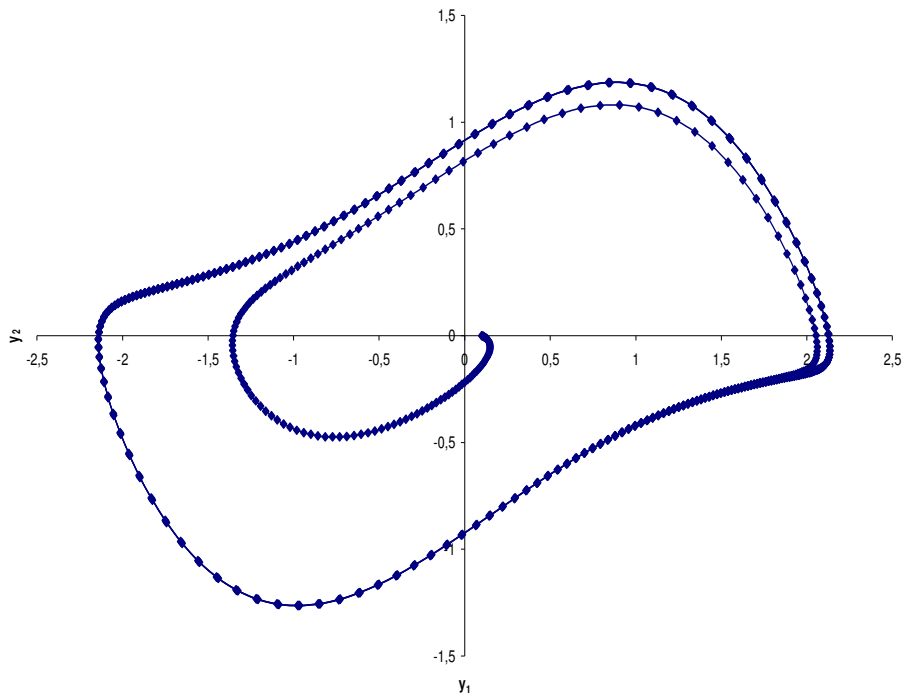


Figure 2.6 Van der Pol equation, (y_1, y_2) phase plane.

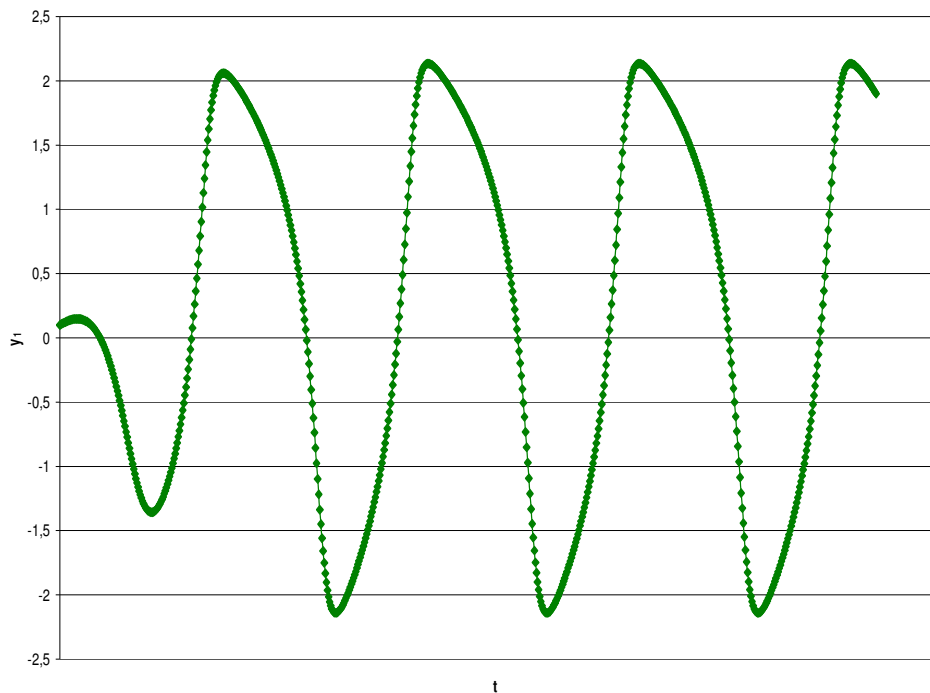


Figure 2.7 The graph of $y_1(t)$.

Such a closed curve toward which the trajectory winds is termed a *limit cycle*. A limit cycle is a *periodic solution* (periodic orbit). That is, after some time period T is elapsed, the values of the solution $\mathbf{y}$ are the same,

$$\mathbf{y}(t+T)=\mathbf{y}(t).$$

The minimum $T > 0$ satisfying this equation is called the *period*. Trajectories starting outside the limit cycle also wind toward it. Limit cycles that are approached by nearby trajectories are called stable; orbits are unstable when trajectories leave their neighbourhoods. We have for

the van der Pol equation a stable limit cycle. Generating this particular limit cycle by means of a simulation is fairly easy, but in general, simulation is not necessarily the best way to create limit cycles.

So far we have discussed two types of attractors –namely, stable equilibria and limit cycles. These are specific trajectories, represented in phase space by points and closed curves. As a consequence of the existence and uniqueness theorems of ODEs there are exactly three kinds of trajectories, namely,

- 1) Stationary solutions: $y(t) \equiv y^*$, $f(y^*) = 0$;
- 2) Periodic solutions: $y(t+T) = y(t)$; and
- 3) One-to one solutions: $y(t_1) \neq y(t_2)$ for $t_1 \neq t_2$.

The last re also called “injective solutions”. Type (3) means that trajectories never intersect, apart from the specific trajectories equilibria and periodic orbits. Injective trajectories are represented in phase space by curves that do not intersect. Since for $n > 2$ graphical illustrations of phase portraits are difficult, one must resort to *projections* of the curves onto two dimensional subspaces, mostly to the (y_1, y_2) plane. The projections of the curves may intersect although the trajectories in n -dimensional space ($n > 2$) do not problems [Seydel, 1994].

2.4 Waves

In addition to stable stationary trajectories and limit cycles, there are limit sets that consists of trajectories connecting equilibria. When distinct saddles are connected, one encounters a *heteroclinic orbit* (illustrated by the phase diagram of Figure 2.8a); a heteroclinic orbit may also join a saddle to a node, or vice versa. A *homoclinic orbit* connects a saddle point to itself. (see Figure 2.8b) For example, the specific Duffing equation $\omega'' - \omega + \omega^3 = 0$ has a homoclinic solution $\omega = \sqrt{2} / \cosh(t)$. Heteroclinic orbits and homoclinic orbits have an infinite “period”, because the motion gets arbitrarily slow ($y' \rightarrow 0$) for trajectories approaching the equilibrium. Several heteroclinic orbits may form a closed path, called a *homoclinic cycle* (see figure 2.8d). In a non-planar two-dimensional case (say, on a torus or on a cylinder in the case of a pendulum), and for $n > 2$, even further limit sets are possible. For example, Figure 2.8c shows a homoclinic orbit of a saddle-focus equilibrium in three-dimensional space; this orbit is also called *Silnikov connection*.

Heteroclinic and homoclinic orbits are of great interest in applications because they form the profiles of travelling wave solutions of many reactor diffusion problems [Seydel, 1994].

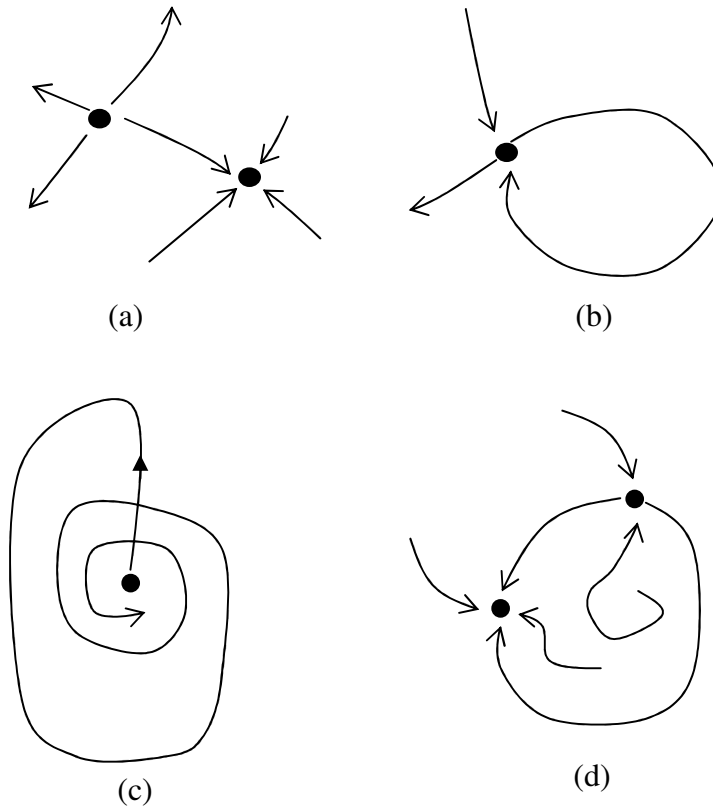


Figure 2.8 Heteroclinic and homoclinic orbits.

2.5 Maps

In many applications, the state $\mathbf{y}$ of a system is determined not for “all” values of t , but for discrete time instances $t_1, t_2, t_3, \dots$. Accordingly the sequence of n -vectors $\mathbf{y}$ forms a discrete *time series*

$$\mathbf{y}(t_1), \mathbf{y}(t_2), \mathbf{y}(t_3), \dots$$

To give an example (scalar case, $n = 1$) we list the number of the human population in the years 1965, 1975, 1985, ... (in millions)

3289, 4070, 4842, ...

Often a law or a differential equation on which the time series is based is unknown. Finding a model equation that matches a time series can be a formidable task. Here a simple model related to the growth of populations is given.

Let's examine the model of Verhulst, an example of a bifurcation diagram. It describes how a population of animals (e.g. insects, hares, or something like that) grows from one generation to the next. This model is one of the simplest ones, and additionally it is very interesting and important (for science) so that very much has been written about it in almost every kind of magazines [<http://www.chaospro.de/bifurcation.php>].

The model looks just like follows:

$$x_{n+1} = ax_n(1 - x_n)$$

with $0 \leq x_n \leq 1$ and $0 \leq a \leq 4$

The biological meaning of x_n is the relative amount of animals in the n^{th} generation, where "1" specifies the maximal amount of animals possible and "0" no animals at all. The index n specifies the time which

goes by in small steps. The parameter ‘ a ’ is a measure for the population growth. If $a < 1$, then the population will die out.

Now how can we work with this model? Let us start with an example:

Let us set $x = 0.1$, $a = 1.5$, $n = 0$, and then let’s apply the model to these values iteratively:

Table 2.2 The change of population values as n increases.

n	population (x_n)
0	0.1
1	$ax_0(1 - x_0) = 1.5 * 0.1 * (1 - 0.1) = 0.1350$
2	$ax_1(1 - x_1) = 1.5 * 0.1350 * (1 - 0.1350) = 0.1752$
3	0.2167
4	0.2546
5	0.2847
6	0.3055
7	0.3182
8	0.3254
9	0.3292
10	0.3313
...	...
50	0.3333

In this example x_n goes to $1/3$ for larger n .

If we repeat this example with $a = 2.5$, then again x_n goes to $1/3$ for large n . But if we examine $x_0, x_1, x_2, \dots, x_n$ using $a = 3.2$, then we will see that the sequence of x_n does not converge to $1/3$ as before, but rather jumps between two values. A more close examination of x_n shows us, that there can happen much more strange things, if we increase ' a ' by small steps. It can happen that $(x_n)_{n \leq 0}$ jumps between m points. These m points are called m -cyclis. Or to say it in other words: We have an attractor consisting of m points. This attractor can even be a much more complicated construct, it need not consist of m discrete points, it can also consist of infinitely many points, a real strange attractor. In such a case we really can say that x_n is attracted by the chaos.

In the model of Verhulst there exists an attractor for every value of ' a ' between 0 and 4 and one can ask how the attractor depends on ' a ', if one increases ' a ' in small steps. It seems as if the attractor stays the same for some time, but then suddenly changes. This phenomenon is known as 'bifurcation' (and that's how these fractals got their name). One can create images showing these bifurcations, so called bifurcation diagrams.

Let's examine the Verhulst model for different intervals:

1st case: $0 < a \leq 1$

In this case x converges to 0, and this is clear, because ‘ a ’ is our growth rate, less than 1 $\Rightarrow$ dying

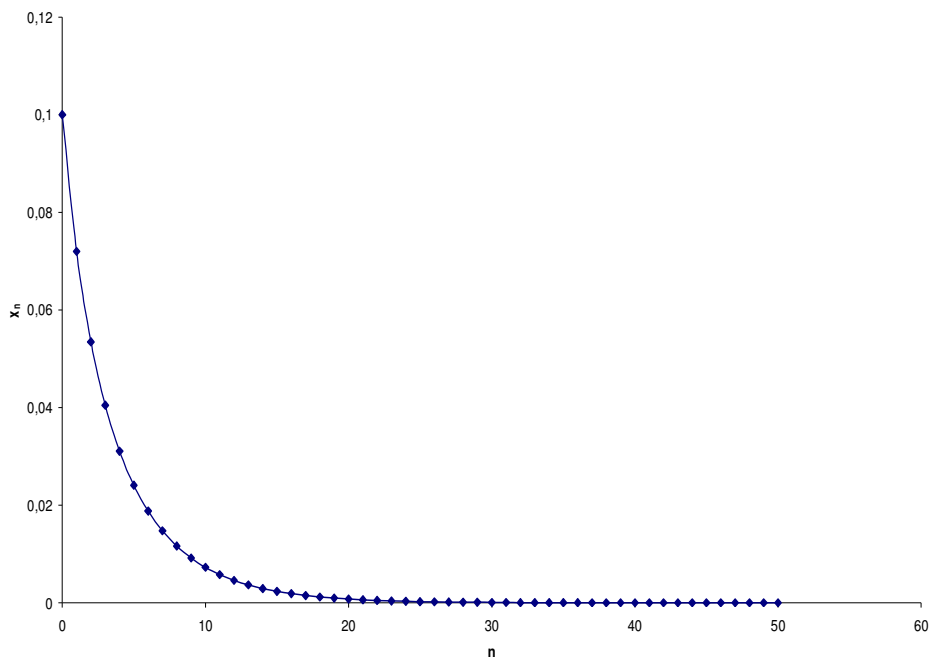


Figure 2.9 Graph of model for $x = 0.1$, $a = 0.8$.

2nd case: $1 < a \leq 2$

Here now the population quickly reaches a balance situation, the population is growing or shrinking (depending on the initial value of x) in a monotone way towards the attractor.

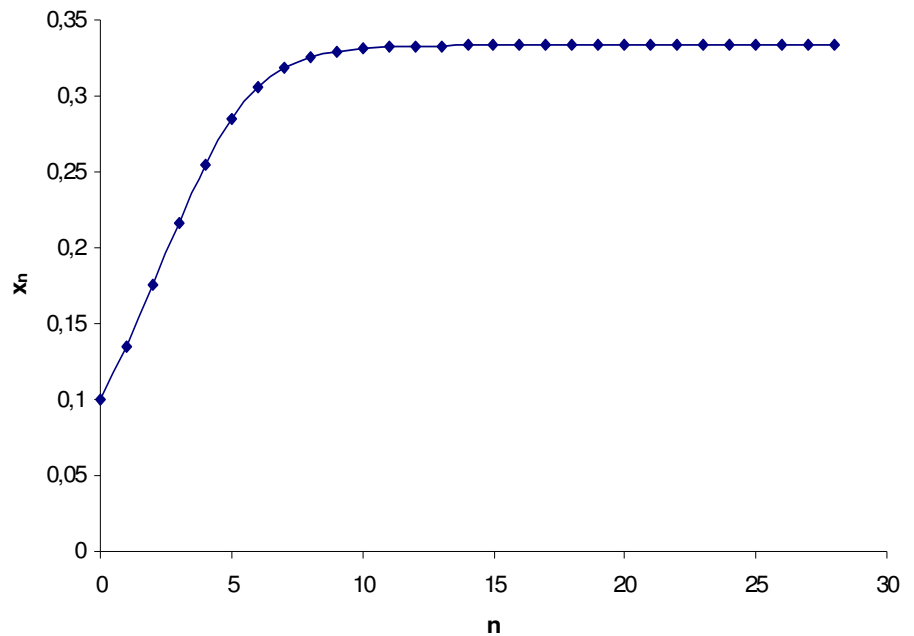


Figure 2.10 Graph of model for $x = 0.1$, $a = 1.5$.

3rd case: $2 < a \leq 3$

Here still balance occurs, but the successive values of ‘ x ’ converge in an oscillating way to the balance-point and not in a monotone way.

Now let ‘ a ’ be greater than 3, e.g. $a = 3.1$

$$x_1 = 0.279$$

$$x_2 = 0.624$$

$$x_3 = 0.727$$

$$x_4 = 0.614$$

$$x_5 = \dots$$

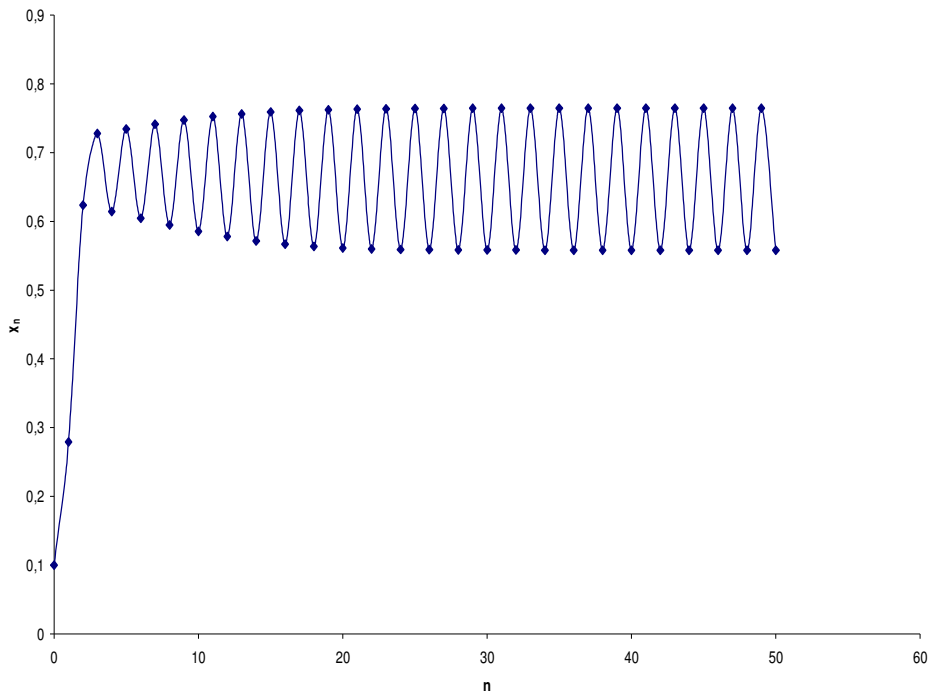


Figure 2.11 Graph of model for $x = 0.1$, $a = 3.1$.

If you continue calculating values, then you will recognize, that ‘ x ’ oscillates between two values, 0.558 and 0.764. So here we do not have a balance, the population is oscillating between these two values.

If you then take a bigger ‘ a ’, but less than 3.449489, then always the population oscillates between two values.

Starting with $a = 3.449489$ something happens. A so called ‘period-doubling’ occurs, that means, ‘ x ’ suddenly oscillates between “four” values instead of “two”. (Figure 2.12)

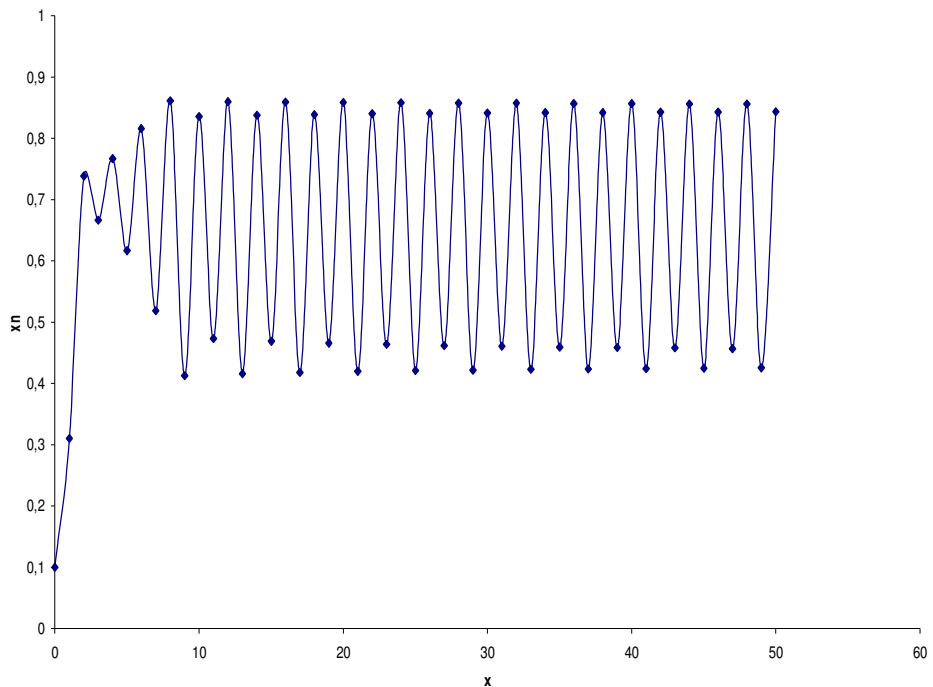


Figure 2.12 Graph of model for $x = 0.1$, $a = 3.449489$.

At $a = 3.5441$ this 4-cyclis changes to an 8-cyclis. All these values, at which the cycle’s length doubles, are called ‘bifurcation nodes’. This 8-cyclis mutates to a 16-cyclis, then to a 32-cyclis, etc., up to a specific value: $a = 3.569946$.

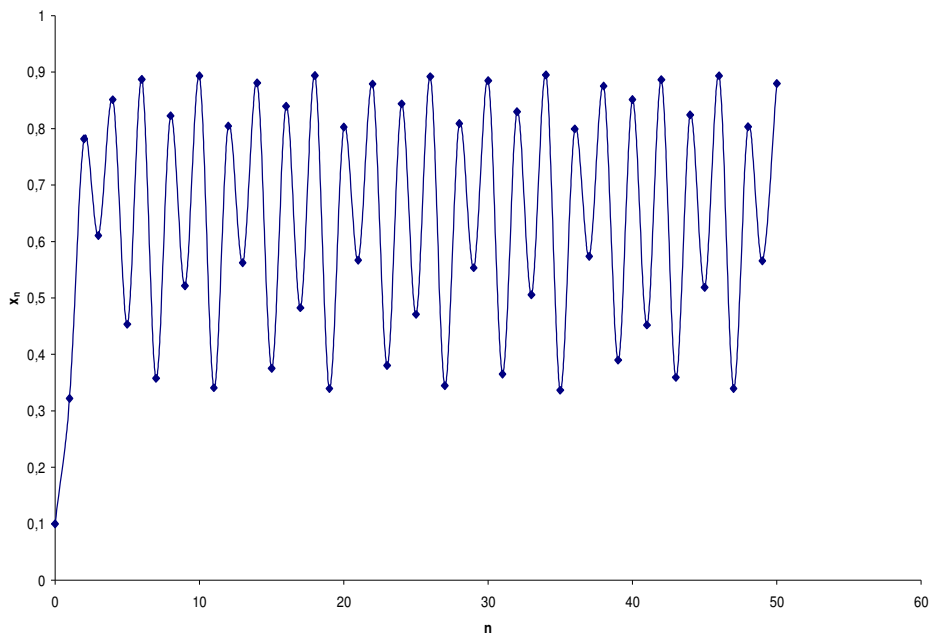


Figure 2.13 Graph of model for $x = 0.1$, $a = 3.5441$.

Now it happens: The whole attractor gets chaotic, that means 'x' oscillates randomly between an infinite amount of unconnected values, here now the attractor is not a cyclus with a fixed length any more, but rather a one dimensional fractal. In this range from 3.569946 up to 4 there are a few 'windows', e.g. at $a = 3.83$, where a 3-cyclus dominates, which mutates to a 6-cyclus, then to a 12-cyclus, a 24-cyclus, etc [Irvin, 2001].

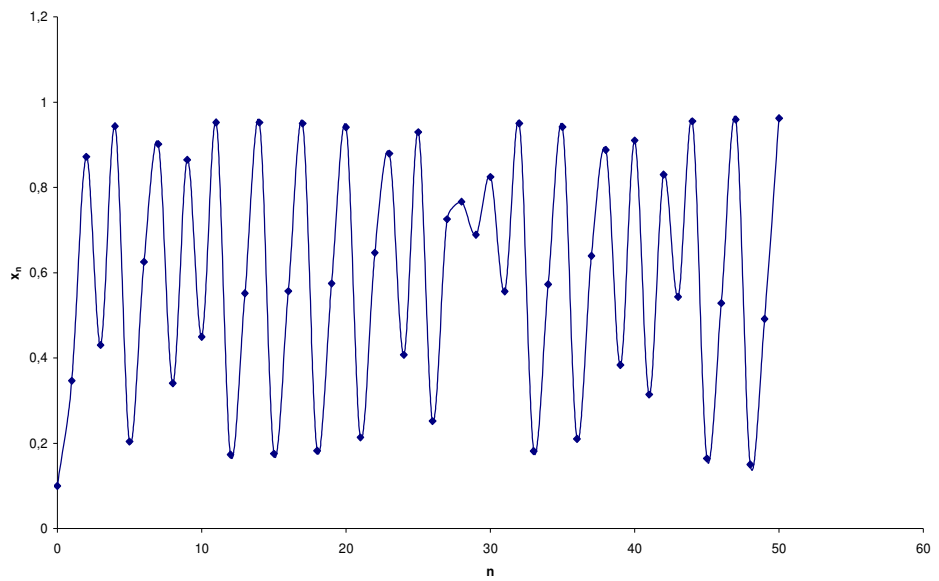


Figure 2.14 Graph of model for $x = 0.1$, $a = 3.57$.

3.0 BIFURCATION OF ONE DIMENSIONAL PHASE SPACE

The function $f(x) = 2x$ is a rule that assigns to each number x a number twice as large. This is a simple mathematical model. It might be imagined that x denote the population of bacteria in a laboratory culture and that $f(x)$ denotes the population one hour later. Then the rule expresses the fact that the population doubles every our. If the culture has an initial population of 10,000 bacteria, then after one hour there will be $f(10,000) = 20,000$ bacteria, after two hour there will be $f(f(10,000)) = 40,000$ bacteria, and so on.

A dynamical system consists of a set of possible states, together with a rule that determines the present state in terms of past states. Let's discuss the simple dynamical system whose states are population levels change with time under the rule $x_n = f(x_{n-1}) = 2x_{n-1}$. Here the variable n stands for time, and x_n designates the population at time n . It will be required that the rule be deterministic, which means that we can determine the present state (population, for example) uniquely from the past states.

No randomness is allowed in our definition of deterministic dynamical system. A possible mathematical model for the price of gold as a function of time would be predict today's price to be yesterday's price plus or minus one dollar, with the two possibilities equally likely. Instead of a dynamical system, this model would be called a random

stochastic, process. A typical realization of such a model could be achieved by flipping a fair coin each day to determine the new price. This type of model is not deterministic, and is ruled out by our definition of dynamical system. [Alligood et al, 1996]

Specifically in the study of dynamical systems, bifurcation occurs when a small smooth change made to the parameter values (the bifurcation parameters) of a system causes a sudden 'qualitative' or topological change in the system's long-term dynamical behaviour. Bifurcations occur in both continuous systems (described by ODEs, DDEs or PDEs), and discrete systems (described by maps). Bifurcation theory is the study of how and when such bifurcations can occur.

Consider the simple one-dimensional dynamical system

$$\frac{dx}{dt} = f(x, r) \tag{3.1}$$

where we will assume that $f = f(x, r)$ is a smooth function and r is a parameter. We wish to study the possible bifurcations for this system, as the parameter r varies. Because the phase portrait for a 1-D system is fully determined by its critical (equilibrium) points, we need only study what happens to the critical points. Bifurcations will (only) occur as these points are created, destroyed, collide, or change stability. For higher dimensional systems, the critical points alone do not determine the phase portrait.

Bifurcations are important scientifically—they provide models of transitions and instabilities as some *control parameter* is varied. For example consider the buckling of beam in Figure 3.1, the beam can support the load and remain vertical. But if the load is too heavy, the vertical position becomes unstable, and the beam may buckle.

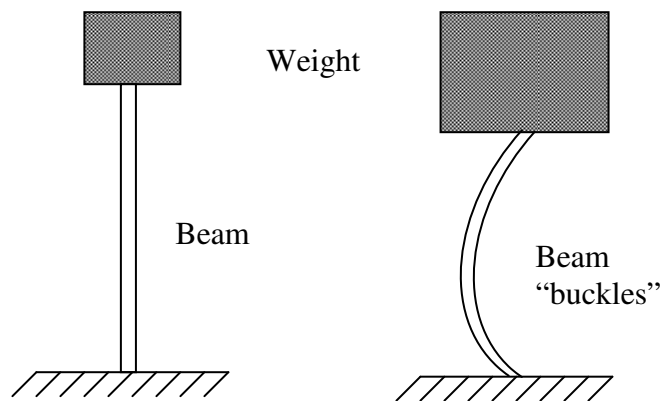


Figure 3.1 Buckling beam.

Here the weight plays the role of the control parameter, and the deflection of the beam from vertical plays the role of the dynamic variable x .

3.1 Saddle Node Bifurcation

In bifurcation theory a saddle-node bifurcation is a local bifurcation in which two fixed points (or equilibria) of a dynamical system collide and annihilate each other. The term 'saddle-node bifurcation' is most often used in reference to continuous dynamical

systems. In discrete dynamical systems, the same bifurcation is often instead called a fold bifurcation.

If the phase space is one-dimensional, one of the fixed points is unstable (the saddle), while the other is stable (the node).

The prototypical example of a saddle-node bifurcation is given by the first order system

$$\frac{dx}{dt} = r + x^2 \quad (3.2)$$

where x is the state variable and r is the bifurcation parameter which may be positive, negative, or zero. When r is negative, there are two fixed points, one stable at $-\sqrt{-r}$ and one unstable at $+\sqrt{-r}$. As “ r ” approaches 0 from below, the parabola moves up and the two fixed points move toward each other. When $r=0$, the fixed points coalesce into a half-stable fixed point at $x^*=0$. This type of fixed point is extremely delicate – it vanishes as soon as $r>0$, and now there are no fixed points at all.

In this example, it is said that a bifurcation occurred at $r=0$, since the vector fields for $r<0$ and $r>0$ are qualitatively different.

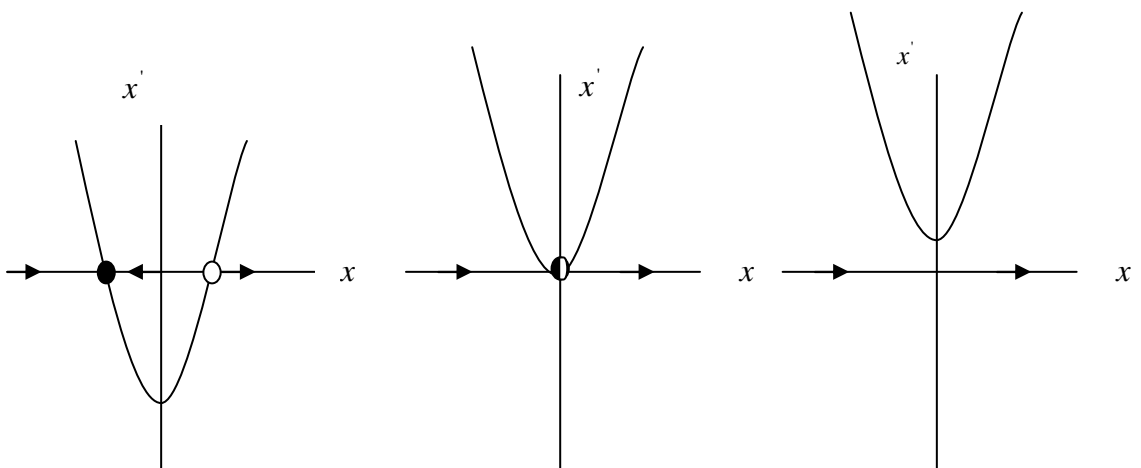


Figure 3.2 Saddle-node bifurcations for $r < 0$, $r = 0$, $r > 0$, respectively.

3.1.1 Graphical conventions

There are several other ways to depict a saddle-node bifurcation. A stack of vector fields for discrete values of r can be shown. (Figure 3.3)

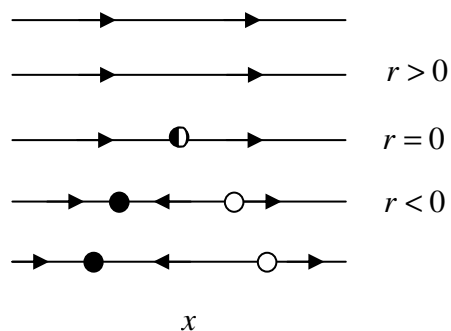


Figure 3.3 Dependence of the fixed points on r .

This representation emphasizes the dependence of the fixed points on r . In the limit of a continuous stack of vector fields, we have a picture like Figure 3.4. The curve shown is $r = -x^2$, i.e., $x' = 0$, which gives the fixed points for different r . To distinguish between stable and unstable fixed points, we use a solid line for stable points and broken line for unstable ones.

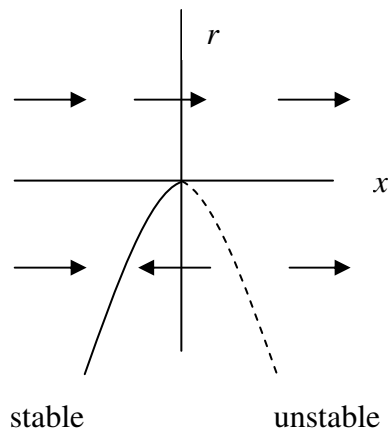


Figure 3.4 Bifurcation diagram for saddle-node bifurcation.

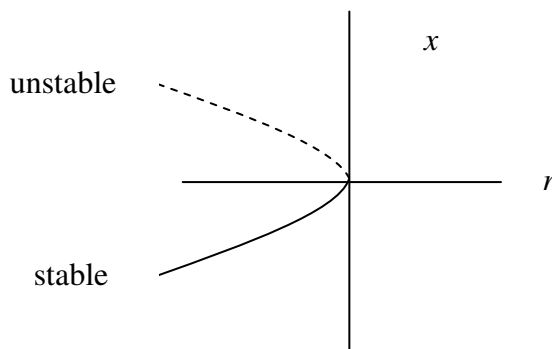


Figure 3.5 Bifurcation diagram for saddle-node bifurcation (x vs. r).

However, the most common way to depict the bifurcation is to invert the axes of Figure 3.4. The rationale is that r plays the role of an independent variable, and so should be plotted horizontally. (Figure 3.5)

The drawback is that now the x -axis has to be plotted vertically, which looks strange at first. Arrows are sometimes included in the picture but not always. This picture is called the ***bifurcation diagram*** for the saddle-node bifurcation.

3.1.2 Terminology

Bifurcation theory is rife with conflicting terminology. The subject really has not settled down yet, and different people use different words for the same thing. For example, the saddle-node bifurcation is sometimes called a *fold bifurcation* (because the curve in Figure 3.5 has a fold in it) or a *turning-point bifurcation* (because the point $(x, r) = (0, 0)$ is a “turning point.”) Admittedly, the term *saddle-node* does not make much sense for vector fields on the line. The name derives from a completely analogous bifurcation seen in a higher-dimensional context, such as vector fields on the plane, where fixed points known as saddles and nodes can collide and annihilate.

3.1.3 Applications

- Give a linear stability analysis of the fixed points in Figure 3.6.

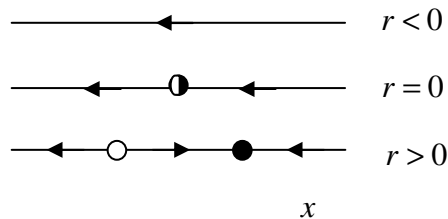


Figure 3.6 An example of bifurcation: ‘splitting into two branches’.

The fixed points for $x' = f(x) = r - x^2$ are given by $x^* = \pm\sqrt{r}$. There are two fixed points for $r \geq 0$, and none for $r < 0$. In order to determine linear stability, we compute $f'(x^*) = -2x^*$. Thus $x^* = +\sqrt{r}$ is stable, since $f'(x^*) < 0$. Similarly $x^* = -\sqrt{r}$ is unstable. At the bifurcation point $r = 0$, we find $f'(x^*) = 0$; the linearization vanishes the fixed points coalesce.

- Show that the first order system $x' = r - x - e^{-x}$ undergoes a saddle-node bifurcation as r is varied, and find the value of r at the bifurcation point.

The fixed points satisfy $f(x) = r - x - e^{-x} = 0$. But now we run into a difficulty, we cannot find the fixed points explicitly as a function of r . Instead we adopt a geometric approach. One method would be graph the function $f(x) = r - x - e^{-x}$ for different value of r , look for its

roots x^* , and then sketch the vector field on the x -axis. This method is fine, but there is an easier way. The point is that; the two functions $r - x$ and e^{-x} have much more familiar graphs than their difference $r - x - e^{-x}$. So we plot $r - x$ and e^{-x} on the same picture. (Figure 3.7) Where the line $r - x$ intersects the curve e^{-x} , we have $r - x = e^{-x}$ and so $f(x) = 0$. Thus, *intersections of the line and the curve correspond to fixed points for the system*. This picture also allows us to read off the direction of flow on the x -axis: the flow is to the right where the line lies above the curve, since $r - x > e^{-x}$ and therefore $\dot{x} > 0$. Hence the fixed point on the right is stable, and the one on the left is unstable.

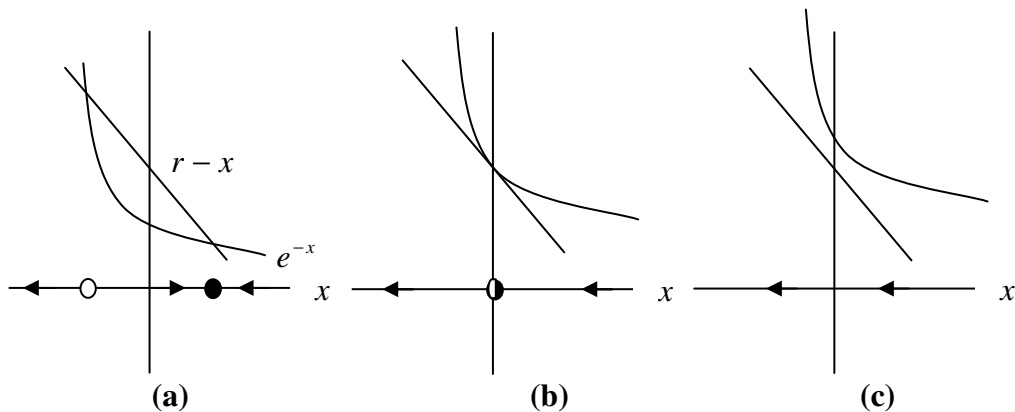


Figure 3.7 Geometric approaches for the application.

If we start decreasing the parameter r , the line $r - x$ slides down and the fixed points approach each other. At some critical value $r = r_c$, the line becomes *tangent* to the curve and the fixed points coalesce in a

saddle-node bifurcation. For r below this critical value, the line lies below the curve and there are no fixed points. (Figure 3.7)

So as to find the bifurcation point r_c , we impose the condition that the graphs of $r - x$ and e^{-x} intersect *tangentially*. Thus we demand equality of the functions and their derivatives.

$$e^{-x} = r - x$$

and

$$\frac{d}{dx} e^{-x} = \frac{d}{dx} (r - x)$$

The second equation implies $-e^{-x} = -1$ so $x = 0$. Then the first equation yields $r = 1$. Hence the bifurcation point is $r_c = 1$, and the bifurcation occurs at $x = 0$.

3.1.4 Normal forms

In a certain sense, the examples $x' = r - x^2$ or $x' = r + x^2$ are representative of *all* saddle-node bifurcations; that's why we called them 'prototypical'. The idea is that, close to saddle-node bifurcation, the dynamics typically look like $x' = r - x^2$ or $x' = r + x^2$.

For instance, considering the second example near the bifurcation at $x=0$ and $r=1$. Using the Taylor expansion for e^{-x} about $x=0$, we find

$$\begin{aligned}x' &= r - x - e^{-x} \\x' &= r - x - \left[1 - x + \frac{x^2}{2!} + \dots \right] \\x' &= (r-1) - \frac{x^2}{2} + \dots\end{aligned}$$

to leading order in x . This has the same algebraic form as $x' = r - x^2$, and can be made to agree exactly by appropriate rescaling of x and r .

It is easy to understand why saddle-node bifurcations typically have this algebraic form. We just ask ourselves: how can two fixed points of $x' = f(x)$ collide and disappear as a parameter r is varied? Graphically, fixed points occur where the graph of $f(x)$ intersects the x -axis. For a saddle-node bifurcation to be possible we need two nearby roots of $f(x)$; this means $f(x)$ must look locally “bowl-shaped” or parabolic.

Now, we use a microscope to zoom in on the behaviour near the bifurcation. As r varies we see a parabola intersecting the x -axis, then becoming tangent to it, and then failing to intersect. This is exactly the scenario in the prototypical Figure 3.8.

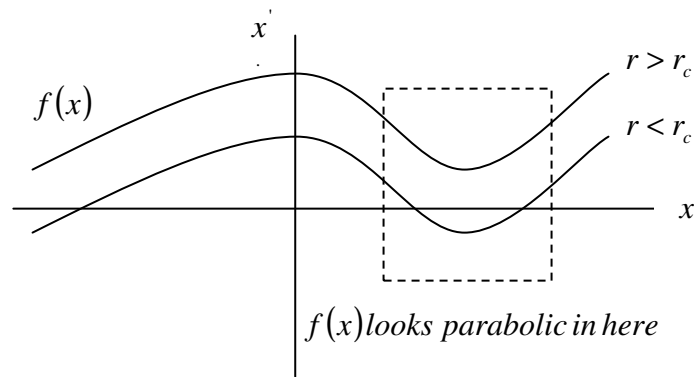


Figure 3.8 The parabolic function.

Here is a more algebraic version of the same argument. We regard f as a function of both x and r , and examine the behaviour of $x' = f(x, r)$ near the bifurcation at $x = x^*$ and $r = r_c$. Taylor's expansion yields

$$\begin{aligned} x' &= f(x, r) \\ &= f(x^*, r_c) + (x - x^*) \left. \frac{\partial f}{\partial x} \right|_{(x^*, r_c)} + (r - r_c) \left. \frac{\partial f}{\partial r} \right|_{(x^*, r_c)} + \frac{1}{2} (x - x^*)^2 \left. \frac{\partial^2 f}{\partial x^2} \right|_{(x^*, r_c)} + \dots \end{aligned}$$

where we have neglected quadric terms in $(r - r_c)$ and cubic terms in $(x - x^*)$. Two of the terms in the equation vanish: $f(x^*, r_c) = 0$ since x^* is a fixed point, and $\left. \frac{\partial f}{\partial x} \right|_{(x^*, r_c)} = 0$ by the tangency condition of saddle-node bifurcation. Thus

$$x' = a(r - r_c) + b(x - x^*)^2 + \dots$$

where $a = \partial f / \partial r|_{(x^*, r_c)}$ and $b = \frac{1}{2} \partial^2 f / \partial x^2|_{(x^*, r_c)}$. Equation above agrees with the form of our prototypical examples. (Assuming that $a, b \neq 0$, which is the typical case; for instance, it would be very special situation if the second derivative $\partial^2 f / \partial x^2$ also happened to vanish at the fixed point.)

What we have been calling prototypical examples is more conventionally known as ***normal forms*** for the saddle-node bifurcation. [Strogatz, 1994]

3.2 Transcritical Bifurcation

There are certain scientific situations where a fixed point must exist for all values of a parameter and can never be destroyed. For example, in the logistic equation and other simple models for the growth of a single species, there is a fixed point at zero population, regardless of the value of the growth rate. However, such a fixed point may change its stability as the parameter is varied. The transcritical bifurcation is the standard mechanism for such changes in stability.

The normal form for a transcritical bifurcation is

$$x' = rx - x^2.$$

Both before and after the bifurcation, there is one unstable and one stable fixed point. However, their stability is exchanged when they collide, so the unstable fixed point becomes stable. Figure 3.9 shows the vector field as r varies. There is a fixed point at $x^* = 0$ for all values of r .

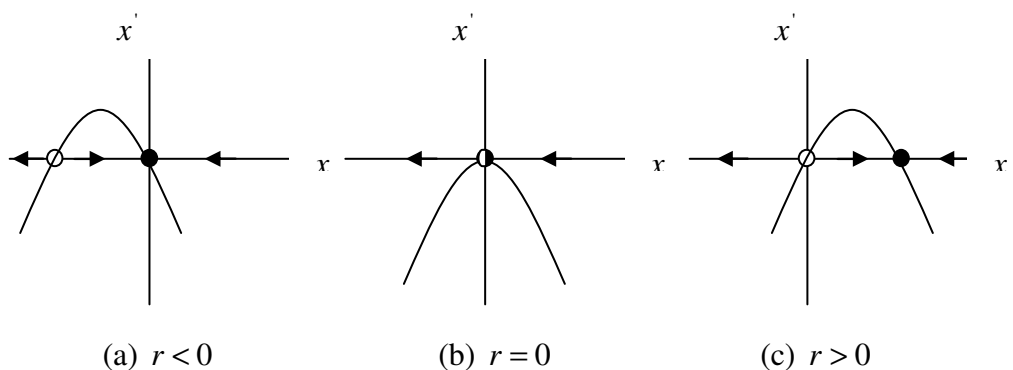


Figure 3.9 Transcritical bifurcations for varying r .

For $r < 0$, there is an unstable fixed point at $x^* = r$ and a stable fixed point at $x^* = 0$. As r increases, the unstable fixed point approaches the origin, and coalesces with it when $r = 0$. Finally, when $r > 0$, the origin has become unstable, and $x^* = r$ is now stable. Some people say that an *exchange of stabilities* has taken place between the two fixed points.

The important difference between the saddle-node and transcritical bifurcations: in the transcritical case, the two fixed points don't disappear after the bifurcation- instead they just switch their stability.

Figure 3.10 shows the bifurcation diagram for the transcritical bifurcation. As in Figure 3.5, the parameter r is regarded as the independent variable and the fixed points $x^* = 0$ and $x^* = r$ are shown as dependent variables.

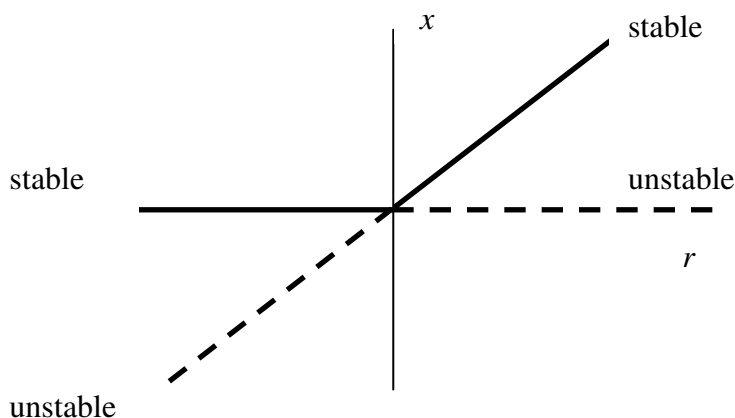


Figure 3.10 Bifurcation diagram for the transcritical bifurcation.

3.2.1 Applications

- Show that the first-order system $x' = x(1 - x^2) - a(1 - e^{-bx})$ undergoes a transcritical bifurcation at $x = 0$ when the parameters a, b satisfy a certain equation, to be determined. (This equation defines a **bifurcation curve** in the (a, b) parameter space.) Then find an approximate formula for the fixed point that bifurcates from $x = 0$, assuming that the parameters are close to the bifurcation point.

$x=0$ is a fixed point for all (a,b) . This makes it plausible that the fixed point will bifurcate transcritically if it bifurcates at all. For small x , we find

$$\begin{aligned} 1 - e^{-bx} &= 1 - \left[1 - bx + \frac{1}{2}b^2x^2 + O(x^3) \right] \\ &= bx + \frac{1}{2}b^2x^2 + O(x^3) \end{aligned}$$

and so

$$\begin{aligned} x' &= x - a \left(bx + \frac{1}{2}b^2x^2 \right) + O(x^3) \\ &= (1 - ab)x + \left(\frac{1}{2}ab^2 \right)x^2 + O(x^3). \end{aligned}$$

Hence a transcritical bifurcation occurs when $ab=1$; this is the equation for the bifurcation curve. The nonzero fixed point is given by the solution of $(1 - ab + \left(\frac{1}{2}ab^2 \right)x) \approx 0$, i.e.,

$$x^* \approx \frac{2(ab-1)}{ab^2}.$$

This formula is approximately correct only if x^* is small, since our series expansions are based on the assumption of small x . Thus the formula holds only when ab is close to 1, which means that the parameters must be close to the bifurcation curve.

- Analyze the dynamics of $x' = r \ln x + x - 1$ near $x=1$, and show that the system undergoes a transcritical bifurcation at a certain value of r . Then find new variables X and R such that the system reduces to the approximate normal form $X' \approx RX - X^2$ near the bifurcation.

$x=1$ is a fixed point for all values of r . Since we are interested in the dynamics near this fixed point, we introduce a new variable $u = x - 1$, where u is small. Then

$$\begin{aligned}
 u' &= x' \\
 &= r \ln(1+u) + u \\
 &= r \left[u - \frac{1}{2}u^2 + O(u^3) \right] + u \\
 &= (r+1)u - \frac{1}{2}ru^2 + O(u^3).
 \end{aligned}$$

Hence a transcritical bifurcation occurs at $r_c = -1$.

So as to put this equation into normal form, we first need to get rid of the coefficient of u^2 . Let $u = av$ where a will be chosen later. Then the equation for v is

$$v' = (r+1)v - \left(\frac{1}{2}ra \right)v^2 + O(v^3).$$

So if we choose $a = 2/r$, the equation becomes

$$v' = (r+1)v - v^2 + O(v^3).$$

Now if we let $R = r+1$ and $X = v$, we have achieved the approximate normal form $X' \approx RX - X^2$, where cubic terms of order $O(X^3)$ have been neglected. In terms of the original variables, $X = v = u/a = \frac{1}{2}r(x-1)$.

To be a bit more accurate, the theory of normal forms assures us that we can find a change of variables such that the system becomes $X' = RX - X^2$, with strict, rather than approximate, equality. Our solution above gives an approximation to the necessary change of variables. If we wanted a better approximation, we would retain the cubic term in the series expansions (and perhaps even higher-order terms if we're really feeling heroic) and we would have to do a more elaborate calculation to eliminate these higher-order terms [Strogatz, 1994].

3.3 Laser Threshold

3.3.1 Physical background

In order to apply our mathematics to a scientific example, a particular type of laser known as a solid-state laser which contains of a collection of special “laser-active” atoms embedded in a solid-state matrix, bounded by partially reflecting mirrors at either end is

considered. An external energy source is used to excite or “pump” the atoms out of their ground states. (Figure 3.11)

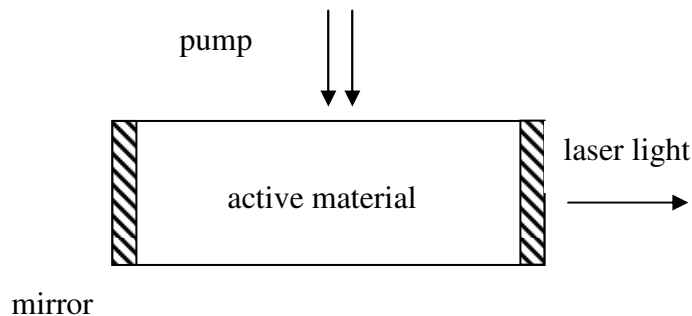


Figure 3.11 An extremely simplified model for a laser.

Each atom can be thought of as a little antenna radiating energy. When the pumping is relatively weak, the laser acts just like an ordinary *lamp*: the excited atoms oscillate independently of one another and emit randomly phased light waves.

Now suppose increasing the strength of the pumping. At first nothing different happens, but then suddenly, when the pump strength exceeds a certain threshold, the atoms begin to oscillate in phase- the lamp has turned into a ***laser***. Now the trillion of little antennas act like one giant antenna and produce a beam of radiation that is much more coherent and intense than that produced below the laser threshold.

This sudden onset of coherence is amazing, considering that the atoms are being excited completely at random by the pump. Hence the

process is *self-organizing*: the coherence develops because of a cooperative interaction among the atoms themselves.

3.3.2 Model

A proper explanation of the laser phenomenon would require delving into quantum mechanics. Instead a simplified model of the essential physics can be considered. The dynamical variable is the number of photons $n(t)$ in the laser field. Its rate of change is given by

$$\begin{aligned} n' &= \text{gain} - \text{loss} \\ &= GnN - kn . \end{aligned}$$

The gain term comes from the process of *stimulated emission*, in which photons stimulate excited atoms to emit additional photons. Because this process occurs via random encounters between photons and excited atoms, it occurs at a rate proportional to n and to the number of excited atoms, denoted by $N(t)$. The parameter $G > 0$ is known as the gain coefficient. The loss term models the escape of photons through the end faces of the laser. The parameter $k > 0$ is a rate constant; its reciprocal $\tau = 1/k$ represents the typical lifetime of a photon in the laser.

Now comes the key physical idea: after an excited atom emits a photon, it drops down to a lower energy level and is no longer excited. Thus N decreases by the emission of photons. To capture this effect, we

need to write an equation relating N to n . Suppose that in the absence of laser action, the pump keeps the number of excited atoms fixed at N_0 . Then the actual number of excited atoms will be reduced by the laser process. Specifically, we assume

$$N(t) = N_0 - \alpha n,$$

where $\alpha > 0$ is the rate at which atoms drop back to their ground states. Then

$$\begin{aligned} n' &= Gn(N_0 - \alpha n) - kn \\ &= (GN_0 - k)n - (\alpha G)n^2. \end{aligned}$$

Figure 3.11 shows the corresponding vector field for different values of the pump strength N_0 . Only positive values of n are physically meaningful.

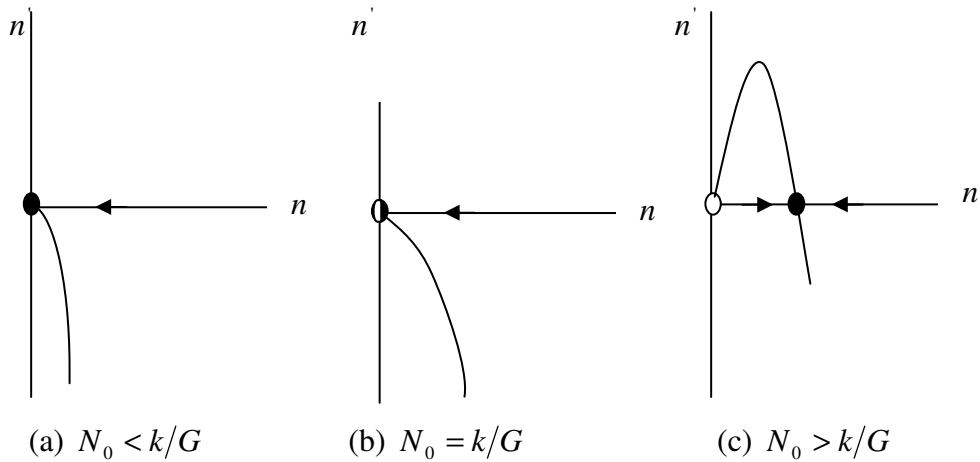


Figure 3.12 First-order systems for $n(t)$.

When $N_0 < k/G$, the fixed point at $n^* = 0$ is stable. This means that there is no stimulated emission and the laser acts like a lamp. As the pump strength N_0 is increased, the system undergoes a transcritical bifurcation when $N_0 = k/G$. For $N_0 > k/G$, the origin loses stability and a stable fixed point appears at $n^* = (GN_0 - k)/\alpha G > 0$, corresponding to spontaneous laser action. Thus $N_0 = k/G$ can be interpreted as the ***laser threshold*** in this model. Figure 3.12 summarizes the result [Strogatz, 1994].

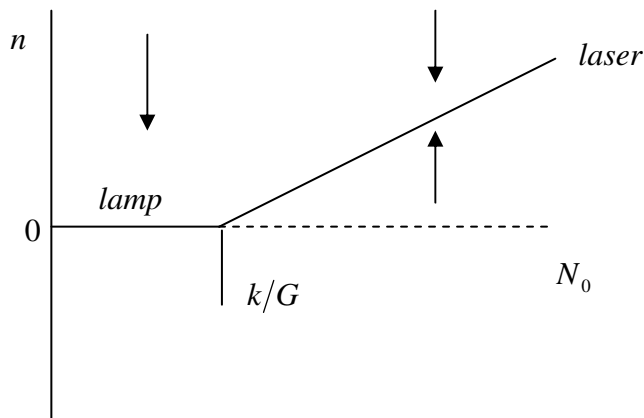


Figure 3.13 The laser threshold.

Although this model correctly predicts the existence of a threshold, it ignores the dynamics of the excited atoms, the existence of spontaneous emission, and several other complications.

3.4 Pitchfork Bifurcation

The third kind of bifurcation is pitchfork bifurcation. It is common in physical problems that have symmetry. For example, many problems have a spatial symmetry between left and right. In such cases, fixed points tend to appear and disappear in symmetrical pairs. In the buckling example, the beam is stable in the vertical position if the load is small. In this case there is a stable fixed point corresponding to zero deflection. But if the load exceeds the buckling threshold, the beam may buckle to either the left or the right. The vertical position has gone unstable, and two new symmetrical fixed points, corresponding to left- and right-buckled configurations, have been born.

There are two very different types of pitchfork bifurcation. The simpler type is called *supercritical*, and will be discussed first.

3.4.1 Supercritical pitchfork bifurcation

The normal form of the supercritical pitchfork bifurcation is

$$\dot{x} = rx - x^3. \quad (3.3)$$

This equation is invariant under the change of variables $x \rightarrow -x$. This is, if we replace x by $-x$ and cancel the resulting minus signs on both sides of the equation, we get (3.3) back again. This invariance is the mathematical expression of the left-right symmetry. (More technically, one says that the vector field is *equivariant*)

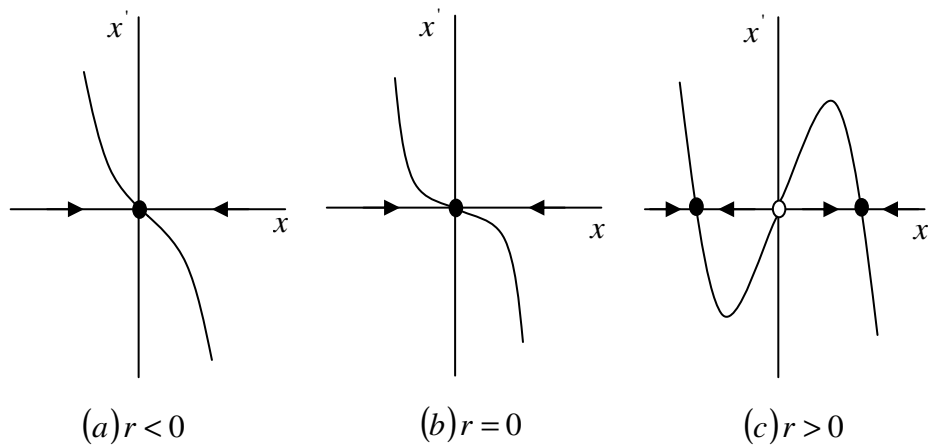


Figure 3.14 Vector field for different values of r .

When $r < 0$, the origin is the only fixed point, and it is stable. When $r = 0$, the origin is still stable, but much more weakly so, since the linearization vanishes. Now solutions no longer decay exponentially fast –instead the decay is a much slower algebraic function of time. This lethargic decay is called critical slowing down in the physics literature. Finally, when $r > 0$, the origin has become unstable. Two new stable fixed points appear on either side of the origin, symmetrically located at $x^* = \pm\sqrt{r}$.

The reason for the term “pitchfork” becomes clear while plotting the bifurcation diagram. Actually pitchfork trifurcation might be a better word.

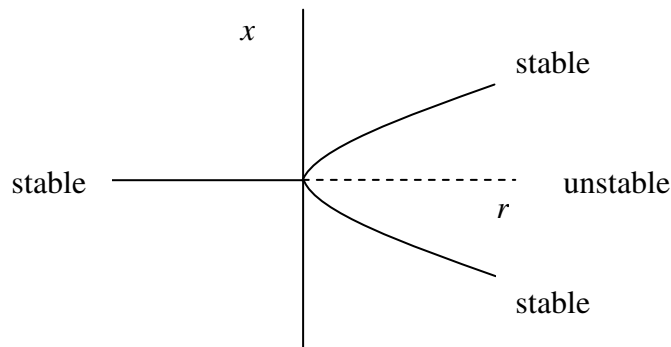


Figure 3.15 The bifurcation diagram of the supercritical pitchfork bifurcation.

3.4.2 Applications

- Equations similar to $x' = -x + \beta \tanh x$ arise in statistical mechanical models of magnets and neural networks. Show that this equation undergoes a supercritical pitchfork bifurcation as β is varied. Then give a numerically accurate plot of the fixed points for each β .

The graphs of $y = x$ and $y = \beta \tanh x$ are shown in Figure 3.15; their intersections correspond to fixed points. The key thing to realize is that as β increases, the $\tanh$ curve becomes steeper at the origin (its slope there is β). Hence for $\beta < 1$ the origin is the only fixed point. A pitchfork bifurcation occurs at $\beta = 1, x^* = 0$, when the $\tanh$ curve develops a slope of 1 at the origin. Finally, when $\beta > 1$, two new stable fixed points appear, and the origin becomes unstable.

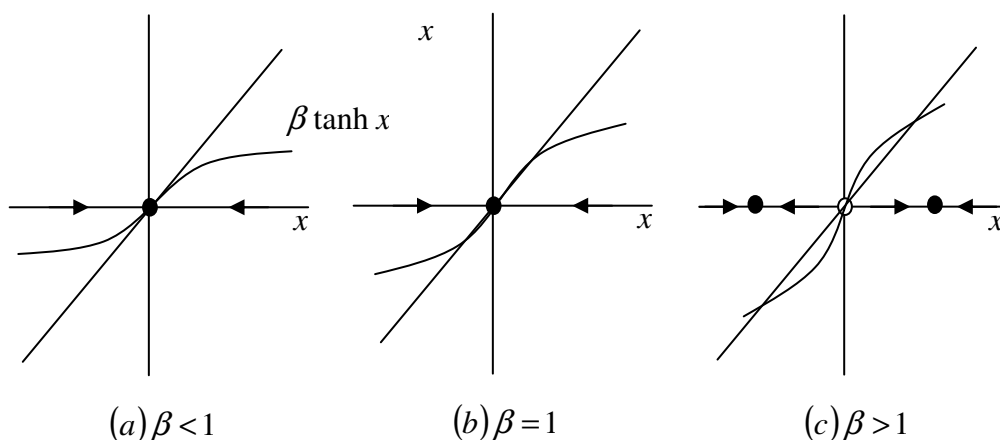


Figure 3.16 The graphical illustration of the first pitchfork bifurcation application.

Now the fixed points x^* for each β can be computed. Of course, one fixed point always occurs at $x^* = 0$; we are looking for the other, nontrivial fixed points. One approach is to solve the equation $x^* = \beta \tanh x^*$ numerically, using the Newton-Raphson method or some other root-finding scheme. But there is an easier way, which comes from changing our point of view. Instead of studying the dependence of x^* on β , we think of x^* as the independent variable, and then compute $\beta = x^* / \tanh x^*$. This gives us a table of pairs (x^*, β) . For each pair, we plot β horizontally and x^* vertically. This yields the bifurcation diagram.

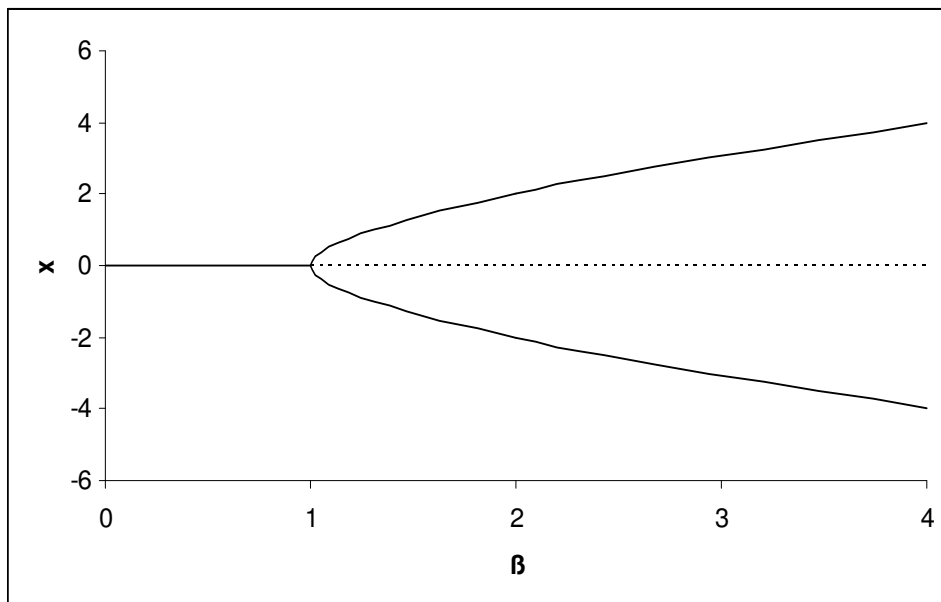


Figure 3.17 Bifurcation diagram according to varying β .

The shortcut used here exploits the fact that $f(x, \beta) = -x + \beta \tanh x$ depends more simply on β than on x . This frequently the case in bifurcation problems –the dependence on the control parameter is usually simpler than the dependence on x .

- Plot the potential $V(x)$ for the system $x' = rx - x^3$, for the cases $r < 0$, $r = 0$, and $r > 0$.

The potential for $x' = f(x)$ is defined by $f(x) = -dV/dx$. Hence we need to solve $-dV/dx = rx - x^3$. Integration yields

$V(x) = -\frac{1}{2}rx^2 + \frac{1}{4}x^4$, where we neglect the arbitrary constant of integration. The corresponding graphs are shown below.

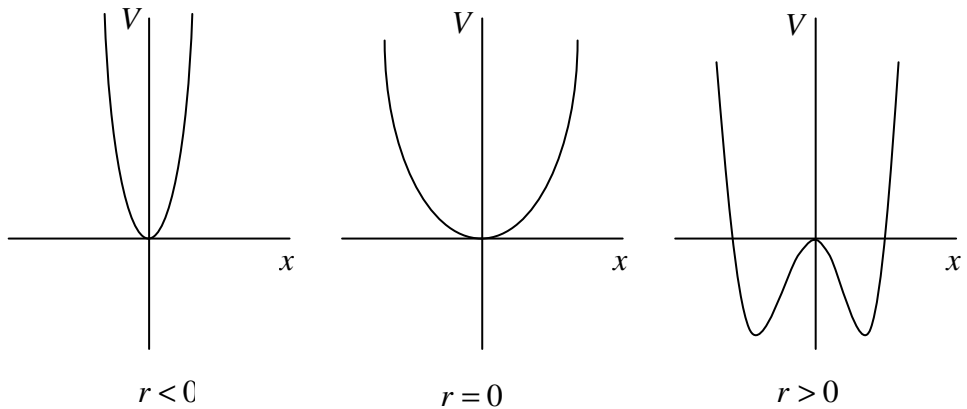


Figure 3.18 The graphs of V with respect to x .

When $r < 0$, there is a quadratic minimum at the origin. At the bifurcation value $r = 0$, the minimum becomes a much flatter quadratic. For $r > 0$, a local maximum appears at the origin, and a symmetric pair of minima occurs to either side of it.

3.4.3 Subcritical Pitchfork Bifurcations

In the supercritical case $x' = rx - x^3$ discussed above, the cubic term is stabilizing: it acts as a restoring force that pulls $x(t)$ back toward $x = 0$. If instead the cubic term were destabilizing, as in

$$x' = rx + x^3, \quad (3.4)$$

Then we'd have a ***subcritical*** pitchfork bifurcation.

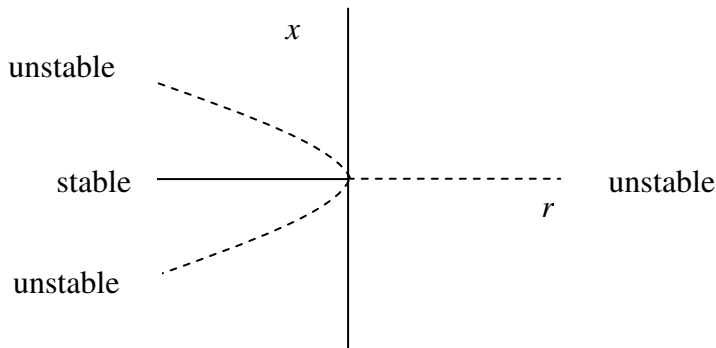


Figure 3.19 Subcritical pitchfork bifurcation diagram.

Compared to Figure 3.14, the pitchfork is inverted. The nonzero fixed points $x^* = \pm\sqrt{r}$ are unstable, and exist only *below* the bifurcation ($r < 0$), which motivates the term “subcritical”. More importantly, the origin is stable for $r < 0$ and unstable for $r > 0$, as in the supercritical case, but now the instability for $r > 0$ is not opposed by the cubic term – in fact the cubic term lends a helping hand in driving the trajectories out to infinity. This effect leads to *blow-up*: one can show that $x(t) = \pm\infty$ in finite time starting from any initial condition $x_0 \neq 0$.

In real physical systems, such an explosive instability is usually opposed by the stabilizing influence of higher-order terms. Assuming that the system is still symmetric under $x \rightarrow -x$, the first stabilizing term

must be x^5 . Thus the canonical example of a system with a supercritical pitchfork bifurcation is

$$\dot{x} = rx + x^3 - x^5. \quad (3.5)$$

There is no loss in generality in assuming that the coefficients of x^3 and x^5 are 1.0.

3.4.4 Terminology

As usual in bifurcation theory, there are several other names for the bifurcation discussed here. The supercritical pitchfork is sometimes called a forward bifurcation, and is closely related to a continuous or second-order phase transition in statistical mechanics. The subcritical bifurcation is sometimes called an inverted or backward bifurcation, and is related to discontinuous or first-order phase transitions. In the engineering literature, the supercritical bifurcation is sometimes called soft or safe, because the nonzero fixed points are born at small amplitude; in contrast, the subcritical bifurcation is hard or dangerous, because of the jump from zero to large amplitude [Strogatz, 1994].

4.0 BIFURCATION OF TWO DIMENSIONAL PHASE SPACE

4.1 Saddle Node, Transcritical, and Pitchfork Bifurcations

The bifurcations of fixed points discussed before have analogs in two dimensions (and indeed, in all dimensions). Yet it turns out that nothing really happens when more dimensions are added –all the action is confined to a one-dimensional subspace along which the bifurcations occur, while in the extra dimensions the flow is either simple attractions or repulsion from the subspace.

4.1.1 Saddle node bifurcation

The saddle node bifurcation is the basic mechanism for the creation and destruction of fixed points. Here's the prototypical example in two dimensions:

$$\begin{aligned}x' &= \mu - x^2 \\ y' &= -y\end{aligned}\tag{4.1}$$

In the x -direction we see the bifurcation behaviour discussed in Section 4.1, while in the y direction the motion is exponentially damped.

Consider the phase portrait as μ varies. For $\mu > 0$, Figure 4.1 shows that there are two fixed points, a stable node approach each other, then collide when $\mu = 0$, and finally disappear when $\mu < 0$.

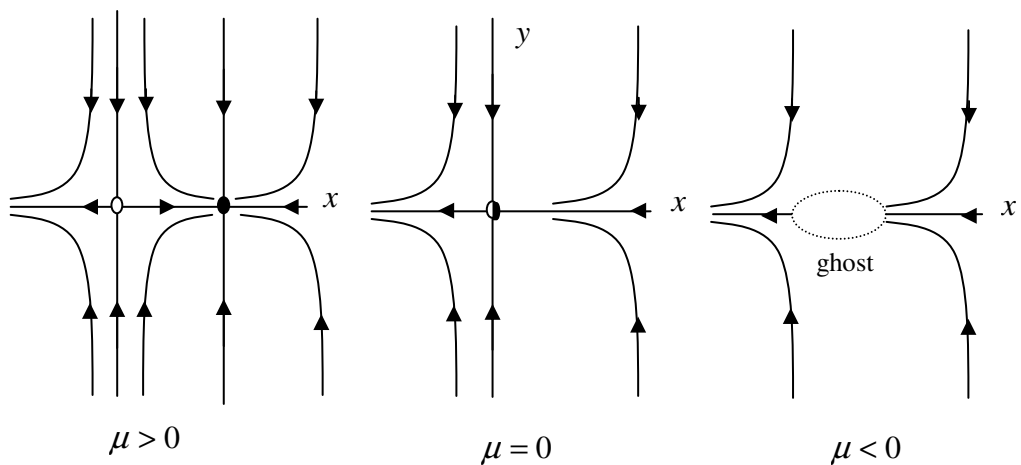


Figure 4.1 Saddle-node bifurcations for $\mu > 0$, $\mu = 0$, $\mu < 0$, respectively.

Even after the fixed points have annihilated each other, they continue to influence the flow, they leave a *ghost*, a bottleneck region that sucks trajectories in and delays them before allowing passage out the other side. The time spent in the bottleneck generically increases as $(\mu - \mu_c)^{-1/2}$, where μ_c is the value at which the saddle-node bifurcation occurs.

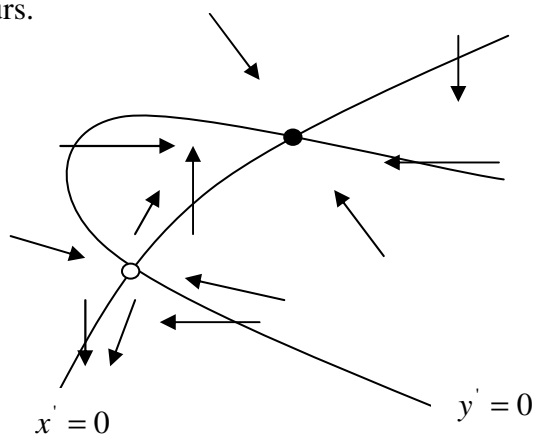


Figure 4.2 Saddle-node situation.

Figure 4.2 is representative of the following more general situation. Consider a two-dimensional system $x' = f(x, y)$, $y' = g(x, y)$ that depends on a parameter μ . Suppose that for some value of μ the nullclines intersect as shown in Figure 4.3. Notice that each intersection corresponds to a fixed point since $x' = 0$ and $y' = 0$ simultaneously. Thus to see how the fixed points move as μ changes, we just have to watch the intersection. Now suppose that the nullclines pull away from each other as μ varies, becoming *tangent* at $\mu = \mu_c$. Then the fixed points approach each other and collide when $\mu = \mu_c$; after the nullclines pull apart, there are no intersections and the fixed points disappear with a bang. The point is that all saddle node bifurcations have this character locally.

4.1.2 Transcritical and pitchfork bifurcations

Using the same idea as above, we can also construct prototypical examples of transcritical and pitchfork bifurcations at a stable fixed point. In the x direction the dynamics are given by the normal forms discussed in Section 2, and in the y direction the motion is exponentially damped. This yields the following examples:

$$x' = \mu x - x^2, \quad y' = -y \quad (\text{transcritical})$$

$$x' = \mu x - x^3, \quad y' = -y \quad (\text{supercritical pitchfork})$$

$$x' = \mu x + x^3, \quad y' = -y \quad (\text{subcritical pitchfork})$$

The analysis in each case follows the same pattern. Let's discuss the supercritical pitchfork for the system $x' = \mu x - x^3$, $y' = -y$, for $\mu < 0$, $\mu = 0$, $\mu > 0$.

For $\mu < 0$, the only fixed point is a stable node at the origin. For $\mu = 0$, the origin is still stable, but we now have very slow (algebraic) decay along the x direction instead of exponential decay; this is the phenomenon of “critical slowing down”. For $\mu > 0$, the origin loses stability and gives birth to two new stable fixed points symmetrically located at $(x^s, y^s) = (\pm\sqrt{\mu}, 0)$. By computing the Jacobean at each point, you can check that the origin is a saddle and the other two fixed points are stable node. The phase portraits are shown in Figure 4.3 [Strogatz, 1994].

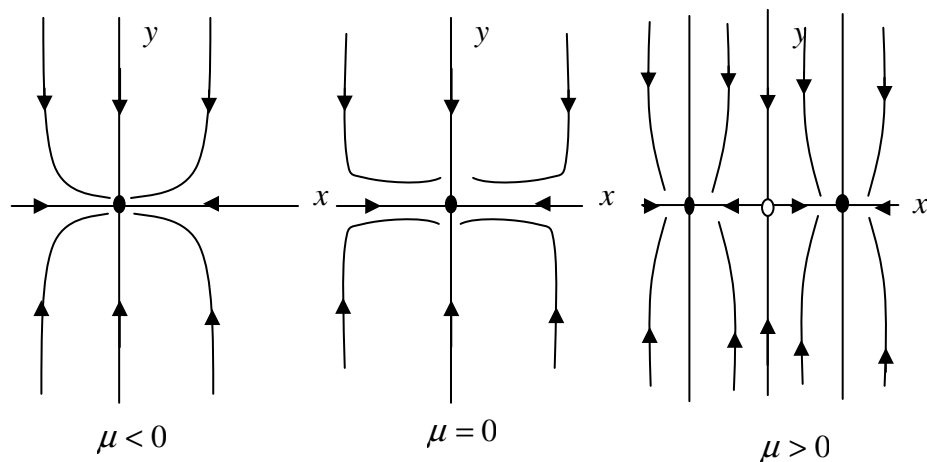


Figure 4.3 Phase portraits for the supercritical pitchfork system.

4.2 Hopf Bifurcations

Suppose a two-dimensional system has a stable fixed point. What are the possible ways it could lose stability as a parameter μ varies? The eigenvalues of the Jacobean are the key. If the fixed point is stable, the eigenvalues λ_1, λ_2 must both lie in the left half plane $\text{Re } \lambda < 0$. Since the λ 's satisfy a quadratic equation with real coefficients, there are two possible pictures: either the eigenvalues are both real and negative or they are complex conjugates. To destabilize the fixed point, we need one or both of the eigenvalues to cross into the right half-plane as μ varies.

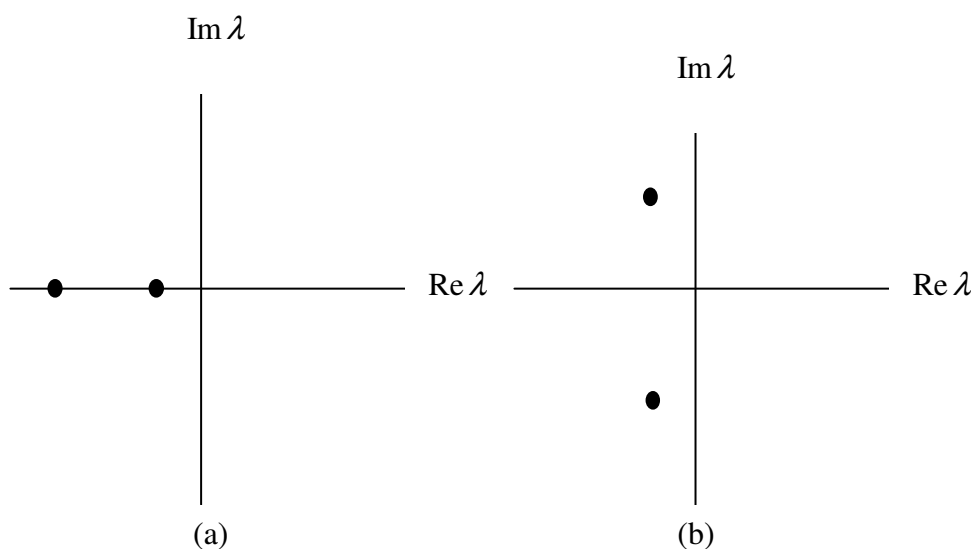


Figure 4.4 Possible pictures of imaginary and real eigenvalues.

In section 4.1 we explored the cases in which a real eigenvalue passes through $\lambda = 0$. These were saddle-node, transcritical, and pitchfork bifurcations. Now we consider the other possible scenario, in

which two complex conjugate eigenvalues simultaneously cross the imaginary axis into the right half-plane.

4.2.1 Supercritical hopf bifurcation

Suppose we have a physical system that settles down to equilibrium through exponentially damped oscillations. In other words, small disturbances decay after “ringing” for a while. (Figure 4.5.a) Now suppose that the decay rate depends on a control parameter μ . If the decay become slower and slower and finally changes to *growth* at a critical value μ_c , the equilibrium state will lose stability. In many cases the resulting motion is small-amplitude, sinusoidal, limit cycle oscillation about the former steady state. (Figure 4.5.b) then we say that the system has undergone a *supercritical Hopf bifurcation*.

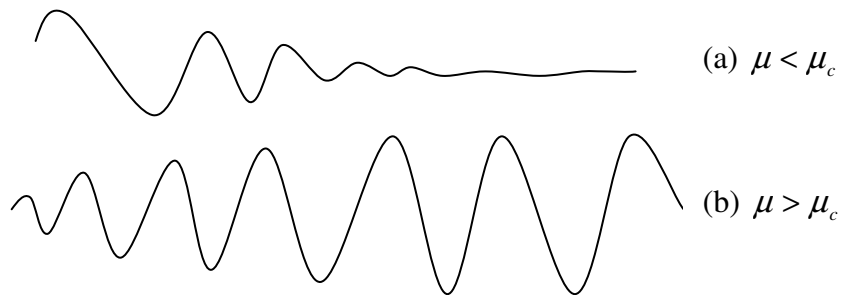


Figure 4.5 Oscillations in Hopf bifurcation.

In terms of the flow in phase space, a supercritical Hopf bifurcation occurs when a stable spiral changes into an unstable spiral

surrounded by a small, nearly elliptical limit cycle. Hopf bifurcations can occur in phase spaces of any dimension $n \geq 2$.

A simple example of a supercritical Hopf bifurcation is given by the following:

$$\begin{aligned}r' &= \mu r - r^3 \\ \theta' &= \omega + br^2.\end{aligned}$$

There are three parameters: μ controls the stability of the fixed points at the origin, ω gives the frequency of infinitesimal oscillations, and b determines the dependence of frequency on amplitude for larger amplitude oscillations.

Figure 4.6 plots the phase portraits for μ above and below the bifurcation. When $\mu < 0$ the origin $r = 0$ is a stable spiral whose sense of rotation depends on the sign of ω . For $\mu = 0$ the origin is still a stable spiral, though a very weak one: the decay is only algebraically fast. Finally, for $\mu > 0$ there is an unstable spiral at the origin and a stable circular limit cycle at $r = \sqrt{\mu}$.

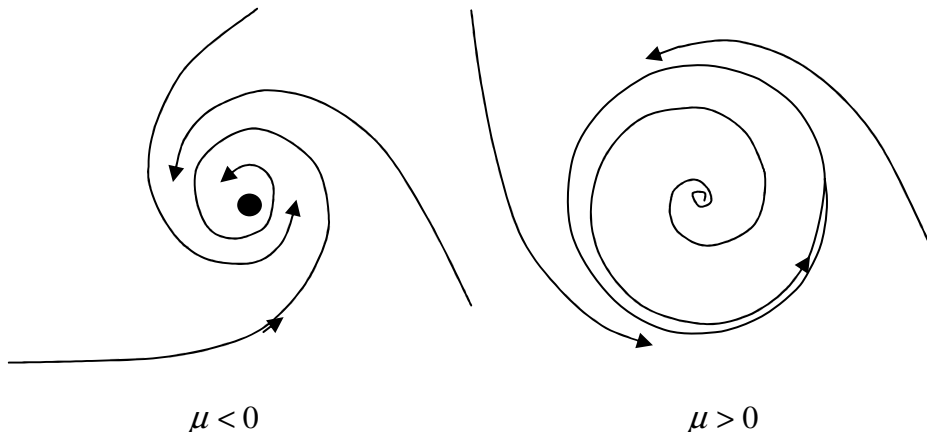


Figure 4.6 Phase portraits for μ above and below the bifurcation.

So as to see how the eigenvalues behave during the bifurcation, we rewrite the system in Cartesian coordinates; this makes it easier to find the Jacobian. We write $x = r \cos \theta$, $y = r \sin \theta$. Then

$$\begin{aligned}
 \dot{x} &= \dot{r} \cos \theta - r \dot{\theta} \sin \theta \\
 &= (\mu r - r^3) \cos \theta - r(\omega + br^2) \sin \theta \\
 &= (\mu - [x^2 + y^2])x - (\omega + b[x^2 + y^2])y \\
 &= \mu x - \omega y + \text{cubic terms}
 \end{aligned}$$

and similarly

$$\dot{y} = \omega x + \mu y + \text{cubic terms}.$$

So the Jacobian at the origin is

$$A = \begin{pmatrix} \mu & -\omega \\ \omega & \mu \end{pmatrix},$$

which has eigenvalues $\lambda = \mu \pm i\omega$.

As expected, the eigenvalues cross the imaginary axis from left to right as μ increases from negative to positive values.

4.2.1.1 Rules of thumb

Our idealized case illustrates two rules that hold *generically* for supercritical Hopf bifurcations:

1. The size of the limit cycle grows continuously from zero, and increases proportional to $\sqrt{\mu - \mu_c}$, for μ close to μ_c .
2. The frequency of the limit cycle is given approximately by $\omega = \text{Im } \lambda$, evaluated at $\mu = \mu_c$. This formula is exact at the birth of the limit cycle, and correct within $O(\mu - \mu_c)$ for μ close to μ_c . The period is therefore $T = (2\pi / \text{Im } \lambda) + O(\mu - \mu_c)$.

But our idealized example also has some artifactual properties. First, in Hopf bifurcations encountered in practice, the limit cycle is elliptical, not circular, and its shape becomes distorted as μ moves away from the bifurcation point. Our example is only typical topologically, not geometrically. Second, in our idealized case the eigenvalues move on horizontal lines as μ varies, i.e., $\text{Im } \lambda$ is strictly independent of μ .

Normally, the eigenvalues would follow a curvy path and cross the imaginary axis with nonzero slope. (Figure 4.7)

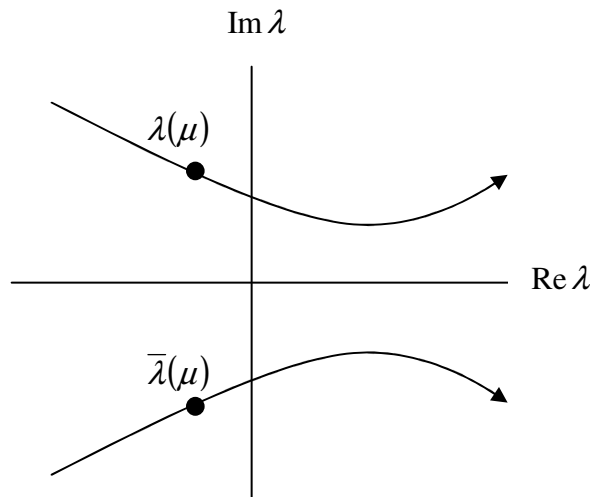


Figure 4.7 Rules of thumb.

4.2.2 Subcritical hopf bifurcation

Like pitchfork bifurcations, Hopf bifurcations come in both super- and subcritical varieties. The subcritical case is always much more dramatic, and potentially dangerous in engineering applications. After the bifurcation, the trajectories must *jump* to a *distant* attractor, which may be a fixed point, another limit cycle, infinity, or –in three and higher dimensions –a chaotic attractor. Consider the two-dimensional example

$$\dot{r} = \mu r - r^3 - r^5$$

$$\dot{\theta} = \omega + br^2.$$

The important difference from the earlier supercritical case is that the cubic term r^3 is now *destabilizing*; it helps to drive trajectories away from the origin.

The phase portraits are shown in Figure 4.8. For $\mu < 0$ there are two attractors, a stable limit cycle and a stable fixed point at the origin. Between them lies an unstable cycle, shown as a dashed curve in Figure 4.8.; it is the player to watch in this scenario. As μ increases, the unstable cycle tightens like a noose around the fixed point. A ***subcritical Hopf bifurcation*** occurs at $\mu = 0$, where the unstable cycle shrinks to zero amplitude and engulfs the origin, rendering it unstable. For $\mu > 0$, the large-amplitude limit cycle is suddenly the only attractor in town. Solutions that used to remain near the origin are now forced to grow into large-amplitude oscillations.

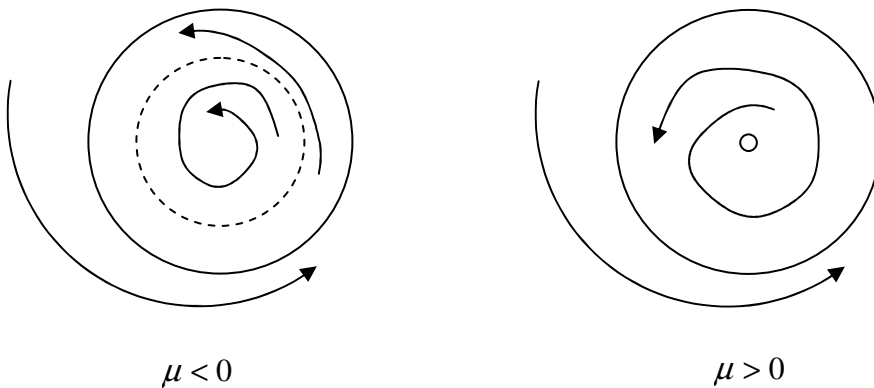


Figure 4.8 Phase portraits of the Hopf bifurcation example.

Note that the system exhibits *hysteresis*: one large-amplitude oscillations have begun; they cannot be turned off by bringing μ back to zero. In fact, the large oscillations will persist until $\mu = -1/4$ where the stable and unstable cycles collide and annihilate. This destruction of the large amplitude cycle occurs via another type of bifurcation.

Subcritical Hopf bifurcations occur in the dynamics of nerve cells, in aero-elastic flutter and other vibrations of airplane wings, and instabilities of fluid flows.

4.2.3 Subcritical, Supercritical, or Degenerate Bifurcation

Given that a Hopf bifurcation occurs, how can we tell if it is sub- or supercritical? The linearised does not provide a distinction: in both cases, a pair of eigenvalues moves from the left to the right half-plane.

An analytical criterion exists, but it can be difficult to use. A quick and dirty approach is to use the computer. If a small, attracting limit cycle appears immediately after the fixed point goes unstable, and if its amplitude shrinks back to zero as the parameter is reversed, the bifurcation is supercritical; otherwise, it is probably subcritical, in which case the nearest attractor might be far from the fixed point, and the system may exhibit hysteresis as the parameter is reversed. Of course, computer experiments are not proofs and you should check the numerics carefully before making any firm conclusions.

Finally a *degenerate Hopf bifurcation* should also be informed. An example is given by the damped pendulum $x'' + \mu x' + \sin x = 0$. As the damping μ is changed from positive to negative, the fixed point at the origin changes from a stable to an unstable spiral. However at $\mu = 0$ a continuous band of closed orbits surrounding the origin is observed. These are not limit cycles.

This degenerate case typically arises when a non-conservative system suddenly becomes conservative at the bifurcation point. Then the fixed point becomes a nonlinear center, rather than the weak spiral required by a Hopf bifurcation.

- Consider the system $x' = \mu x - y + xy^2$, $y' = x - \mu y + y^3$. Show that a Hopf bifurcation occurs at the origin as μ varies. Is the bifurcation subcritical, supercritical, or degenerate?

The Jacobean at the origin is $A = \begin{pmatrix} \mu & -\omega \\ \omega & \mu \end{pmatrix}$, which has $\tau = 2\mu$, $\Delta = \mu^2 + 1 > 0$, and $\lambda = \mu \pm i$. Hence, as μ increases through zero, the origin changes from a stable spiral to an unstable spiral. This suggests that some kind of Hopf bifurcation takes place at $\mu = 0$.

In order to decide whether the bifurcation is subcritical, supercritical, or degenerate, we use simple reasoning and numerical integration. If we transform the system to polar coordinates, we find that

$$r' = \mu r + r y^2$$

as you should check. Hence $r' = \mu r$. This implies that for $\mu > 0$, $r(t)$ grows *at least* as fast as $r_0 e^{\mu t}$. In other words, all trajectories are repelled out to infinity. So there are certainly no closed orbits for $\mu > 0$. In particular, the unstable spiral is not surrounded by a stable limit cycle; hence the bifurcation cannot be supercritical.

Could the bifurcation be degenerate? That would require that the origin be a nonlinear center when $\mu = 0$. But r is strictly positive away from the x -axis, so closed orbits are still impossible.

By process of elimination, we expect that the bifurcation is *subcritical*. This is confirmed, which is a computer-generated phase portrait for $\mu = -0.2$ [Strogatz, 1994].

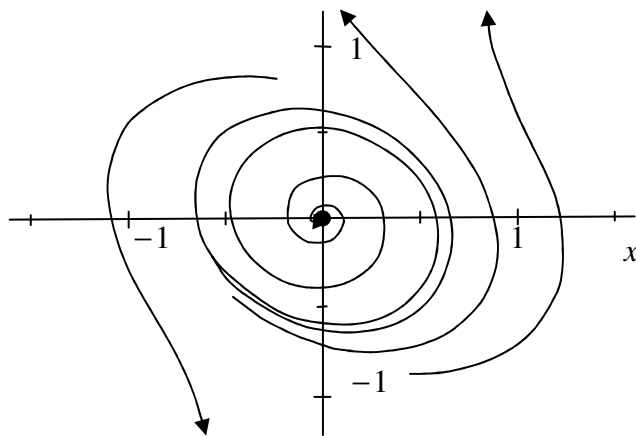


Figure 4.9 Computer generated phase portrait.

Note that an *unstable* limit cycle surrounds the stable fixed point, just as expected in a subcritical bifurcation. Furthermore, the cycle is nearly elliptical and surrounds a gently winding spiral –these are typical features of either kind of Hopf bifurcation.

5.0 APPLICATIONS

5.1 Chemical Pattern Formation of Gray-Scott Model

5.1.3 Introduction to Gray-Scott Model

We consider the Gray-Scott model corresponding to the following two hypothetical chemical reactions



i.e., agent U reacts with two parts of agent V to form three units of V , which are subsequently converted into a precipitate P . U is fed into the reaction at a constant feed rate F and the precipitate is removed. We shall henceforth denote the concentrations of the agents U and V by u and v , respectively.

If the concentrations of the reagents were spatially uniform then the change in the concentration of agent U would be simply

$$\frac{du}{dt} = -uv^2 + F(1-u).\tag{5.2}$$

Since the amount of U removed per time unit is proportional to uv^2 and the amount of u added per time unit is proportional to the feed

rate F and $1-u$, assuming that 1 is the saturation concentration of U . Similarly, we would have

$$\frac{dv}{dt} = uv^2 - (F + k)v \quad (5.3)$$

where k is the rate constant of the 2nd reaction.

5.1.4 Linear Stability Analysis

The reaction diffusion equations (5.4) form a set of coupled non-linear PDE's. We shall first investigate the equilibria and stability of the system. Neglecting the diffusion terms, the system is in a steady state if

$$\begin{aligned} 0 &= -uv^2 + F(1-u) \\ 0 &= +uv^2 - (F + k)v \end{aligned} \quad (5.4)$$

Adding these equations leads to

$$\begin{aligned} F(1-u) &= (F + k)v \\ v^* &= \frac{F}{F + k}(1-u^*). \end{aligned}$$

Plugging the last expression back into (5.4) and setting $\delta = \frac{F + k}{F}$

gives

$$(1 - u^*)((u^*)^2 - u^* + \delta^2 F) = 0.$$

The solutions of this equation are $u^* = 1$ and

$$u^* = \frac{1}{2} \left(1 \pm \sqrt{1 - 4\delta^2 F} \right). \quad (5.5)$$

The corresponding values for v are $v^* = 0$ and

$$v^* = \frac{1}{2\delta} \left(1 \mp \sqrt{1 - 4\delta^2 F} \right), \quad (5.6)$$

respectively. The trivial solution $u = 1$ and $v = 0$ exists for any value of F and k , but the other two steady states exist only when

$$1 - 4\delta^2 F \geq 0 \quad \Leftrightarrow \quad (k + F) \leq F/4 \quad (5.7)$$

i.e., saddle node bifurcation occurs when

$$k_c = -F + \frac{1}{2}\sqrt{F}, \quad 0 \leq F \leq \frac{1}{4} \quad (5.8)$$

If the concentrations are not spatially uniform then u and v depend not only on time but also on the spatial coordinates, i.e., we have $u = u(x; y; z; t)$ and $v = v(x; y; z; t)$ and we must account for changes in the spatial dependence of the concentrations due to diffusion, i.e., our evolution equations for the system become

$$\begin{aligned}\frac{\partial u}{\partial t} &= D_u \nabla^2 u - uv^2 + F(1-u) \\ \frac{\partial v}{\partial t} &= D_v \nabla^2 v + uv^2 - (F+k)v\end{aligned}\tag{5.9}$$

where D_u and D_v are the dimensionless diffusion coefficients of U and V , respectively.

In order to analyze the stability of these equilibria, let u^* and v^* be one of the steady-state solutions of (5.9). If we perturb this solution as in the follow:

Let's say $f_1(u, v) = uv^2$ then,

$$\begin{aligned}f_1(u, v) &= f_1(u^*, v^*) + \left. \frac{\partial f_1}{\partial u} \right|_* (u - u^*) + \left. \frac{\partial f_1}{\partial v} \right|_* (v - v^*) \\ f_1(u, v) &= u^* (v^*)^2 + (v^*)^2 (u - u^*) + 2u^* v^* (v - v^*)\end{aligned}$$

where $u - u^* = \bar{u}$ and $v - v^* = \bar{v}$.

$$f_1(u, v) = u^* (v^*)^2 + (v^*)^2 \bar{u} + 2u^* v^* \bar{v}.$$

By using $f_1(u, v)$, we can write

$$\frac{\partial \bar{u}}{\partial t} = D_u \nabla^2 \bar{u} - u^* (v^*)^2 - (v^*)^2 \bar{u} - 2u^* v^* \bar{v} + F - F(u^* + \bar{u}) + O(\varepsilon)$$

$$\frac{\partial \bar{u}}{\partial t} = D_u \nabla^2 \bar{u} - \left((v^*)^2 + F \right) \bar{u} - 2u^* v^* \bar{v} - u^* (v^*)^2 - F u^* + F + O(\varepsilon)$$

According to Equation (5.4); $-u^* (v^*)^2 - F u^* + F = 0$.

$$\frac{\partial \bar{v}}{\partial t} = D_v \nabla^2 \bar{v} + u^* (v^*)^2 + (v^*)^2 \bar{u} + 2u^* (v^*)^2 \bar{v} - (F + k)(v^* + \bar{v}) + O(\varepsilon)$$

$$\frac{\partial \bar{v}}{\partial t} = D_v \nabla^2 \bar{v} - (F + k - 2u^* v^*) \bar{v} - (v^*)^2 \bar{u} + u^* (v^*)^2 - (F + k)v^* + O(\varepsilon)$$

Again according to Equation (5.4); $u^* (v^*)^2 - (F + k)v^* = 0$. As a result:

$$\begin{aligned} \frac{\partial \bar{u}}{\partial t} &= D_u \nabla^2 \bar{u} - \left((v^*)^2 + F \right) \bar{u} - 2u^* v^* \bar{v} + O(\varepsilon) \\ \frac{\partial \bar{v}}{\partial t} &= D_v \nabla^2 \bar{v} - (F + k - 2u^* v^*) \bar{v} - (v^*)^2 \bar{u} + O(\varepsilon) \end{aligned} \quad (5.10)$$

Making the ansatz

$$\bar{u} = u_0 e^{\lambda t - i(k_1 x + k_2 y)}, \quad \bar{v} = v_0 e^{\lambda t - i(k_1 x + k_2 y)} \quad (5.11)$$

where u_0 and v_0 are the perturbation amplitudes and k_1 and k_2 are the wave numbers for the variations in the x and y direction, respectively.

Equation (5.10) leads to the eigenvalue problem

$$\begin{aligned}\frac{\partial \bar{u}}{\partial t} &= D_u \left(\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} \right) - \left((v^*)^2 + F \right) \bar{u} - 2u^* v^* \bar{v} + O(\varepsilon) \\ \frac{\partial \bar{v}}{\partial t} &= D_v \left(\frac{\partial^2 \bar{v}}{\partial x^2} + \frac{\partial^2 \bar{v}}{\partial y^2} \right) - \left(F + k - 2u^* v^* \right) \bar{v} - (v^*)^2 \bar{u} + O(\varepsilon)\end{aligned}$$

By the derivation:

$$\begin{aligned}\frac{\partial \bar{u}}{\partial t} &= D_u \left(\bar{u} k_1^2 i^2 + \bar{u} k_2^2 i^2 \right) - \left((v^*)^2 + F \right) \bar{u} - 2u^* v^* \bar{v} + O(\varepsilon) \\ \frac{\partial \bar{v}}{\partial t} &= D_v \left(\bar{v} k_1^2 i^2 + \bar{v} k_2^2 i^2 \right) - \left(F + k - 2u^* v^* \right) \bar{v} - (v^*)^2 \bar{u} + O(\varepsilon)\end{aligned}$$

$$\begin{aligned}\frac{\partial \bar{u}}{\partial t} &= -D_u \left(k_1^2 + k_2^2 \right) \bar{u} - \left((v^*)^2 + F \right) \bar{u} - 2u^* v^* \bar{v} + O(\varepsilon) \\ \frac{\partial \bar{v}}{\partial t} &= -D_v \left(k_1^2 + k_2^2 \right) \bar{v} - \left(F + k - 2u^* v^* \right) \bar{v} - (v^*)^2 \bar{u} + O(\varepsilon)\end{aligned}$$

If we set $\kappa^2 = k_1^2 + k_2^2$

$$\begin{aligned}\frac{\partial \bar{u}}{\partial t} &= -D_u \left(\kappa^2 - (v^*)^2 - F \right) \bar{u} - 2u^* v^* \bar{v} + O(\varepsilon) \\ \frac{\partial \bar{v}}{\partial t} &= \left(-D_v - F - k + 2u^* v^* \right) \bar{v} - (v^*)^2 \bar{u} + O(\varepsilon)\end{aligned}$$

$$\begin{bmatrix} \bar{u} \\ \bar{v} \end{bmatrix} = \begin{bmatrix} -D_u \kappa^2 - (v^*)^2 - F & -2u^* v^* \\ -(v^*)^2 & -D_v \kappa^2 - F - k + 2u^* v^* \end{bmatrix} \begin{bmatrix} \bar{u} \\ \bar{v} \end{bmatrix}$$

$$\det \begin{bmatrix} -D_u \kappa^2 - (v^*)^2 - F - \lambda & -2u^* v^* \\ -(v^*)^2 & -D_v \kappa^2 - F - k + 2u^* v^* - \lambda \end{bmatrix} = 0 \quad (5.12)$$

$$\left(-D_u \kappa^2 - (v^*)^2 - F - \lambda\right) \left(-D_v \kappa^2 - F - k + 2u^* v^* - \lambda\right) - 2u^* (v^*)^3 = 0$$

$$\lambda^2 + \left(D_u \kappa^2 + (v^*)^2 + F + D_v \kappa^2 + F + k - 2u^* v^*\right) \lambda + \left(-D_u \kappa^2 - (v^*)^2 - F\right) \left(D_v \kappa^2 - F - k + 2u^* v^* - \lambda\right) - 2u^* (v^*)^3 = 0$$

This is a quadratic equation $\lambda^2 + p\lambda + q = 0$ with

$$p = (D_u + D_v) \kappa^2 + 2F + k + (v^*)^2 - 2u^* v^*$$

$$q = \left(D_u \kappa^2 + (v^*)^2 + F\right) \left(D_v \kappa^2 + F + k - 2u^* v^*\right) - 2u^* (v^*)^3$$

$$\lambda_1 = -\left(\frac{p + \sqrt{p^2 - 4q}}{2}\right), \quad \lambda_2 = -\left(\frac{p - \sqrt{p^2 - 4q}}{2}\right)$$

For the trivial steady state $u^* = 1, v^* = 0$.

$$p = (D_u + D_v) \kappa^2 + 2F + k$$

$$q = \left(D_u \kappa^2 + F\right) \left(D_v \kappa^2 + F + k\right)$$

$$\lambda_1 = -\frac{p + \sqrt{p^2 + 4q}}{2}$$

$$\lambda_1 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k + \left[\begin{aligned} &(D_u^2 + 2D_u D_v + D_v^2) \kappa^4 + 4F^2 + k^2 + \\ &4(D_u + D_v) F \kappa^2 + 4Fk + 2(D_u + D_v) k \kappa^2 \\ &- 4D_u \kappa^4 D_v - 4D_u \kappa^2 F - 4D_u \kappa^2 k - \\ &4FD_v \kappa^2 - 4F^2 - 4Fk \end{aligned} \right]^{\frac{1}{2}}}{2}$$

$$\lambda_1 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k + \left[\begin{aligned} &D_u^2 \kappa^4 + 2D_u D_v \kappa^4 + D_v^2 \kappa^4 + 4F^2 \\ &+ k^2 + 4D_u F \kappa^2 + D_v F \kappa^2 + 4Fk \\ &+ 2D_u k \kappa^2 + 2D_v k \kappa^2 - 4D_u \kappa^4 D_v \\ &- 4D_u \kappa^2 F - 4D_u \kappa^2 k - 4FD_v \kappa^2 \\ &- 4F^2 - 4Fk \end{aligned} \right]^{\frac{1}{2}}}{2}$$

$$\lambda_1 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k + \left[\begin{aligned} &D_u^2 \kappa^4 + D_v^2 \kappa^4 + k^2 + 2D_v k \kappa^2 \\ &- 2D_u D_v \kappa^4 - 2D_u \kappa^2 k \end{aligned} \right]^{\frac{1}{2}}}{2}$$

$$\lambda_1 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k + \left[\begin{aligned} &k^2 + (D_u^2 + D_v^2 - D_u D_v) \kappa^4 + \\ &2(D_v - D_u) k \kappa^2 \end{aligned} \right]^{\frac{1}{2}}}{2}$$

$$\lambda_1 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k + \left[\begin{aligned} &k^2 + 2k \kappa^2 (D_v - D_u) + \\ &(\kappa^2 (D_v - D_u))^2 \end{aligned} \right]^{\frac{1}{2}}}{2}$$

$$\lambda_1 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k + \left[k + \kappa^2 (D_v - D_u)^2 \right]^{\frac{1}{2}}}{2}$$

$$\lambda_1 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + 2k + \kappa^2 D_v - \kappa^2 D_u}{2}$$

$$\lambda_1 = -\frac{2D_v \kappa^2 + 2F + 2k}{2} = -D_v \kappa^2 + F + k$$

$$\therefore \lambda_1 = -D_v \kappa^2 + F + k$$

$$\lambda_2 = -\frac{p - \sqrt{p^2 + 4q}}{2}$$

$$\lambda_2 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k - \left[\begin{aligned} &(D_u^2 + 2D_u D_v + D_v^2) \kappa^4 + 4F^2 + \\ &k^2 + 4(D_u + D_v) F \kappa^2 + 4Fk \\ &+ 2(D_u + D_v) k \kappa^2 - 4D_u \kappa^4 D_v - \\ &4D_u \kappa^2 F - 4D_u \kappa^2 k - 4FD_v \kappa^2 \\ &- 4F^2 - 4Fk \end{aligned} \right]^{\frac{1}{2}}}{2}$$

$$\lambda_2 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k - \left[\begin{aligned} &D_u^2 \kappa^4 + 2D_u D_v \kappa^4 + D_v^2 \kappa^4 + 4F^2 \\ &+ k^2 + 4D_u F \kappa^2 + D_v F \kappa^2 + 4Fk \\ &+ 2D_u k \kappa^2 + 2D_v k \kappa^2 - 4D_u \kappa^4 D_v \\ &- 4D_u \kappa^2 F - 4D_u \kappa^2 k - 4FD_v \kappa^2 \\ &- 4F^2 - 4Fk \end{aligned} \right]^{\frac{1}{2}}}{2}$$

$$\lambda_2 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k - \left[D_u^2 \kappa^4 + D_v^2 \kappa^4 + k^2 + 2D_v k \kappa^2 \right]^{\frac{1}{2}}}{2}$$

$$\lambda_2 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k - \left[k^2 + (D_u^2 + D_v^2 - D_u D_v) \kappa^4 \right]^{\frac{1}{2}}}{2}$$

$$\lambda_2 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k - \left[k^2 + 2k \kappa^2 (D_v - D_u) \right]^{\frac{1}{2}}}{2}$$

$$\lambda_2 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k - \left[k + \kappa^2 (D_v - D_u)^2 \right]^{\frac{1}{2}}}{2}$$

$$\lambda_2 = -\frac{D_u \kappa^2 + D_v \kappa^2 + 2F + k - k - \kappa^2 D_v + \kappa^2 D_u}{2}$$

$$\lambda_2 = -\frac{2D_u \kappa^2 + 2F}{2} = -D_u \kappa^2 - F$$

$$\therefore \lambda_2 = -D_u \kappa^2 - F$$

i.e., both eigenvalues are negative. Hence the trivial steady states is a stable equilibrium for all values of k and F .

For the other steady states $u^* = \frac{1}{2} \left(1 \pm \sqrt{1 - 4\delta^2 F} \right)$ and

$v^* = \frac{1}{2\delta} \left(1 \mp \sqrt{1 - 4\delta^2 F} \right)$, we observe that we have

$$u^* v^* = \frac{1}{4\delta} (1 - (1 - 4\delta^2 F)) = \delta F = F + k$$

$$(v^*)^2 = \frac{1}{4\delta^2} (1 \mp 2\sqrt{1 - 4\delta^2 F} + 1 - 4\delta^2 F) = \frac{1}{\delta} v^* - F.$$

Thus, neglecting the diffusion terms, the eigenvalue equation for these two fixed points becomes

$$0 = \lambda^2 + \lambda \left(\frac{v^*}{\delta} - F - k \right) - \frac{v^*}{\delta} + (F + k) - \left(\frac{v^*}{\delta} - F \right) 2(F + k).$$

The system undergoes a Hopf bifurcation when the real part of λ vanishes, i.e., when

$$\frac{1}{\delta} v^* - F - k = 0$$

and

$$-\frac{v^*}{\delta} + (F + k) - \left(\frac{v^*}{\delta} - F \right) 2(F + k) > 0.$$

Algebraic simplifications show that this bifurcation occurs when

$$F_c = \frac{\sqrt{k} - 2k - \sqrt{(2k - \sqrt{k})^2 - 4k^2}}{2} \quad (5.13)$$

and $0 \leq k \leq k_c$.

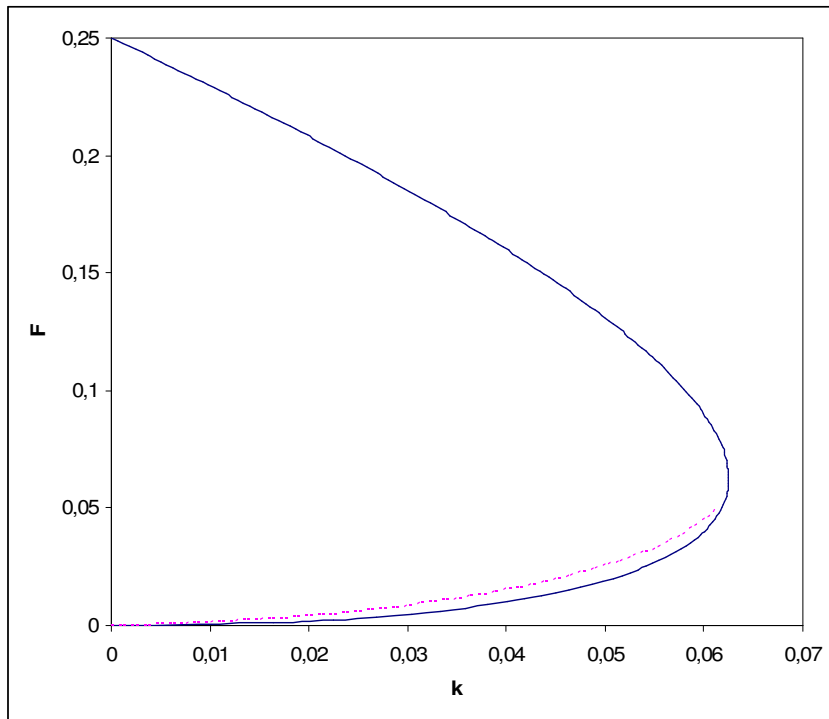


Figure 5.1 Bifurcation diagram of F versus k .

In reactor dynamics it is particularly important to find out if multiple stationary points exist or if sustained oscillations can arise. Bifurcation analysis is aimed at locating the set of parameter values for which multiple steady states will occur. We apply bifurcation analysis to learn whether or not multiple steady states are possible. A *bifurcation point* is a point at which two branches of a curve coalesce as a parameter is varied.

Figure 5.1 shows the bifurcation diagram. The solid line represents the saddle node bifurcation. For parameter values outside the region bounded by this curve, there exists only the trivial, linearly stable

equilibrium. As the solid line is crossed from above, the system undergoes a saddle node bifurcation and two additional steady states are born. One is stable and the other is unstable. As the dashed line is crossed from above, the nontrivial stable equilibrium loses its stability in a Hopf bifurcation and a stable limit cycle is born. Finally, as the solid line is crossed again, the two non-trivial equilibria collide leaving only the stable trivial steady state.

In practice, designs near the bifurcation points are dangerous, since changing operating conditions or uncertain design parameters can lead to behaviour that is different from the expected one. Such a design, close to the fold (saddle-node) point, can suffer from serious operability problems. If the reaction rate constant overestimated, or the feed flow rate deviates from the nominal design value, the operating point falls. In this case infinite reactant accumulation occurs.

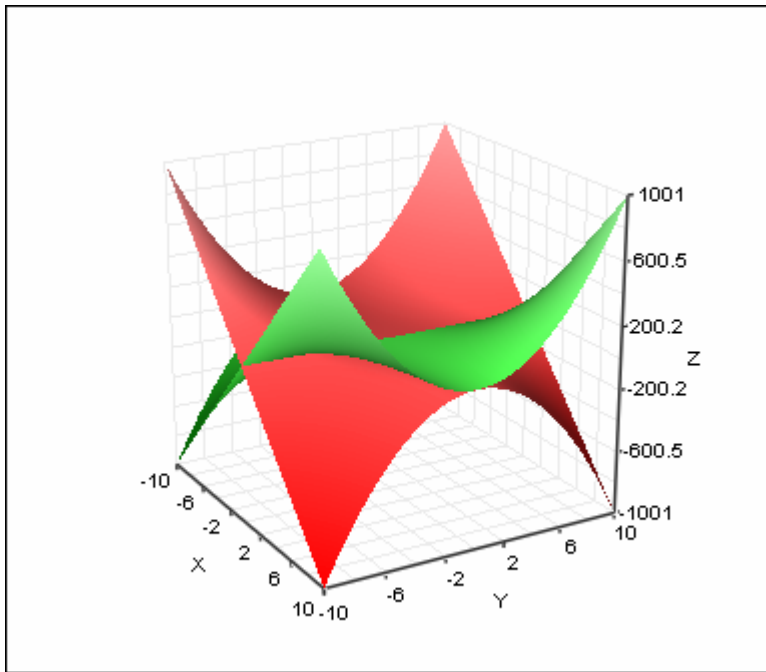


Figure 5.2 Bifurcation diagram in 3-D.

5.2 Dynamical Analysis of Brusselator

5.2.1 Equations

The dynamics of the Brusselator reaction can be described by a system of two ODE's. In dimensionless form, they are:

$$x' = 1 - (b + 1)x + ax^2y \quad (5.14)$$

$$y' = bx - ax^2y \quad (5.15)$$

where $x, y \in \Re$ and $a, b \in \Re$ are constants with $a, b > 0$. x and y represent the dimensionless concentrations of two of the reactants.

5.2.2 Equilibria

The equilibria of (5.14) and (5.15) are given by solving the system,

$$1 - (b+1)x + ax^2y = 0 \quad (5.16)$$

$$bx - ax^2y = 0 \quad (5.17)$$

Adding (5.15) and (5.16) and simplifying;

$$1 - bx - x + ax^2y = 0 \quad (5.18)$$

$$bx - ax^2y = 0$$

gives $x = 1$. Plugging $x = 1$ into (5.17) gives $y = b/a$. Hence $(1, b/a)$ is the equilibrium of the system, and in fact, the only equilibrium of the system.

5.2.3 Stability

Compute the Jacobean of the system:

$$\mathbf{J} = \begin{bmatrix} -b-1+2axy & ax^2 \\ b-2axy & -ax^2 \end{bmatrix} \quad (5.19)$$

Evaluated at $(x, y) = (1, b/a)$,

$$\mathbf{J} = \begin{bmatrix} b-1 & a \\ -b & -a \end{bmatrix} \quad (5.20)$$

So as to analyze the stability, we compute the trace and the determinant of (5.20)

$$\tau = \text{Trace} \left(\mathbf{J} \left(1, \frac{b}{a} \right) \right) = b - a - 1 \quad (5.21)$$

$$\Delta = \det \left| \mathbf{J} \left(1, \frac{b}{a} \right) \right| = a \quad (5.22)$$

$\Delta > 0$, since $a > 0$, which implies that $(1, b/a)$ is not a saddle point. If $b < 1 + a^2$, then $\tau < 0$, and the equilibrium is an attractor. If $b > 1 + a^2$, then $\tau > 0$, and it is a repellor. (Strogatz, 1994) (See Figure 5.3)

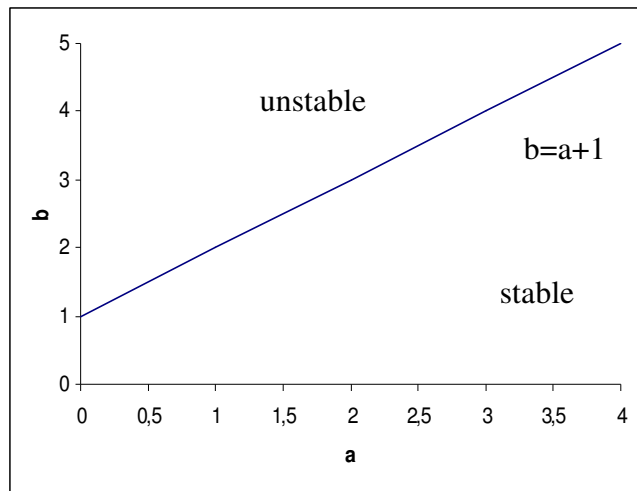


Figure 5.3 Stability analysis in parameter space.

5.2.4 Nullclines

Compute the x' -nullcline by setting $x' = 0$

$$1 - (b+1)x + ax^2y = 0$$

$$y = \frac{(b+1)x - 1}{ax^2} \quad (5.23)$$

Compute the y' -nullcline by setting $y' = 0$

$$bx - ax^2y = 0$$

$$x(b - axy) = 0$$

$$x = 0 \text{ or } y = \frac{b}{ax} \quad (5.24)$$

This nullcline consists of the y -axis and a hyperbola. For $(a,b) = (1,2.5)$ the nullclines are shown in Figure 5.4.

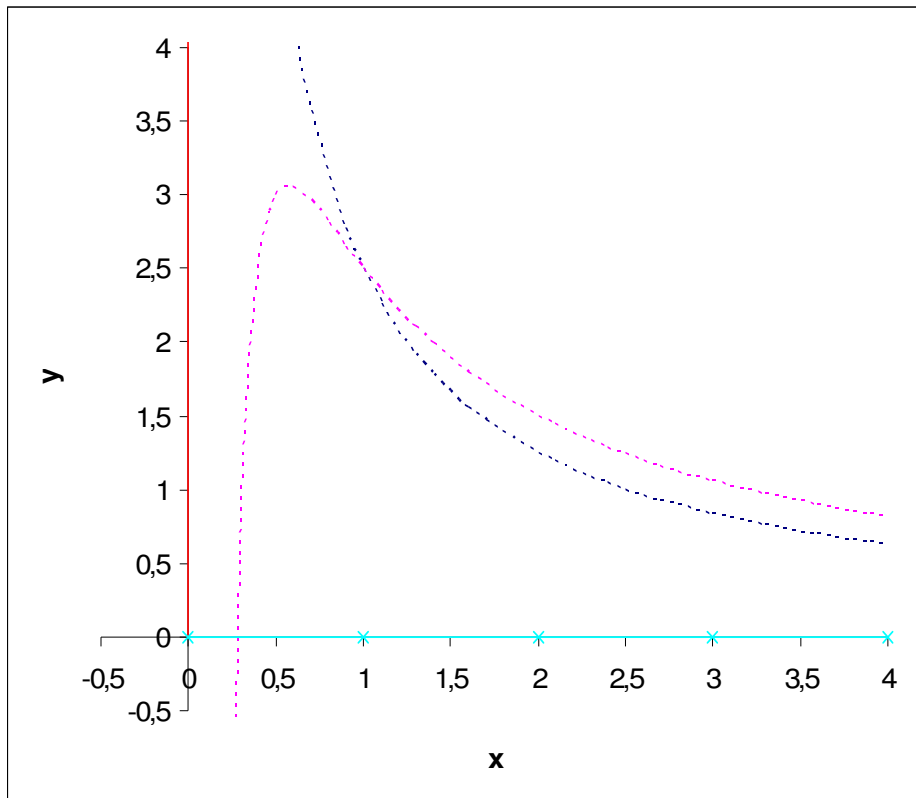


Figure 5.4 Nullclines for $(a,b) = (1,2.5)$.

5.2.5 Bifurcation Analysis

First, fix a constant. As b varies, the equilibrium $(1, b/a)$ undergoes a change in stability. Since there are no other equilibria in the system, it is reasonable to guess that a Hopf bifurcation occurs at $b_c = a + 1$. To prove this conjecture, we need to:

1. Show that the eigenvalues of (5.20) are pure imaginary and non-zero at $b_c = a + 1$, and
2. Show that the rate of change of the real part of the eigenvalues is non-zero at $b_c = a + 1$.

The eigenvalues of (5.20) will be pure imaginary and non-zero if and only if and only if $\tau^2 - 4\Delta < 0$. From (5.21), $\tau = b - a - 1$. But, at $b_c = a + 1$, τ vanishes. From (5.22), $\Delta = a$. Thus, $\tau^2 - 4\Delta = -4a < 0$, as required.

For an eigenvalue, λ , $\text{Re}(\lambda) = \frac{1}{2}\tau$. Since we fix a , we need

$$\frac{\partial \text{Re}(\lambda)}{\partial b} \neq 0.$$

$$\frac{\partial \text{Re}(\lambda)}{\partial b} = \frac{1}{2} \frac{\partial}{\partial b} [b - a - 1] = \frac{1}{2} \neq 0,$$

As required. Hence, bifurcation occurs at $b_c = a + 1$.

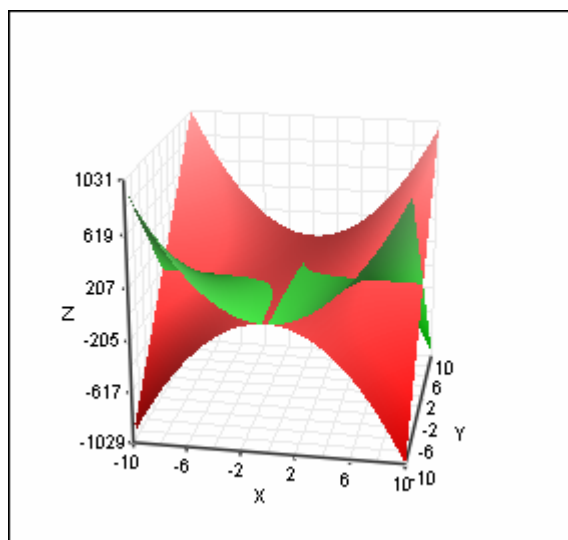
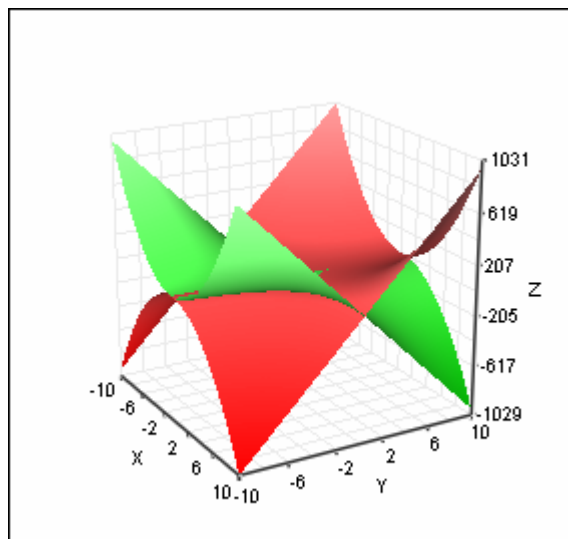


Figure 5.5 The bifurcation diagrams of the Brusselator.

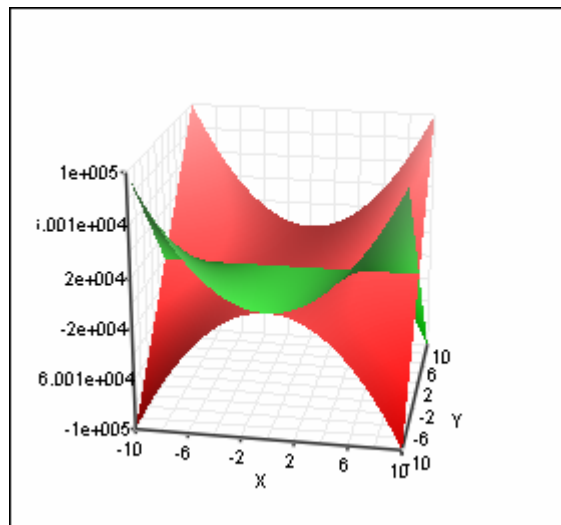
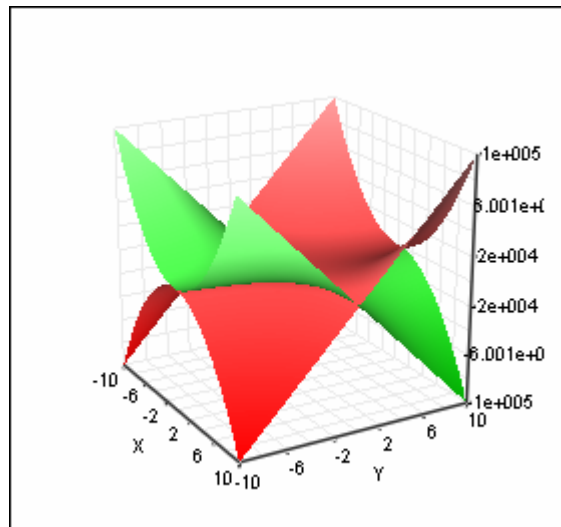


Figure 5.6 The bifurcation diagrams for $b < a + 1$.

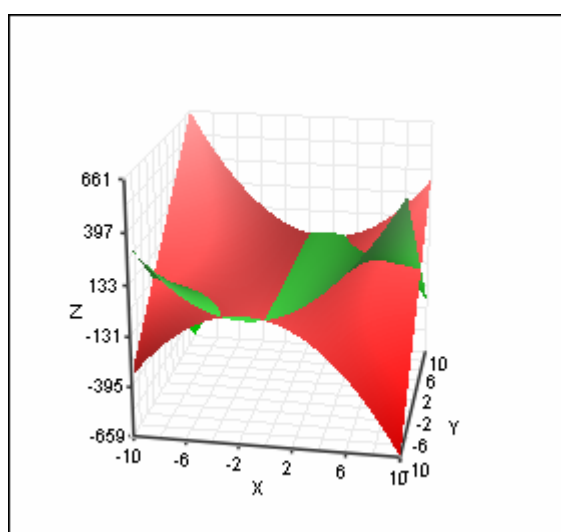
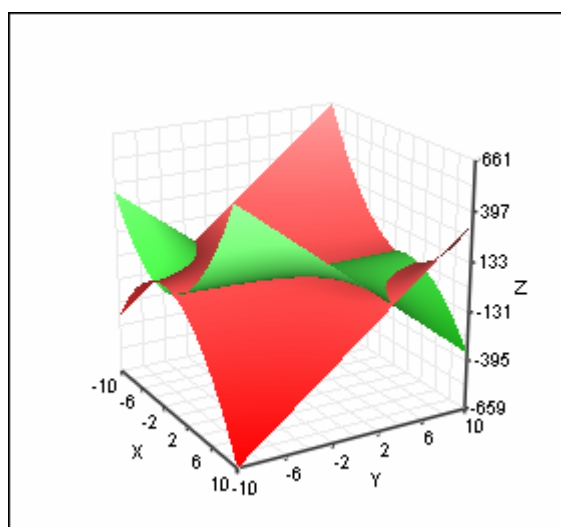


Figure 5.7 The bifurcation diagrams for $b > a + 1$.

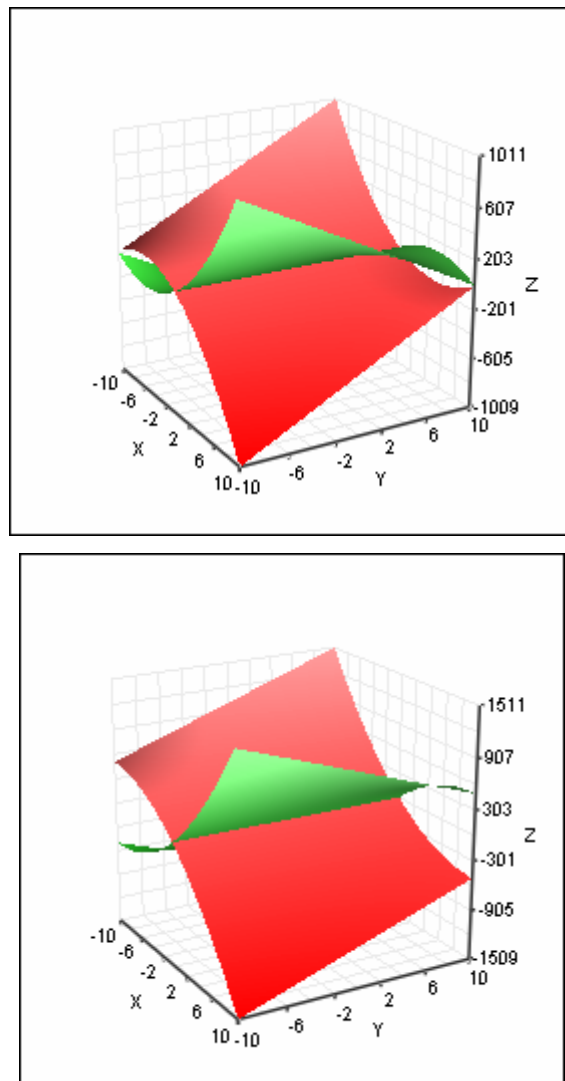


Figure 5.8 The bifurcation diagrams (continuing to increase b value).

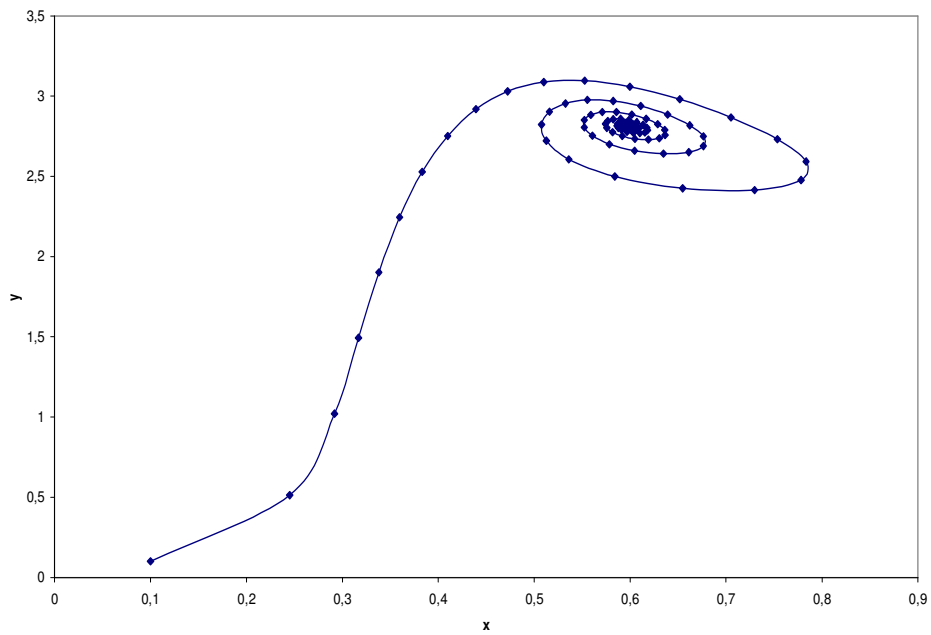


Figure 5.9 x-y graph for $a = 1$ & $b = 2.5$.

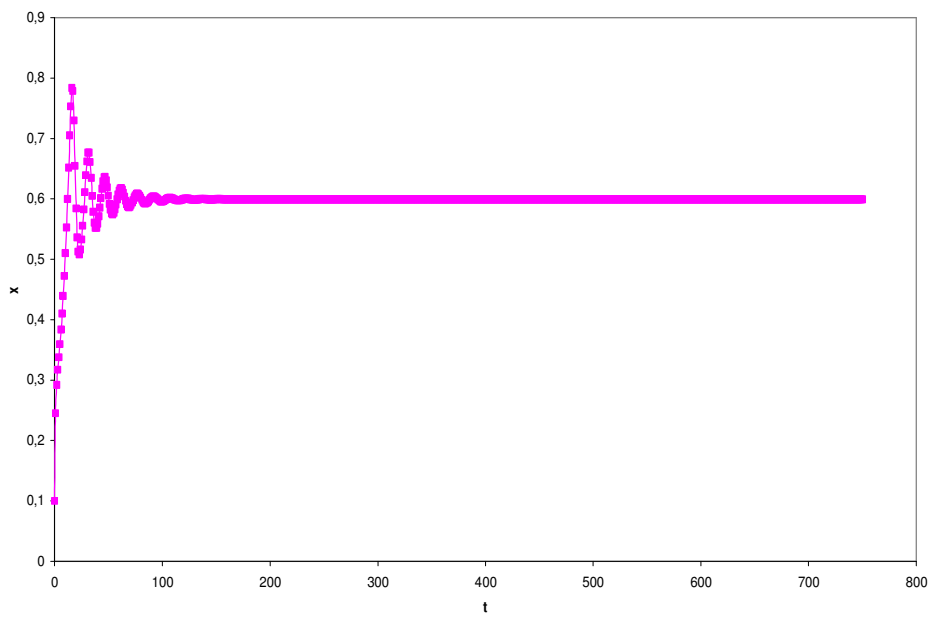


Figure 5.10 x-t graph for $a = 1$ & $b = 2.5$.

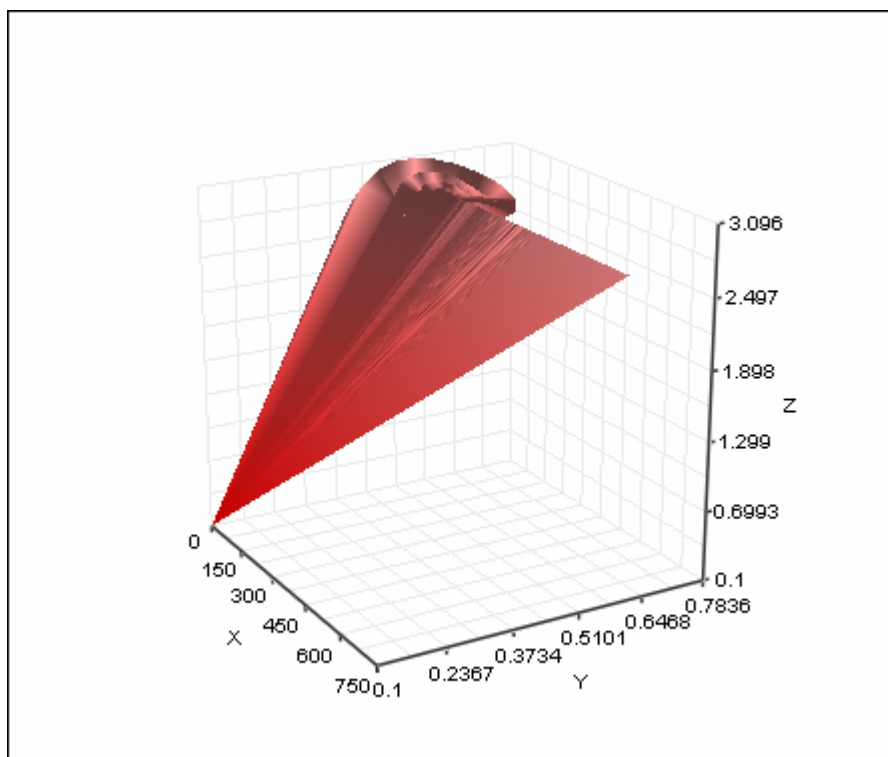


Figure 5.11 t-x-y graph for $a = 1$ & $b = 2.5$.

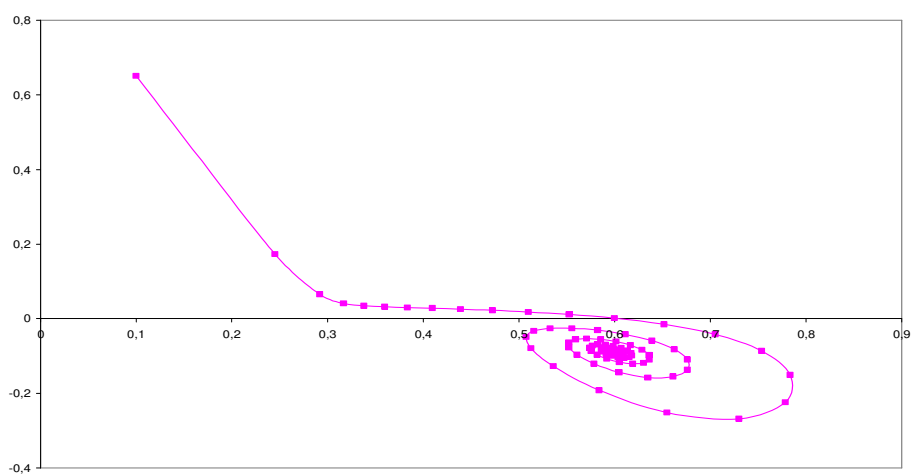
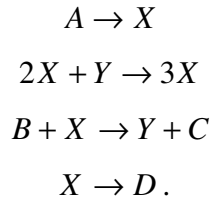


Figure 5.12 $x' - x$ graph for $a = 1$ & $b = 2.5$.

5.3 Stability Analysis of Reaction Diffusion Equations

The mechanism for the Brusselator



The two species of interest us are X and Y , the autocatalytic species. In dimensionless form, the Brusselator ODEs are

$$x' = a - bx + x^2y - x, \quad (5.25)$$

$$y' = bx - x^2y. \quad (5.26)$$

At equilibrium,

$$x' = a - bx + x^2y - x = 0 \quad (5.27)$$

$$y' = bx - x^2y = 0 \quad (5.28)$$

This model has a single equilibrium point at $(x^*, y^*) = (a, b/a)$.

If we want to study the reaction-diffusion version of this model, we just add diffusion terms to the two equations. We can immediately obtain a dimensionless form by setting one of the diffusion coefficients to unity:

$$\frac{\partial x}{\partial t} = \frac{\partial^2 x}{\partial z^2} + a - bx + x^2 y - x \quad (5.29)$$

$$\frac{\partial y}{\partial t} = D \frac{\partial^2 y}{\partial z^2} + bx - x^2 y \quad (5.30)$$

Here, z is our spatial variable, while D is the relative diffusion coefficient of Y , i.e. the ratio of Y to D_x . Note that the steady state of the well-mixed model is also a steady state of the reaction-diffusion model: If $(x, y) = (x^*, y^*)$, then the spatial derivatives of this constant function are zero, as are the reaction terms, so the time derivatives must be zero too. This solution is called the **homogeneous steady state**. Analyzing the stability of the homogeneous steady state assumes that the boundary conditions are consistent with this steady state.

In order to linearise these equations, let

$$x = \delta x + x^* = \delta x + a \quad (5.31)$$

$$y = \delta y + y^* = \delta y + b/a. \quad (5.32)$$

Here, δx and δy are the displacements from equilibrium, which now depend *both* on time and space. As usual, we will ask what happens when δx and δy are small. Because the above definitions are linear in δx and δy , we have

$$\frac{\partial x}{\partial t} = \frac{\partial(\delta x)}{\partial t}, \quad \frac{\partial^2 x}{\partial z^2} = \frac{\partial^2(\delta x)}{\partial z^2}, \quad \text{etc.}$$

The linearization of the reaction terms is just $\mathbf{J}^*[\delta x \quad \delta y]^T$, where $\mathbf{J}^*$ is the Jacobean evaluated at the equilibrium point, and the superscripted T represents the transpose operation. Thus we have the linearised equation

$$\frac{\partial}{\partial t} \begin{bmatrix} \delta x \\ \delta y \end{bmatrix} = \mathbf{D} \frac{\partial^2}{\partial z^2} \begin{bmatrix} \delta x \\ \delta y \end{bmatrix} + \mathbf{J}^* \begin{bmatrix} \delta x \\ \delta y \end{bmatrix}, \quad (5.33)$$

where $\mathbf{D}$ is the matrix that has the diffusion coefficients on its diagonal, and zeros everywhere else:

$$\mathbf{D} = \begin{bmatrix} 1 & 0 \\ 0 & D \end{bmatrix}. \quad (5.34)$$

Also the Jacobean for the Brusselator is

$$\mathbf{J}^* = \begin{bmatrix} b-1 & a^2 \\ -b & -a^2 \end{bmatrix}. \quad (5.35)$$

We again want to determine if the steady state is stable against small perturbations, but this time we want to introduce a spatial aspect. Suppose therefore that our perturbations are inhomogeneous in space. One convenient form is

$$\begin{bmatrix} \delta x & \delta y \end{bmatrix} = \begin{bmatrix} \delta x_0 & \delta y_0 \end{bmatrix} e^{\lambda t} e^{ikz} \quad (5.36)$$

The $e^{\lambda t}$ part is easily recognizable from our previous work. The term $e^{ikz} = \cos(kz) + i \sin(kz)$ is a convenient way to represent a spatial wave. Our question now will be whether or not conditions can be found under which the steady state is unstable ($\text{Re}(\lambda) > 0$) when a wiggly disturbance is introduced. Since any disturbance over a finite domain can be synthesized by adding up sine waves, this will answer the question of whether the steady state is stable against small, but otherwise arbitrary perturbations.

If we substitute the perturbation into the linearised equation, we get, after cancelling off the common factors of $e^{\lambda t} e^{ikz}$,

$$\lambda e^{\lambda t} e^{ikz} \begin{bmatrix} \delta x_0 \\ \delta y_0 \end{bmatrix} = i^2 k^2 e^{\lambda t} e^{ikz} \mathbf{D} \begin{bmatrix} \delta x_0 \\ \delta y_0 \end{bmatrix} + \mathbf{J}^* \begin{bmatrix} \delta x_0 \\ \delta y_0 \end{bmatrix} e^{\lambda t} e^{ikz} \quad (5.37)$$

$$\lambda \begin{bmatrix} \delta x_0 \\ \delta y_0 \end{bmatrix} = -k^2 \mathbf{D} \begin{bmatrix} \delta x_0 \\ \delta y_0 \end{bmatrix} + \mathbf{J}^* \begin{bmatrix} \delta x_0 \\ \delta y_0 \end{bmatrix} \quad (5.38)$$

After rearranging,

$$\{\lambda \mathbf{I} + k^2 \mathbf{D} - \mathbf{J}^*\} \begin{bmatrix} \delta x_0 \\ \delta y_0 \end{bmatrix} = 0$$

where $\mathbf{I}$ is the identity matrix. This is a homogeneous equation in $[\delta x_0 \quad \delta y_0]$ which only has nontrivial solutions if

$$|\lambda \mathbf{I} + k^2 \mathbf{D} - \mathbf{J}^*| = 0$$

where again the bars represent the determinant operation. Note that we haven't done anything so far that is specific to the Brusselator, so that this is a *general characteristic equation for reaction-diffusion equations in one spatial dimension*. Our task will be to determine whether this characteristic equation has solutions for which the real part of λ is positive, and if so, under what conditions. Because of the appearance of the unknown wave number k in this equation, this equation has a different solution for every k , so again we are faced with equations where we can't simply find a finite number of roots and stop there.

Let us plug in our $\mathbf{J}^*$ and complete the analysis for the Brusselator:

$$\begin{vmatrix} \lambda + k^2 + 1 - b & -a^2 \\ b & \lambda + Dk^2 + a^2 \end{vmatrix} = 0 \quad (5.39)$$

$$(\lambda + k^2 + 1 - b)(\lambda + Dk^2 + a^2) + a^2 b = 0$$

$$\lambda^2 + Dk^2 \lambda + a^2 \lambda + k^2 \lambda + Dk^4 + a^2 k^2 + \lambda + Dk^2 + a^2 - b\lambda - Dbk^2 - a^2 b + a^2 b = 0$$

$$\lambda^2 + [k^2(1+D)+1-b+a^2] + Dk^4 + k^2[D(1-b)+a^2] + a^2 = 0 \quad (5.40)$$

This quadratic equation is of the form

$$\lambda^2 + q\lambda + p = 0$$

The solutions are

$$\lambda = \frac{1}{2} \left\{ -q \pm \sqrt{q^2 - 4p} \right\}.$$

There will be at least one root with a positive real part provided one of the following two conditions is met:

1. $q < 0$. If this is the case, then $-q$ is positive, and the root of the quadratic equation which uses the plus sign certainly has a positive real part, regardless of whether the discriminant of the equation is positive or negative.

For our characteristic equation, this condition reduces to

$$b > 1 + a^2 + k^2(1+D) > 1 + a^2$$

since $k^2(1+D) > 0$. To be clear: If $b > 1 + a^2$, then there exist values of k such that the steady state is unstable. This is just the Andronov-Hopf bifurcation condition, which is not very

interesting since we get this instability without the diffusion terms.

2. $q > 0$ and $p < 0$. If $p < 0$, then the discriminant is both positive and greater in magnitude than $|q|$. Again, this makes the root with the positive sign positive overall.

For the Brusselator, the condition $q > 0$ is realized when $b < 1 + a^2$. Note that this will take us out of the regime where we expect to see an Andronov-Hopf bifurcation. The condition $p < 0$ is

$$Dk^4 + k^2[D(1-b) + a^2] + a^2 < 0$$

Note that the left-hand side of this inequality is a concave parabola in the variable $\gamma = k^2$.

$$f(\gamma) = D\gamma^2 + \gamma[D(1-b) + a^2] + a^2 < 0$$

There will be a range of γ (i.e. k^2) where this is negative provided the minimum of the parabola is itself negative. That is not quite enough though. Since $\gamma = k^2$, only positive values of γ are physically significant. Thus we want to know under what conditions $f(\gamma)$ is negative for some positive values of γ . Note

that $f(0) = a^2 > 0$. This means that, if the minimum lies in the region $\gamma < 0$, the entire range containing negative values also lies in this range. We must therefore insist that the minimum lie to the right of the axis. Let us find this minimum:

$$\frac{df}{d\gamma} = 2D\gamma + D(1-b) + a^2 = 0 \quad (5.41)$$

$$\therefore \gamma = \frac{1}{2}(b-1-a^2/D). \quad (5.42)$$

Since we want γ at the minimum to be positive, we must insist that $b > 1 + a^2/D$.

$$\begin{aligned} f_{\min} &= \frac{D}{4}(b-1-a^2/D) + \frac{1}{2}(b-1-a^2/D)[D(1-b)+a^2] + a^2 \\ &\quad (5.43) \\ &= \frac{D}{4}(b-1-a^2/D) - \frac{D}{2}(b-1-a^2/D)^2 + a^2 \\ &= a^2 - \frac{D}{4}(b-1-a^2/D)^2 < 0 \\ 4a^2/D &< (b-1-a^2/D)^2 \\ \therefore 2a/\sqrt{D} &< b-1-a^2/D \end{aligned} \quad (5.44)$$

Note that this last step is only legitimate because we are restricting ourselves to values of b such that $b > 1 + a^2/D$. Continuing, we have

$$2a/\sqrt{D} < b-1-a^2/D.$$

$$b > 1 + \frac{2a}{\sqrt{D}} + \frac{a^2}{D}$$

$$b > \left(1 + \frac{a}{\sqrt{D}}\right)^2.$$

Since we must also have $b < 1 + a^2$, this gives the following bifurcation condition:

$$\left(1 + \frac{a}{\sqrt{D}}\right)^2 < b < 1 + a^2. \quad (5.45)$$

Note that this bifurcation occurs *only* when the steady state would be stable in the absence of diffusion. Thus, this is a purely diffusive instability. Moreover, it occurs for a finite range of wave numbers k . This instability will therefore form a spatial pattern of some sort since adding up a bunch of sine waves within a finite range of wavelengths should produce a nontrivial wave pattern. This is a **Turing bifurcation**. Technically, a Turing bifurcation is the destabilization of another stable steady state by diffusive terms, leading to pattern formation.

Suppose that D is small. Then

$$\left(1 + \frac{a}{\sqrt{D}}\right)^2 = 1 + \frac{2a}{\sqrt{D}} + \frac{a^2}{D} > 1 + a^2,$$

and it becomes impossible to satisfy both parts of condition (21) at the same time. We conclude that D must be sufficiently large in order to

make a Turing bifurcation possible. In other words, Y must diffuse faster than X in the Brusselator model. How much faster? We want

$$1 + \frac{2a}{\sqrt{D}} + \frac{a^2}{D} < 1 + a^2.$$

$$\therefore \sqrt{D} - \frac{1}{\sqrt{D}} > \frac{2}{a}.$$

In two-variable systems, and in the absence of other complications, Turing bifurcations always require that one of the chemicals diffuse faster than the other.

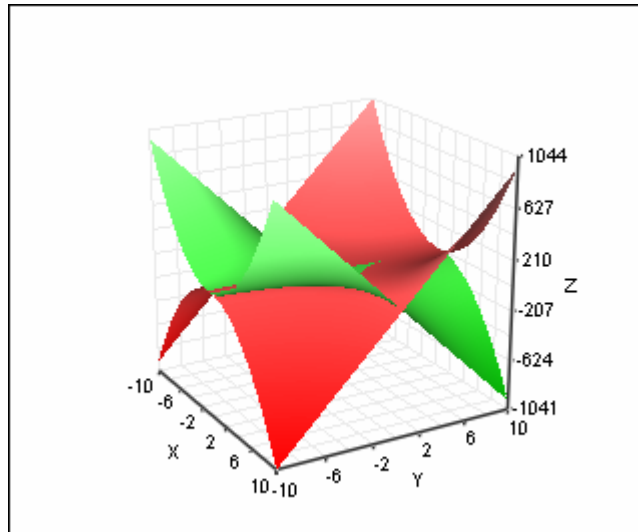


Figure 5.13 Bifurcation diagram of the model.

5.4 A Lotka-Volterra Food Chain

Predation and parasitism are examples of antagonistic ecological interactions in which one species takes advantage of another species. Predators use their prey as a source of food only, whereas parasites use their hosts both as a food and as a habitat. Predation and parasitism are stage-specific interactions rather than species-specific. Many species are predators or parasites only on specific stages in their life cycle.

Lotka-Volterra model is the simplest model of predator-prey interactions. The model was developed independently by Lotka (1925) and Volterra (1926):

$$\begin{aligned}\frac{dH}{dt} &= rH - aHP \\ \frac{dP}{dt} &= bHP - mP\end{aligned}\tag{5.46}$$

It has two variables (P, H) and several parameters:

H : density of prey

P : density of predators

r : intrinsic rate of prey population increase

a : predation rate coefficient

b : reproduction rate of predators per one prey eaten

m : predator mortality rate

To analyze this system in a straightforward manner, divide the second equation of (5.46) by the first,

$$\frac{dP}{dH} = \frac{dP}{dt} \bigg/ \frac{dH}{dt} = \frac{P(-m + bH)}{H(r - aP)}$$

and solve the resulting separable ODE. This gives the family of equations

$$a \ln y - by + c \ln x - dx = C$$

where C is the constant of integration. It can be shown that the maximum value C^* of the left-hand side of the above equation occurs at $(c/d, a/b)$. Figure 5.14 depicts the family of trajectories of (5.46) in the xy -plane with parameters $a = b = c = d = 1$. Figure 5.15 plots the behaviour of a particular solution over time.

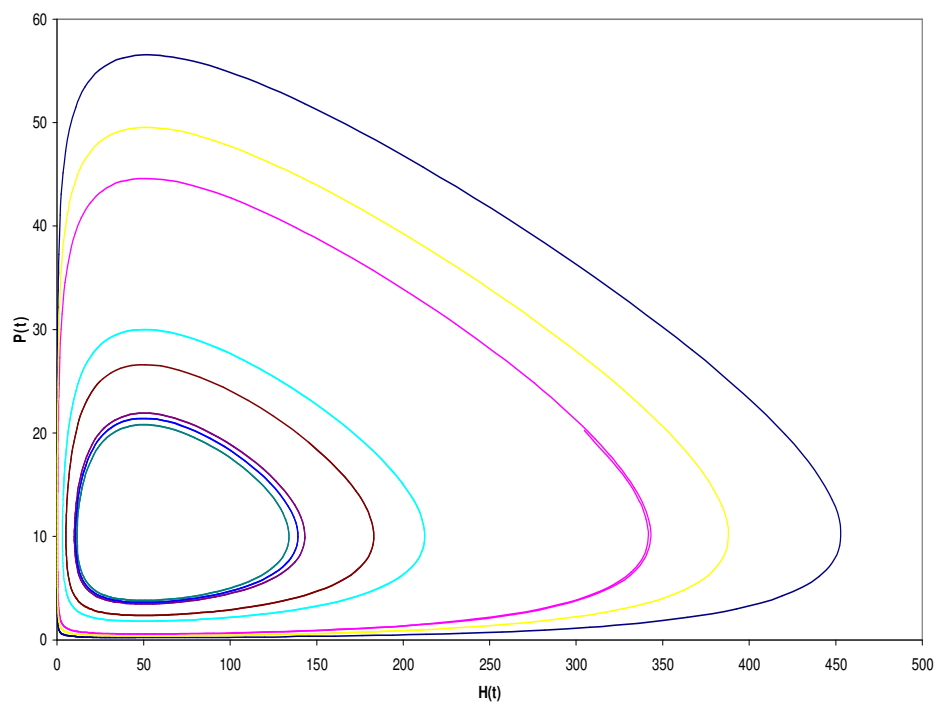


Figure 5.14 A family of closed orbits in the xy -plane circulating about $(1,1)$ with $r = m = a = b = 1.0$.

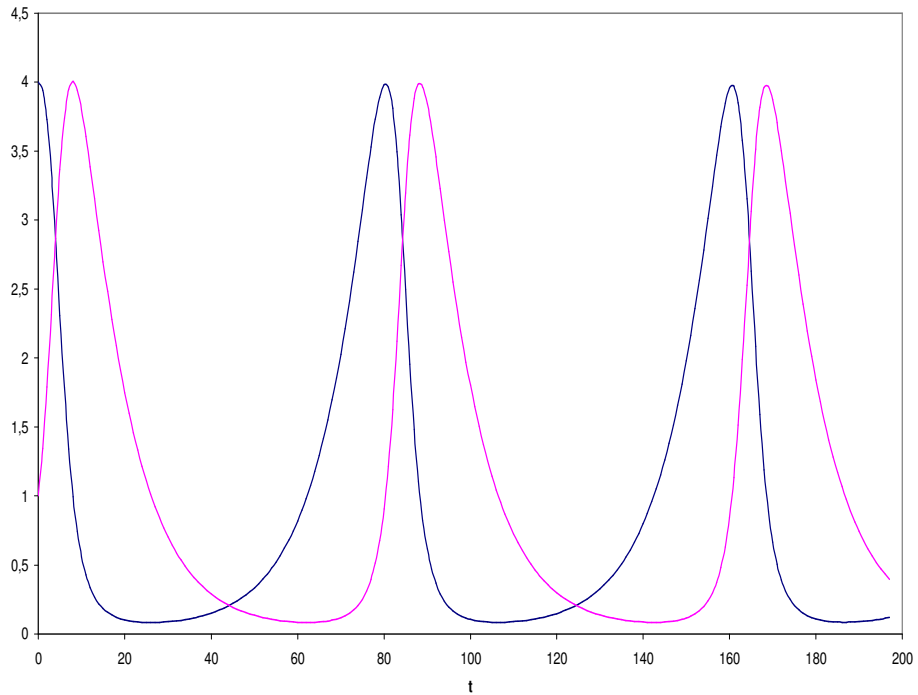


Figure 5.15 A solution with initial conditions $(x, y) = (4, 1)$ with parameters $r = m = a = b = 0.1$.

The predator-prey model predicts a phase-shifted periodic behaviour in the populations of both species with a common period. In this study, we completely characterize the qualitative behaviour of a linear three species food chain where the dynamics are given by classic Lotka-Volterra type equations. The Lotka-Volterra equations are typically modified by making the prey equation a logistic equation to eliminate the possibility of unbounded growth of the prey in the absence of the predator.

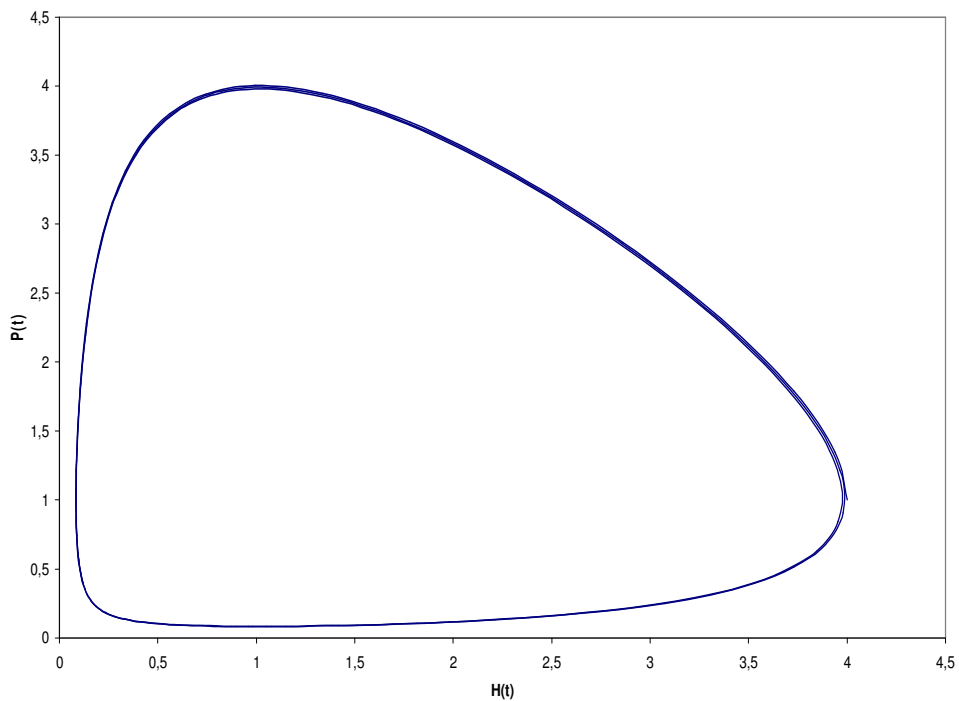


Figure 5.16 A closed orbit in the xy -plane.

This figure shows relative changes in prey predator density for both initial conditions. Trajectories are closed lines.

The model of Lotka and Volterra is not very realistic. It does not consider any competition among prey or predators. As a result, prey population may grow infinitely without any resource limits. Predators have no saturation: their consumption rate is unlimited. The rate of prey consumption is proportional to prey density. Thus, it is not surprising that model behaviour is unnatural showing no asymptotic stability. However numerous modifications of this model exist which make it more realistic.

5.5 A Full Model of Prey-Predator System

Now we can build a full model of predator-prey system that includes both the functional and numerical responses.

We will start with the prey population. Predation rate is simulated using the Holling's "disc equation" of functional response:

$$H_a = \frac{aHT}{1 + aHT_h}$$

The rate of prey consumption by all predators per unit time equals to

$$\frac{H_a P}{T} = \frac{aHP}{1 + aHT_h}$$

The equation of prey population dynamics is:

$$\frac{dH}{dt} = r_H H \left(1 - \frac{H}{K} \right) - \frac{aHP}{1 + aHT_h}$$

Here we assumed that without predators, prey population density increases according to logistic model.

Predator dynamics is represented by a logistic model with carrying capacity proportional to the number of prey:

$$\frac{dP}{dt} = r_p P \left(1 - \frac{P}{kH} \right)$$

This equation represents the numerical response of predator population to prey density.

r_H : Growth rate of prey population

K : Carrying capacity of prey population

r_p : Growth rate of predator population

a : Search rate of predators

T_h : Handling time

k : Carrying capacity of predators per 1 prey

Simulation results are presented below. This model exhibits more various dynamic regimes than the Lotka-Volterra model.

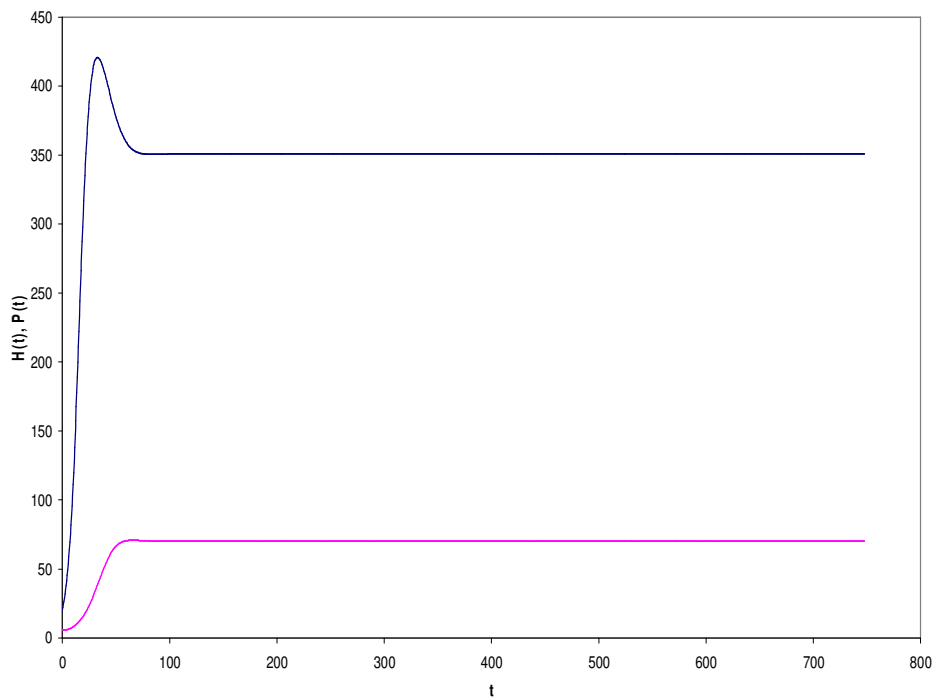


Figure 5.17 $H(t)$ & $P(t)$ vs. time.

This graph shows that there are no oscillations for the parameter values. When we change the parameter a values we can observe damping oscillations converging to a stable equilibrium.

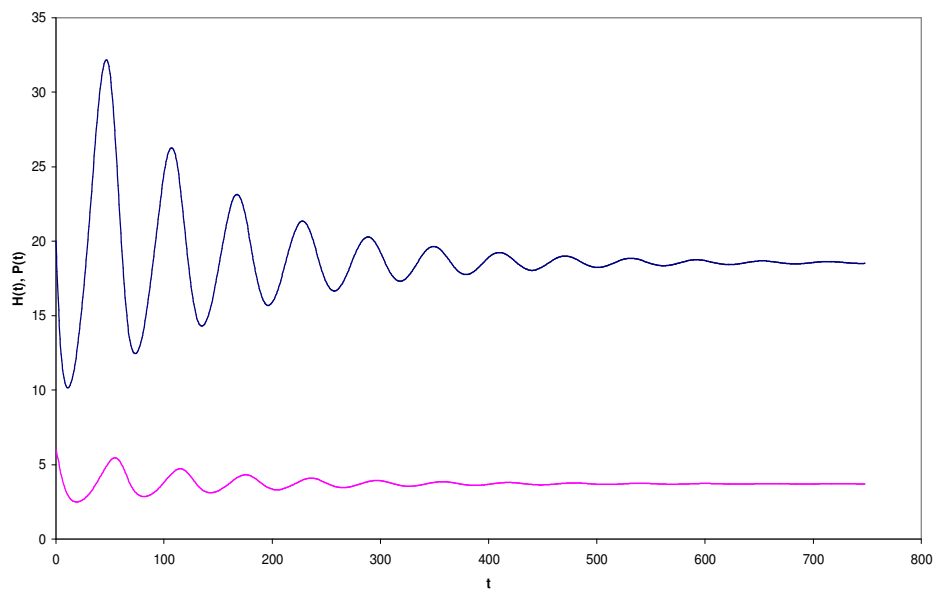


Figure 5.18 $H(t)$ & $P(t)$ vs. time.

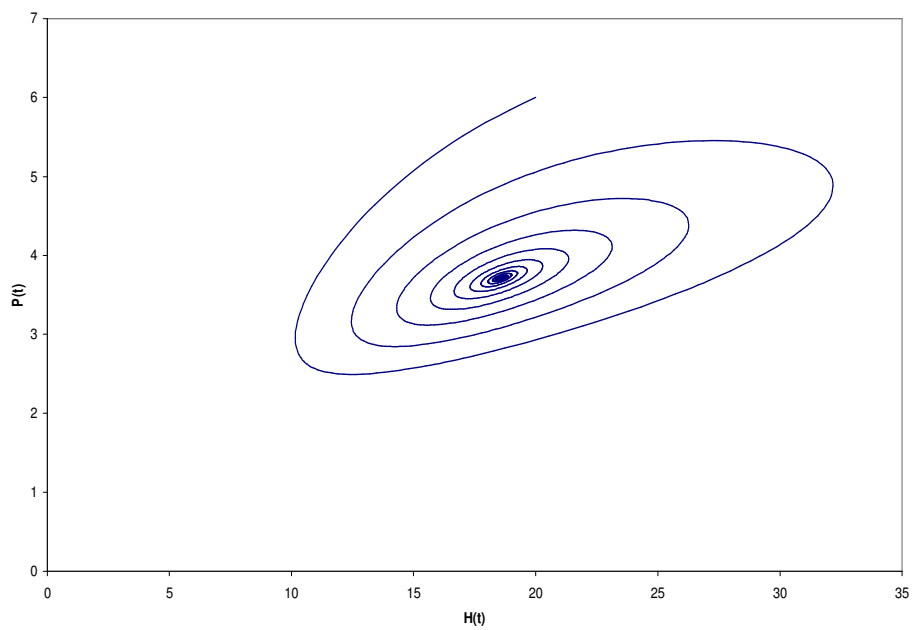


Figure 5.19 $P(t)$ vs. $H(t)$.

If we increase the value of parameter a values we have a limit cycle as shown below.

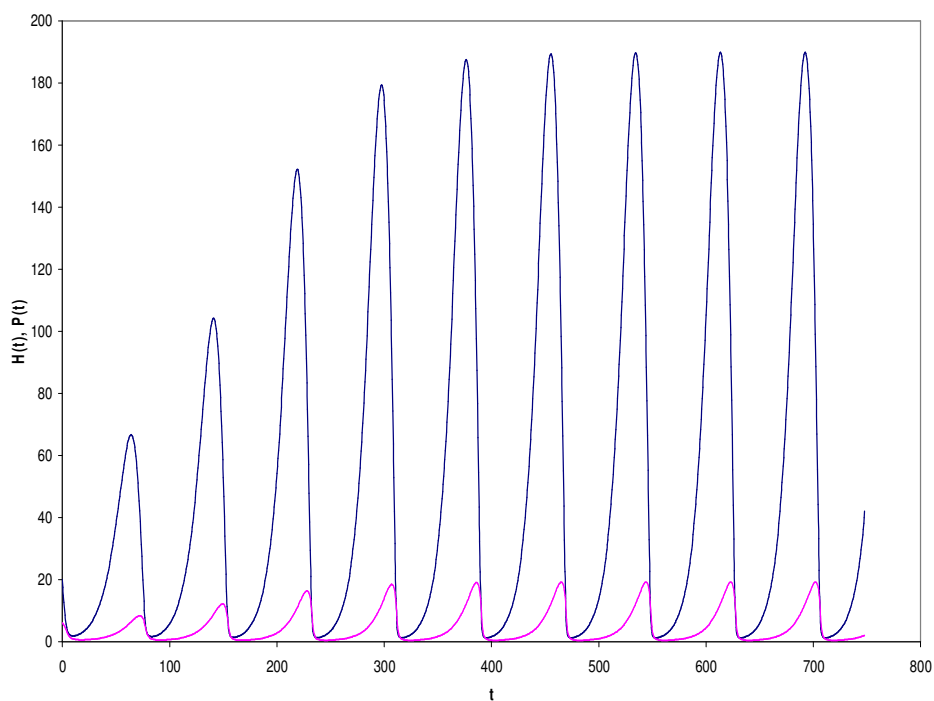


Figure 5.20 $H(t)$ & $P(t)$ vs. time as a value increases.

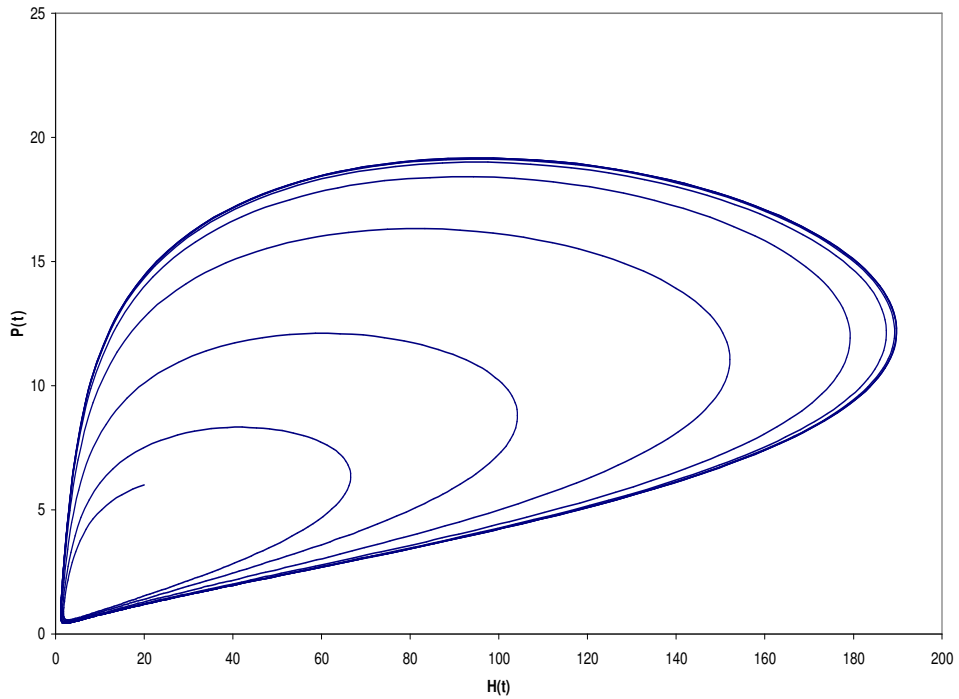


Figure 5.21 $H(t)$ & $P(t)$ vs. time.

This model can be used to simulate biological control. The goal of biological control is to suppress the density of the pest population using natural enemies. We will assume that the prey in our model is a dangerous pest, and that the predator was introduced to suppress its density. Without predators the density of prey population is equal to the carrying capacity, $K = 500$. After a predator with a search rate, $a = 0.001$, was introduced, the equilibrium population density, N^* declined to the value of 351. Beddington suggested measuring the degree of pest suppression by the ratio:

$$q' = \frac{N^*}{K}$$

For example, if $a = 0.001$, then $q' = \frac{N^*}{K} = \frac{351}{500} = 0.702$.

Biological control is successful if the value of q' is low (at least, $q' < 0.5$). If we increase the search rate of the predator (i.e., we introduced a more effective predator species) to $a = 0.1$, then the pest population is suppressed to the density of 18.52 ($q' \approx 0.037$).

It could be expected that more effective predators will cause more suppression of the prey population density. But this is not true, because more effective natural enemies also cause larger oscillations in population density. For example, at $a = 0.3$, the equilibrium is not stable and populations exhibit periodic cycles (Figure 5.20). Periodically pest density reaches the value of 190.

The transition between the stable equilibrium and the limit cycle occurs approximately at $a = 0.244$. The transition from one type of dynamics to another one is often called "phase transition" (e.g., transitions between liquid and gas phases or between solid and liquid phases). The phase transition in our model will be less abrupt if we introduce noise. With noise, the system will exhibit oscillations even if the equilibrium is stable. The closer we are to the critical value, $a = 0.244$, the larger will be these oscillations. These oscillations result from the interaction of predators with prey.

6.0 CONCLUSIONS

The concepts of stability and chaos are commonplace in the scientific community. Stability is a classical subject, whereas chaos is a recent field. There is one class of mechanisms that control both, namely, bifurcations. Solutions of nonlinear equations bifurcate at critical values of parameters. At these bifurcation points, stability may be lost or gained. On the other hand, chaos sets in after a sequence of certain bifurcations. The wide range of states, with equilibrium as the most rigid state and chaos as the most flexible state, is governed by bifurcations.

In mathematics, bifurcation theory has been developed over several decades. In this discipline the emphasis traditionally was placed on theoretical investigations. Inspired by the discovery of numerous applications and stimulated by new emerging fields, bifurcation theory had to renew and reshape some of its results. The availability of powerful computers was driving forces that gave bifurcation theory a practical significance.

Methods for the analysis of the dynamics of nonlinear process models are well established in the chemical engineering community. While these methods are very mature and powerful, they rely on visualizing numerical data and on subsequently interpreting diagrams. Unfortunately, an approach which depends on manual visualization and experience-based interpretation cannot be used systematically in process

design. Further, nonlinear analysis becomes tedious or even impossible if the dimension of the space of relevant parameter is large. This thesis has included the ideas behind a new approach to taking dynamics into account at the design stage.

Bifurcation analysis has been employed to identify and characterize the qualitative nonlinear behaviour of chemical process systems. The phenomena of interest include steady states and periodic or even chaotic oscillations. The analyses have been aiming at proper understanding of the relation between the observed behaviour on the one and the process parameters as well as the underlying physical-chemical phenomena on the other hand.

This thesis presented an introduction into a practical bifurcation and stability analysis of states and phenomena between equilibrium and chaos. The first part of this study introduced chaos and bifurcation generally.

The second section was thought of as a tutorial of a significant part of applied mathematics. Since the analysis of nonlinear phenomena requires, on the one hand, tools that provide qualitative results and, on the other hand, the theoretical knowledge of nonlinear behaviour that allows one to interpret these qualitative results.

The model, $x_{n+1} = ax_n(1 - x_n)$, was also introduced in this section and its dynamical properties at various fixed values of the parameter

a were investigated. It was found that, a certain parameter values, including $0 < a < 2$, x_n had a fixed point attractors; for larger a values, x_n had periodic or chaotic attractors. The parameter value at which the number or stability of fixed point or periodic points changes was called ‘bifurcation value’ of the parameter.

Of all possible motions in dynamical systems, a fixed point or equilibrium is the simplest. If the fixed point is stable, the system is likely to persist in that state, even in the face of minor disturbances. However, the behaviour of the systems changes. In the logistics diagram (given because the curve can be defined via the recursive relationship: $x_{n+1} = ax_n(1 - x_n)$, which is known as a logistics relationship since it occurs so often in resource management settings) there was an interesting phenomenon –as you pump more and more energy into the system, the number of states increase to a point where they create a cloud of points that seem surprisingly dense – it becomes harder to model the characteristics of the system, because the system can be in *so* many states.

However, when you pump in a certain critical threshold of energy, you end up with voids where the number of states ends up clustering around only a handful of possible values. It took us a while to realize that this was not a matter of the number of states decreasing –they do not go away –but the states are all so close in value that for all intents

and purposes the bifurcations start over as if from a considerably simpler part of the graph.

The third section included the simplest examples: bifurcations of fixed points for flows on the line. The most fundamental bifurcation of all was the saddle-node bifurcation that is the basic mechanism in which two fixed points of a dynamical system collide and annihilate each other. In this section the studied phase space was one-dimensional, so one of the fixed points was unstable (the saddle), while the other was stable (the node). In this part, the additional types of bifurcations and their scientific applications were also investigated in one-dimensional phase space.

The bifurcations of fixed points discussed in the third section had analogs in two dimensions (and indeed, in all dimensions). Yet it turns out that nothing really new happens when more dimensions are added. It was observed in the fourth section that, the bifurcation is a fundamentally one dimensional event, with the fixed points sliding toward each other along the unstable manifold like beads on a string.

Bifurcation, a word introduced into nonlinear dynamics by Poincare, is used to indicate a qualitative change in the features of a system, such as the number and type of solutions, under the variation of one or more parameters on which the considered system depends. The existence of stable or unstable periodic solutions to a set of nonlinear ordinary differential equations was proven by Hopf. Recognizing earlier

contributions by Poincare and Andronov, the theorem is sometimes called the Poincare-Andronov-Hopf bifurcation theorem. This theorem guarantees the existence of periodic (stable or unstable) solutions to nonlinear differential equations if certain conditions are satisfied. Details of this theorem are presented in the fourth section.

Hopf bifurcations come in several types, depending on what happens to orbit near the equilibrium at the bifurcation point. Two types are important in experimental work, because they explain the important phenomenon of the creation of periodic behaviour. At a supercritical bifurcation, the equilibrium at the bifurcation value of the parameter, which we might call the bifurcation orbit, is stable. The formerly stable equilibrium starts to wobble in extremely small oscillations that grow into a family of stable periodic orbits as the parameter changes. When the bifurcation orbit is unstable, the bifurcation is called subcritical. A subcritical Hopf bifurcation was seen experimentally as a sudden jump in behaviour.

In the fifth section of this thesis, applications of bifurcation theory were presented. The bifurcation diagrams that provided lots of useful information were drawn. They helped to find regions of parameters with specific behaviours.

Models of chemical reactors vary from a pair of ODEs (CSTR) to a large set of 3-D PDEs (reactive flows). Due to the strong transport/reaction coupling and the nonlinear dependence of the reaction rates on temperature and concentration these models exhibit very

complex bifurcation behaviour. Multiple steady-states, spatio-temporal oscillations, and chaos are frequently encountered. One of the goals of this study was to develop numerical methods and bifurcation techniques especially for models of high dimension by application of direct linearization and operator methods.

The classical, irreversible Gray-Scott model which describes the kinetics of a simple autocatalytic reaction in an unstirred flow reactor was studied. There was a substance V whose concentration was kept fixed outside the reactor and which was supplied through the walls into the reactor with rate F . The product P of the reaction was removed from the reactor with the same rate. Inside the reactor V undergoes a reaction involving an intermediate substance U . Furthermore, V reacts at the rate k to change into P . Both reactions are irreversible, so P was an inert product. As the model was investigated both a saddle node bifurcation and hopf bifurcation were observed since a limit cycle was born.

The physical, chemical and biological systems were mostly considered depending upon one parameter. The bifurcation analyses of these systems mean the construction of their one parameter bifurcation diagram in particular, studying the dependence of equilibria and limit cycles on the parameter, as well as locating and analyzing their bifurcation.

So as to show the diffusion effect to reaction mechanism by bifurcation, another reaction diffusion model, Brusselator, was studied. It was shown by this application that bifurcation occurs *only* when the steady state was stable in the absence of diffusion. Thus, this was a purely diffusive instability. Moreover, it occurs for a finite range of wave numbers k . This instability will therefore form a spatial pattern of some sort since adding up a bunch of sine waves within a finite range of wavelengths should produce a nontrivial wave pattern. This is a Turing bifurcation. Technically, a Turing bifurcation is the destabilization of another stable steady state by diffusive terms, leading to pattern formation.

It was also aimed to improve this study by studying on control bifurcation in the future work. It was shown that, an important objective in the study of dynamic systems depending on parameters and particularly of nonlinear systems was the investigation of system bifurcations. These are qualitative changes in the system dynamics that occur when the parameters are varied. Due to avoid unpredictable or sometimes undesirable consequences in systems, the control of bifurcation has become an important topic. The bifurcations express the transition among different operating regions and their knowledge is essential both in the analysis of system dynamics, where possible kinds of behaviour of a given process need to be predicted, and in control design, where a regulator must be carried out and added to a process to guarantee the required dynamics.

The objective of this study was to provide an introduction to the nonlinear phenomena of bifurcation theory. The use of bifurcation analysis for physical, chemical and biological system design was discussed, proposing that bifurcation analysis could be used to assess and understand the structural stability of engineering systems of interest. The examples and geometrical interpretations were essential ingredients.

A new field of research was introduced and a theoretical background was established in this thesis. The research done throughout of the thesis aimed to foresee the possibilities in industrial applications. It was shown that the behaviour of models that included differential equations could be investigated qualitatively without using quantitative solutions. Using these fresh approaches, a general investigation on engineering problems was possible. By this way, before making a solution, an opportunity to examine possible bifurcations and chaotic behaviour was afforded as a preliminary design stage. The idea about the investigated physical system could also be improved by the graphical support and, in this way theoretical and practical knowledge in design stages may be enriched.

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RESUME

Evrin YAVUZ was born in Gölcük in 1982. She graduated from Atakent Anatolian High School in 2000. She received the degree Bachelor of Science from Chemical Engineering Department of Ege University in 2005. At the same year, she was accepted to Chemical Engineering Department of Ege University for the degree of Master of Science. The subject of her thesis was “Bifurcation Analysis in Chemical Engineering”. She has completed her M. Sc. thesis successfully in June 2007.