Mathematical Modelling and Simulation of Biological Systems

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Contents

Preface

This Workbook for Students is designed to teach students how to apply mathematics by formulating, analysing, criticizing and simulating mathematical models. The book requires elementary calculus, matrix theory, elementary differential equations and knowledge of programming in MATLAB. Although the level of mathematics required is not high, this is not an easy text: Setting up and manipulating models require thought, effort, and usually discussion - purely mechanical approaches usually end in failure. Since a firmly believe in learning by doing, all the problems require creating and studying models by students. A possible fields application of mathematics are physics, technology, chemistry, economics, management, geography, demography, biology/medicine and sport. The book concentrates on mathematical modelling and simulation of biological systems, mainly on continuous population models, chemostat models and application of control theory. The core of the book, which should be included in any begining modelling course is *Chapter* 2, 3, 4. Students should find numerical methods quite interesting and useful. Computer calculations using MATLAB are presented in the form of graphs whenever possible so that the resulting numerical simulations are easier to visualize and interpret. The book is meant to be an introduction to the principle and practice of mathematical modelling and simulation in the biological science.

Chapter 1

Teaching and learning mathematical modelling

The world to which mathematics is applied is in a process of dynamic change. Besides the traditional physical sciences and engineering, the social sciences, the biological and ecological sciences, and it seems all areas of human endeavour are susceptible to quantitative reasoning or mathematical modelling.

The unifying theme for application of mathematics to these subjects is the translation of the "real world" problem to the mathematical one by the formulation of a mathematical model. The process of modelling is illustrated in *Table* 1.1 .

The left-hand column represents the real world, the right-hand column the mathematical world and the middle column provides the translation between the two states. The art of the good applied mathematician is to get the optimum balance between manageability and reality.

If the mathematical model is made as a too simple one there would be poor agreement between observed and predicted data at the validation stage and the cycle must be traversed again with an improved model. On the other hand as the model becomes more complicated so does the resulting mathematics.

Definition 1.1 *Model is an object or concept that is used to present something else. It is reality scaled down and converted to a form we can comprehend.*

Definition 1.2 *A mathematical model is a model whose parts are mathematical concepts, such as constants, variables, functions, equations, inequalities*

Table 1.1: Process of modelling

Formulate the real problem	$\longrightarrow$	Assumption made	$\longrightarrow$	Formulate the mathematical problem
$\uparrow$				$\downarrow$
Validate and refining model	$\longleftarrow$	Interpret solution	$\longleftarrow$	Solve the mathematical problem

a representation in mathematical terms of the behaviour of real devices and subjects.

Mathematical models can be divided into two categories: descriptive and prescriptive. A descriptive model is one which describes or predicts how something actually works or how it will work. A prescriptive model is one, which is meant to help us choose the best way for something to work. Alternative names which are sometimes used for prescriptive models are *normative* or *optimisation* models. The differences between descriptive and prescriptive models do not lie primarily in the mathematics. The main difference is in what the model is used for. A prescriptive model is a tool for human decision-making, while a descriptive model just tell us "what makes it tick". Often a descriptive model can be turned into a prescriptive one.

Mathematical modelling is a process that involves responding to a real situation, abstracting a problem using some simplification and assumption, establishing a response to the problem (which may involve the use of mathematical visualization and symbols) and evaluating and communicating that response to self and others.

Modelling cannot be done mechanically. Nevertheless, there are some guidelines for how to go about it. We can divide the modelling process into

three main steps:

- formulation
- mathematical manipulation
- evaluation

. Formulation can, in turn, be divided into three smaller steps.

Formulation

1. Starting the question. The question we start with is often too vague or too "big". If it is vague, make it precise. If it is too big, subdivide it into manageable parts.

2. Identifying relevant factors. Decide which quantities and relationships are important for your question and which can be neglected.

3. Mathematical description. Each important quantity should be represented by a suitable mathematical entity, e.g., a variable, a function, a geometric figure, etc. Each relationship should be represented by an equation, inequality, or other suitable mathematical assumption.

Mathematical Manipulation

The mathematical formulation rarely gives us answers directly. We usually have to do some mathematics. This may involve a calculation, solving an equation, proving a theorem, etc.

Evaluation

In deciding whether our model is a good one, there are many things we could take into account. The most important question concerns whether or not the model gives the correct answer. If the answers are not accurate enough or if the model has other shortcomings, then we should try to identify the sources of the shortcomings. It is possible that mistakes have been made in the mathematical manipulation. But in many cases we need a new formulation. For example, it can occur that some quantity or relationships which we neglected, were more important than we thought. After a new formulation we need to do new mathematical manipulations and a new evaluation. Thus, mathematical modelling can be a repeated cycle of the three modelling steps.

Amongst the activities undertaken in mathematical modelling are Formulate the real-world problem, Formulate the mathematical problem and Solve the mathematical problem. In order to solve a modelling problem we need a number of skills, amongst which are the ability to *abstract* a mathematical problem from real-world situation, *identify* the appropriate mathematical tools needed to solve the problem, and *use* the appropriate mathematical tools to solve problems.

Mathematics is often thought to consist of finding formulas for quantities of interest to us. In that approach, called the analytical *approach*, we rely heavily on mathematical theory. There is another approach, which might almost be called *experimental mathematics*, which can sometimes be used. One form of mathematical experiment is called *simulation*. There are two great pillars upon which the experimental sciences rest, theory and experiments. By contrast, the mathematical manipulation in a mathematical model often seems to be based wholly on one pillar, the theory. This is largely true, but not completely. In fact, the experimental approach finds some use when we do mathematics.

Definition 1.3 *An analytic solution involves finding a formula that relates the quantity we are trying to estimate to other quantities known to us (We rely heavily on mathematical theory). A simulation solution attempts to estimate the value of a quantity by mimicking (simulating) the dynamic behaviour of the system involved (It needs less theory but lots of patience and/or computer time).*

Mathematical modelling is the activity of translating a real problem into a mathematical form. The mathematical form is solved and then interpreted back to help explain the behaviour of the real problem.

When a model is used, it may lead to incorrect prediction. The model is often modified, frequently discarded, and sometimes used anyway because it is better than nothing. This is the way science develops. What makes mathematical models useful? If we "speak in mathematics" then:

1. We must formulate our ideas precisely and so are less likely to let implicit assumption slip by.

2. We have a concise "language" which encourages manipulation.

3. We have a large number of potentially useful theorems available.

4. We have high-speed computers available for carrying out calculations.

There is a trade-off between items 3 and 4: Theory is useful for drawing general conclusions from simple models and computers are useful for drawing specific conclusions from complicated models.

There are two approaches to teaching a syllabus in applicable mathematics.

One way is to consider a particular mathematical topic and to illustrate its application in a variety of different situation. For examples, the differential equation

$$dy/dx = ky$$

has not only an impotent application in carbon carbon dating, but it is also the governing equation for mathematical models which represent (i) the population changes of a single species, (ii) the way in which a drug loses its concentration in the body and (iii) the manner in which water cools.

This is one of the powers of mathematical analysis: the actual governing equations can be representative for many situations in different disciplines, so that by solving this one equation we have effectively solved a wide range of problems.

A second approach to teaching applicable mathematics is to consider the application of mathematics to different disciplines divided up on a subject basis.

There are many good reasons to include modelling in the school curriculum. In general, five arguments have been presented as a rationale for modelling in schools: motivation, facilitating learning, preparation for the use of mathematics in different areas, developing general competencies, and comprehension of the socio-cultural role of mathematics. Modelling literature has characterized modelling activities according to the duration and extent of the task as the teacher poses it.

Like problem solving modelling is a difficult skill to teach. In authentic modelling situation, modellers typically:

1. extract the problem from the underlying real-word situation,

2. construct a simplified version of the initial problem,

3. construct a mathematical model of the simplified problem,

4. identify solution within the framework of the mathematical model,

5. interpret these solutions in terms of the simplified problem,

6. verify that the solutions generated for the idealised problem are solutions to the initial problem.

We can speak about three cases afforded by a modelling task as it is presented to students. In case 1, the teacher presents problem with quantitative and qualitative information, and the students are expected to investigate the situation. Case 2 provides other different possibilities for students engagement. The teacher poses an initial question to the students and they become responsible for collecting data and for presenting their solutions. In this case, the students are mostly responsible for regulating their own activities. The third case entails project with non-mathematical themes that may be chosen either by a teacher or students. The students are responsible for formulating problem, collection information and solving the problem.

Freudenthal rightly demands that pupils should not learn applied mathematics but should learn how to apply mathematics. Only their own active engagement can, in the end, make a difference for pupils. The well-known quotation from Chinese philosopher Confucius points out:

1. Tell it to me and I forget it.

2. Show it to me and I recall it.

3. Let me do it and I remember it.

Chapter 2

Continuous Population Models

2.1 Exponential Growth

In this chapter we look at a population in which all individual develops independently of one another. For this situation to occur these individuals must live in an unrestricted environment, where no form of competitions is possible. The population size of a single species at time t we will denote by $x(t)$, where it is assume that x is an everywhere differentiable, that is a *smooth* function on t. The rate of change of population size can be computed if the births and deaths and the migration rate are known. A *closed* population has no migration either into or out of population. For microorganisms, which reproduce by splitting, it is reasonable to assume that the rate of births of new organisms is proportional to the number of organisms present. In mathematical terms this assumption we can express by saying that if the population size at time t is x, then over a short time interval of duration h from time t to $t+h$ the number of births is approximately bhx for a some constant b, the *per capacity birth rate*. Similarly, we may assumed that the number of deaths over the same time interval is approximately μhx for some constant μ, the *per capacity dealt rate*. Hence, the net change in population size from time t to time $t+h$, which is $x(t+h)-x(t)$ may be approximated by $(bh-\mu h)x(t)$.

We obtain the approximate equations

$$\frac{x(t+h)-x(t)}{h} \approx (b-\mu)x(t) \tag{2.1}$$

and passage to the limit as $h \to 0$ gives

$$\frac{dx}{dt} = (b - \mu)x(t) \tag{2.2}$$

under the assumption that the function $x(t)$ is differentiable.
If the net growth rate is naturally defined as

$$r \equiv b - \mu$$

then we arrive again at the differential equation

$$\frac{dx}{dt} = rx(t) \tag{2.3}$$

This differential equation has the infinite of solution given by the one parameter family of function

$$x(t) = ke^{rt} \tag{2.4}$$

The most convenient way to impose a condition that will describe the population dynamics of a specific population is by specifying the initial population size at time $t = 0$ as

$$x(0) = x_0 \tag{2.5}$$

this choose select the solution,

$$x(t) = x_0 e^{rt}. \tag{2.6}$$

Condition (2.5) is call an *initial condition* and the problem consisting of the differential equation (2.3) together with the initial condition (2.5) is called an *initial value problem*. The above initial value problem has the unique solution

$$x(t) = x_0 e^{rt},$$

where $r > 0$ implies that the population size will grow as $t \to \infty$, while $r < 0$ implies that population size will approach zero as $t \to \infty$. Population that grow exponentially at first are commonly observed in nature. However, their growth rates usually tend to decrease as population size increases. In fact exponential growth or decay may be considered *typical* local behaviour. The next section considers nonlinear assumptions on the rate of population growth rate, which lead to quite different qualitative prediction.

2.2 The Logistic Population Model

As before $x(t)$ denotes the size of a population at time t, and dx/dt, or $\dot{x}$ the rate of change of population size. Here we study models in which the growth rate depends only on population size, because, in spite of their shortcoming, these do predict qualitative behaviour of many real problems. The *per capacity growth rate*, is given by $\dot{x}/x(t)$, which we are assuming is a function of $x(t)$. The simplest population model in which per capacity growth rate is a decreasing function of population size is $\nu - ax$. This assumption leads to the *logistic* differential equation

$$\dot{x} = x(\nu - ax).$$

This equation is commonly written in the form

$$\dot{x} = rx(1 - \frac{x}{K}). \tag{2.7}$$

In analysing equation (2.7), we first observe that the constant function $x(t) = 0$ and $x(t) = K$ are solutions. In seeking the remaining solutions, we can assume that $x(t) \neq 0$ and $x(t) \neq K$. We rewrite equation (2.7) as

$$\frac{\dot{x}}{x(1 - x/K)} = r.$$

By the method of partial fractions, we transform this to

$$\frac{\dot{x}}{x} + \frac{\dot{x}}{K - x} = r.$$

Integrated we get

$$\int \frac{\dot{x}}{x} dt + \int \frac{\dot{x}}{K - x} dt = \int r dt + c.$$

A little more algebra yields the logistic function for initial value $x(0) = x_0$

$$x(t) = \frac{x_0 K}{x_0 + (K - x_0)e^{-rt}}. \tag{2.8}$$

The parameters r and K appearing in equation 2.8 we can fit for a given set of experimental data using the following two $M - file$:

```
global t x
t=[0,1,2,3,4,5,6,7,8,9];
x=[9.6,29.0,71.1,174.6,350.7,513.3,594.4,640.8,655.9,661.8];
start=[1,10];
estimates = fminsearch(@expfun,start)
plot(t,x,'*')
z=x(1)*estimates(2)./(x(1)+(estimates(2)-x(1)).*exp(-estimates(1)*t));
z1=abs(z-x);
hold on
plot(t,z,'r')
plot(t,z1,'+')
xlabel('t')
ylabel('Number of yeast cells x(t)')
hold off

function sse = expfun(params)
global t x
r = params(1);
K= params(2);
FittedCurve = x(1)*K./(x(1)+(K-x(1)).*exp(-r*t));
ErrorVector=FittedCurve - x;
sse= sum(ErrorVector.^2);
end
```

2.3 Qualitative Analysis

Differential equations are commonly used for mathematical modelling in science and engineering. Consider the equation

$$\dot{x} = f(x,t). \tag{2.9}$$

It is a differential equations because it involves the derivative dx/dt of the *unknown* function $x(t)$. Only the independent variable t appears on the right side of equation (2.9)

Definition 2.1 *A solution of the initial value problem* $\dot{x} = f(x,t)$ *with* $x(0) = x_0$ *on the interval* $[0,b]$ *is a differentiable function* $x = x(t)$ *such that* $x(0) = x_0$ *and* $\dot{x}(t) = f(x(t),t)$ *for all* $t \in [0,b]$.

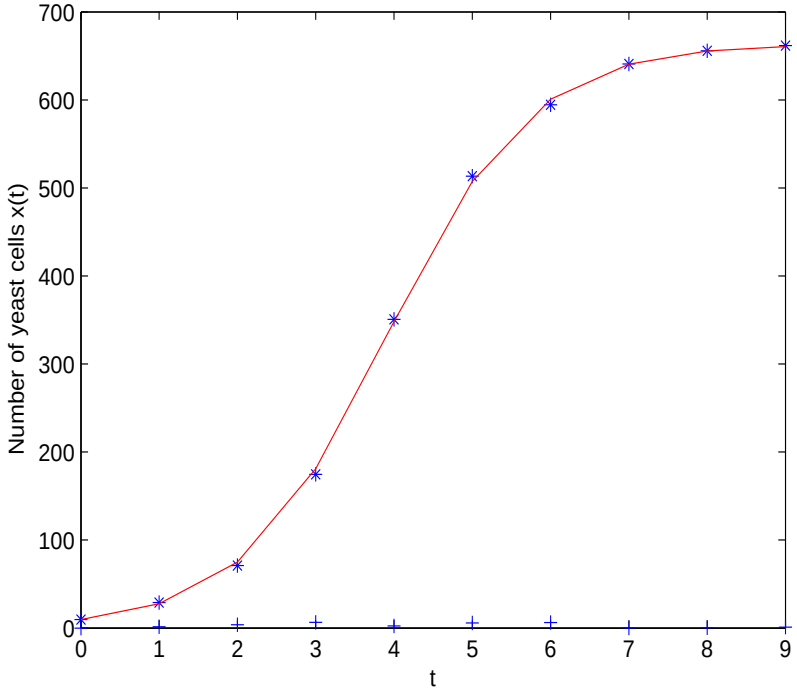

Figure 2.1: Actual yeast growth compared to logistic function (2.8)

At each point (t, x) in the rectangular region

$$R = \{(t, x) : 0 \leq t \leq b, c \leq x \leq d\},$$

the slope of the solution curve $x = x(t)$ can be found using the implicit formula $m = f(x(t), t)$. Hence the values $m_{i,j} = f(x_i, t_j)$ can be computed throughout the rectangle, and each value $m_{i,j}$ represents the slope of the line tangent to a solution curve $x(t)$ that passes through the point (t_j, x_i). It can be used to visualise how a solution curve $fits$ the slope constraint. Sketches of the slope field and solution can be constructed by using the MATLAB. The following $M - file$ will generate a graph analogous to $Figure$ 2.2.

```
[t,x] = meshgrid(0:1.:8,1:-0.25:0);
dt=ones(5,9);
```

```
K=0.5; % satutation coefficient
r=0.3; %growth rate
x1=0.2; %initial condition
x2=0.9; %initial condition
dx=r*(x-x.^2/K)
quiver(t,x,dt,dx);
hold on
y=0:0.01:8;
z1=0.;
z2=0.5;
z3=x1*K ./(x1+(K-x1)*exp(-r*y));
z4=x2*K ./(x2+(K-x2)*exp(-r*y));
plot(y,z1,y,z2,y,z3,y,z4)
hold off.
```

Definition 2.2 *Given the rectangle* $R = \{(t, x) : 0 \leq t \leq b, c \leq x \leq d\}$*, assume that* $f(x, t)$ *is continuous on* R*. The function* f *is said to satisfy a Lipschitz condition in the variable* x *on* R *provided that a constant* $L > 0$ *exists with the property that*

$$|f(x_1, t) - f(x_2, t)| \leq L\,|x_1 - x_2|$$

Theorem 2.1 *Assume that* $f(x, t)$ *is continuous in a region* R*. If* f *satisfies a Lipschitz condition on* R *in the variable* x *and* $(t_0, x_0) \in R$*, then the initial value problem has a unique solution* $x = x(t)$ *on the some subinterval* $t_0 \leq t \leq t_0 + \delta$*.*

Intuitively, a dynamic system is said to be in equilibrium if it does not change as time proceeds. Thus, a population is in equilibrium if it stays the some size. The mathematical way to put this would be: let $x(t)$ denote the population at time t; if $x(t)$ is a constant function, equally if $dx/dt = 0$ for all t, then the population is in equilibrium. Here is the formal definition used for the kinds of differential equations of interest to us.

Definition 2.3 *For the differential equation of the form*

$$\frac{dx}{dt} = f(x) \tag{2.10}$$

the value $\bar{x}$ *is called an equilibrium if* $f(\bar{x}) = 0$*.*

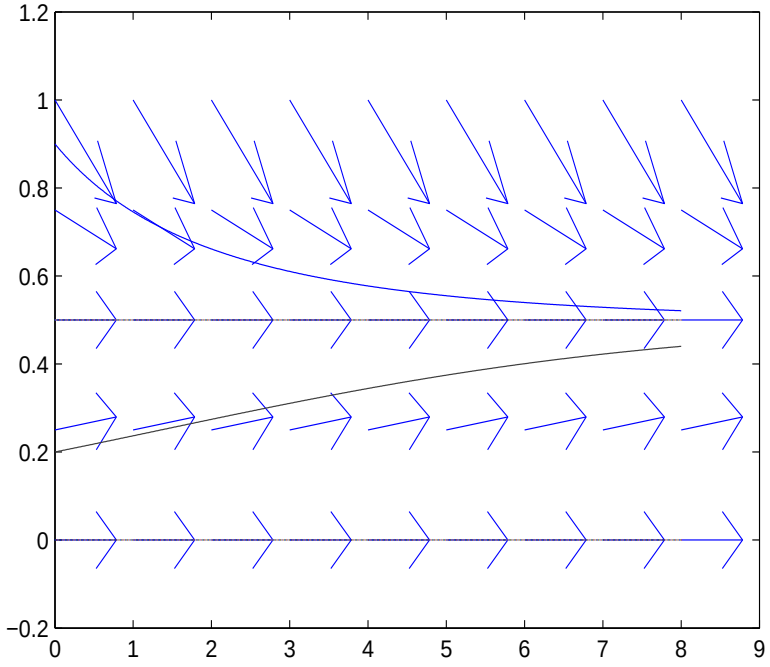

Figure 2.2: The slope field for the differential equation (2.7)

Observe that if $\bar{x}$ is an equilibrium, then the constant function $x(t) = \bar{x}$ satisfies equation (2.10) and so $x(t) = \bar{x}$ is called an equilibrium solution of (2.10).

In order to describe the behaviour of the solution near an equilibrium we introduce the process of *linearization*. If $\bar{x}$ is an equilibrium of the differential equation $\dot{x} = f(x)$ so that $f(\bar{x}) = 0$, we make the change of variable $u(t) = x(t) - \bar{x}$. Substitution gives

$$\frac{dx}{dt} = f(u(t) + \bar{x})$$

The *linearization* of the differential equation at the equilibrium $\bar{x}$ is defined to be the linear homogeneous differential equation

$$\frac{dv}{dt} = \frac{df(\bar{x})}{dx} v \tag{2.11}$$

The importance of the linearization lies in the fact that the behaviour of its solution is easy to analyse.

Theorem 2.2 *If all solution of the linearization* (2.11) *at an equilibrium* $\bar{x}$ *tend to zero as* $t \to \infty$ *then all solution of* (2.10) *with x(0)sufficiently close to* $\bar{x}$ *tend to the equlibrium* $\bar{x}$ *as* $t \to \infty$.

Definition 2.4 *An equilibrium* $\bar{x}$ *is said to be stable if for every* $\epsilon > 0$ *there exists* $\delta > 0$ *such that* $|x(0) - \bar{x}| < \delta$ *implies* $|x(t) - \bar{x}| < \epsilon$ *for all* $t > 0$. *An equilibrium is said to be asymptotically stable if it is stable and if in addition* $|x(0) - \bar{x}| < \delta$ *implies* $\lim_{t\to\infty} x(t) = \bar{x}$.

For differential equation $\dot{x}(t) = f(x(t))$ an equilibrium $\bar{x}$ is asymptotically stable if and only if

$$\frac{df(x)}{dx}_{x=\bar{x}} = \frac{df(\bar{x})}{dx} < 0.$$

If the population governed by logistic equations (2.7) is at equilibrium K at some point of time, say $t = 0$ for convenience, then it will at the equilibrium and the function $x(t) = K$ is a solution with the initial condition $x(0) = K$. We get

$$\frac{df(x)}{dx} = r\left(1 - \frac{x}{K}\right) - \frac{xr}{K}.$$

For $\bar{x} = 0$ $\frac{df(0)}{dx} = r > 0$ and for $\bar{x} = K$ $\frac{df(K)}{dx} = -r < 0$. As follows from *Figure* 2.2 all solutions of the logistic equation trends to equilibrium $\bar{x} = K$ as $t \to \infty$ and the only solution that trends to $\bar{x} = 0$ is the identically zero solution $x(t) = 0$.

2.4 Continuous Single-Species Population Models with Time Delay

Up to now in our study of continuous population models we have been assuming that $\dot{x}(t)$, the growth rate of population size at a same time t, depends only on $x(t)$. However, there are situation in which the growth rate does not respond instantaneously to change in population size. If we assume that the per capacity growth rate $\dot{x}(t)/x(t)$ is a function of $x(t-\tau)$, as may be approximate for example in modelling a population whose food supply requires a time τ. We are led to a model of the form

$$\dot{x}(t) = x(t)g(x(t-\tau)) \tag{2.12}$$

a differential-difference equation. For example, the delay logistic equation is

$$\dot{x}(t) = rx(t)(1 - \frac{x(t-\tau)}{K}) \tag{2.13}$$

Definition 2.5 *An equilibrium of the differential-difference equation*

$$\dot{x}(t) = x(t)g(x(t-\tau))$$

is a value such that $\bar{x}(t)g(\bar{x}) = 0$, so that $x(t) \equiv \bar{x}$ is a constant solution of the differential-difference equation.

Observe that for the differential-difference equation (2.12) implies that $x = 0$ is always an equilibrium. The delay logistic equations has two equilibria $\bar{x} = 0$ and $\bar{x} = K$. For differential equation $\dot{x}(t) = x(t)g(x(t))$ an equilibrium $\bar{x}$ is asymptotically stable if and only if

$$\frac{d\,(xg(x))}{dx}_{x=\bar{x}} = \bar{x}\frac{dg(\bar{x})}{dx} + g(\bar{x}) < 0,$$

so that the equilibrium $x = 0$ is asymptotically stable if $g(0) < 0$ and an equilibrium $\bar{x}$ is asymptotically stable if $g'(\bar{x}) < 0$. The asymptotic stability of equilibrium $\bar{x}$ of the differential-difference equations

$$\dot{x}(t) = x(t)g(x(t-\tau))$$

requires additional condition. We let $u(t) = x(t) - \bar{x}$ and obtain the equivalent differential-difference equation

$$\begin{aligned} \dot{u}(t) &= (\bar{x}(t) + u(t))g(\bar{x} + u(t-\tau)) \\ &= (\bar{x}(t) + u(t))(g(\bar{x}) + g'(\bar{x})u(t-\tau)) + fracg''(c)2u(t-\tau)^2 \\ &= u(t))(g(\bar{x}) + \bar{x}g'(\bar{x})u(t-\tau)) + h(, u(t), u(t-\tau)) \end{aligned}$$

The linearization of the differential-difference equation $\dot{x}(t) = x(t)g(x(t-\tau))$ is defined to be the linear differential-difference equation

$$\dot{v}(t) = g(\bar{x})v(t) + \bar{x}g'(\bar{x})v(t-\tau))$$

Theorem 2.3 *If all solutions of the linearization*

$$\dot{v}(t) = g(\bar{x})v(t) + \bar{x}g'(\bar{x})v(t-\tau))$$

at an equilibrium $\bar{x}$ tend to zero as $t \to \infty$, then every solutions $x(t)$ of $\dot{x}(t) = x(t)g(x(t-\tau))$ with $|x(t) - \bar{x}|$ sufficiently small for $-\tau \leq t \leq 0$ trends to the equilibrium $\bar{x}$ as $t \to \infty$.

In order to describe the behaviour of solution of linearization, we must study a problem more general

$$\dot{v}(t) = av(t) + bv(t-\tau)$$

We look for solution of the form $v(t) = ce^{\lambda t}$ and obtain the *characteristic equation*

$$\lambda = a + be^{-\lambda\tau}$$

In order that all solution of $\dot{v}(t) = av(t) + bv(t-\tau)$ tend to zero as $t \to \infty$, all solution of the characteristic equation must have negative real part. It is possible to prove the following result.

Theorem 2.4 *All roots of the equation* $(z+a)e^z + b = 0$, *where* a *and* b *are real, have negative real parts if and only if*

$$\begin{aligned} a &> -1 \\ a+b &> 0 \\ b &< \zeta \sin\zeta - a\cos\zeta \end{aligned}$$

where ζ *is the root of* $\zeta = -a\tan\zeta$, $0 < \zeta < \pi$, *if* $a \neq 0$ *and* $\zeta = \frac{\pi}{2}$ *if* $a = 0$.

The following similar theorem holds

Theorem 2.5 *If a,b are real number, then all roots* z *of*

$$ae^z + b - ze^z = 0$$

have negative real parts if and only if $a < 1$ *and* $a < -b < \sqrt{\alpha^2 + a^2}$, *where* α *is a root of* $\alpha = a\tan\alpha$, *such that* $0 < \alpha < \pi/2$. *If* $a = 0$, *then take* $\alpha = \pi/2$.

For the equilibrium $\bar{x} = 0$ the linearization is

$$\dot{v}(t) = g(\bar{x})v(t).$$

Since $g(0) > 0$ for most model of this type, the equilibrium $\bar{x} = 0$ is unstable. For the equilibrium $\bar{x} > 0$, $g(\bar{x}) = 0$ end the linearization is

$$\dot{v}(t) = \bar{x}g'(\bar{x})v(t-\tau))$$

or in general form with $a = 0$

$$\dot{v}(t) = bv(t-\tau))$$

Using *Theorem* 2.4 it is possible to show that the condition that all roots of the characteristic equation have negative real part is

$$0 < -b\tau < \frac{\pi}{2}.$$

For the delay-logistic equation this stability condition is $0 < r\tau < \frac{\pi}{2}$.

A graphic display of the solution is often helpful for obtaining insights into the behavior of solution. For delay-logistic equation, here is a display of the solution with $r = 1,\ K = 2, \tau = 1$.

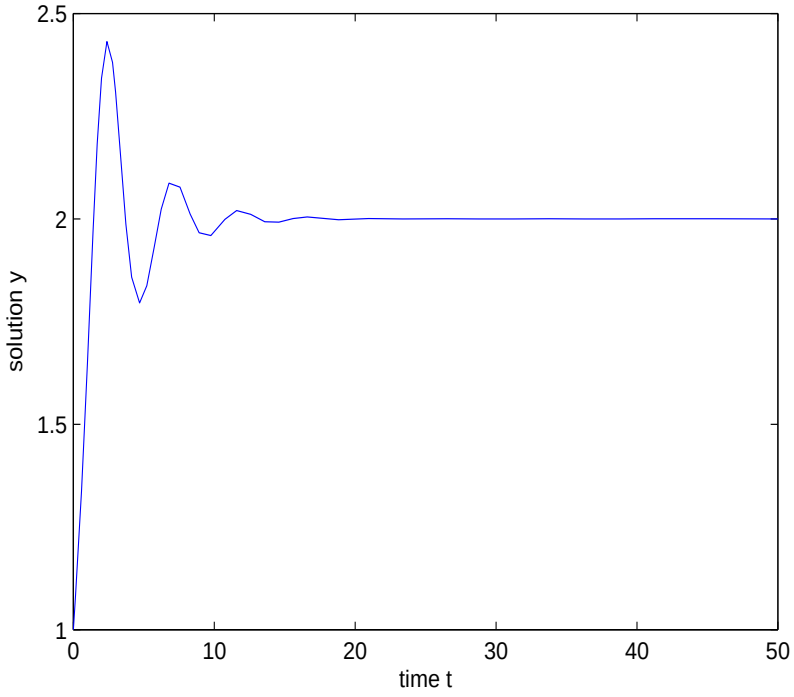

Figure 2.3: Numerical solution of logistic-delay equation

```
%   logist_delay
```

```
%   The differential equations
%
%        y'(t) = r* y(t)*(1- y(t-1)/K)
%
%
%   are solved on [0, 10] with history y = 1 for
%   t <= 0.
%
%   The lags are specified as a vector [1], the delay differential
%   equations are coded in the subfunction DDEfun, and the history is
%   evaluated by the function DDEHIST. Because the history is constant it
%   could be supplied as a vector:
%       sol = dde23(@ddefun,[1],1,[0, 10]);
%       K=2, T=1, r=1
global r K
r=0.5;
K=2;
sol = dde23(@ddefun,[1],@ddehist,[0, 50]);
figure;
plot(sol.x,sol.y)
xlabel('time t');
ylabel('solution y');

function s = ddehist(t)
% Constant history function.
s = 1;

function dydt = ddefun(t,y,Z,r,K)
% Differential equations function.
global r K
ylag1 = Z(:,1);
dydt =  r*y(1)*(1-ylag1(1)/K);
```

2.5 Partial functional logistic equation in one space dimension

Let us consider the following delayed logistic equation in one space dimension with diffusion and a discrete time delay

$$\frac{\partial}{\partial t}u(x,t) = D\frac{\partial^2}{\partial x^2}u(x,t) + \alpha u(x,t)(1-u(x,t-1)) \tag{2.14}$$

with Neumann boundary condition

$$\frac{\partial}{\partial x}u(x,t) = 0,\ x = 0,\pi,\ t \geq 0, \tag{2.15}$$

and initial conditions

$$u\,(x,t) \ = \ \phi\,(x,t) \geq 0,\ 0 \leq x \leq \pi,\ t \in \langle -1,0\rangle \tag{2.16}$$

where D, τ, α are all positive constant.

We investigate the stability of the equilibrium $u \equiv 1$ by changing variables $v = u - 1$ to obtain

$$\frac{\partial}{\partial t}v(x,t) = D\frac{\partial^2}{\partial x^2}v(x,t) - \alpha v(x,t-1)(1+v(x,t)) \tag{2.17}$$

The linearization around the equilibrium $v \equiv 0$ takes the form

$$\frac{\partial}{\partial t}v(x,t) = D\frac{\partial^2}{\partial x^2}v(x,t) - \alpha v(x,t-1) \tag{2.18}$$

We look for the solution of the form $v(x,t) = ce^{\lambda t}\cos kx$ and obtain the *characteristic equation*.

Let $X = C([0,\pi]\,;R)$ As the Laplace operator has eigennvalues $-k^2,\ k = 0,1,...$ with corresponding eigenfunctions $coskx$, λ is a characteristic value of the linearization if and only if for some $k = 0,1,...$ λ is a solution of characteristic equation

$$\lambda + \alpha e^{-\lambda} + Dk^2 \ = \ 0.$$

We need the following result:

Theorem 2.6 *Consider the equation*

$$\lambda + \alpha e^{-\lambda} + Dk^2 \;\; = \;\; 0,$$

where $D > 0$. *If* $0 < \alpha < \pi/2$, *then every solution of the equation has a negative real part. If* $\alpha > \pi/2$, *then there is a root* $\gamma(\alpha)+i\eta(\alpha)$ *of the equation, which is continuous together with its first derivative in* α *and satisfies* $0 < \eta(\alpha) < \pi$, $\eta(\pi/2) = \pi/2$, $\gamma(\pi/2) = 0$, $\gamma'(\pi/2) > 0$, *and* $\gamma(\alpha) > 0$ *for* $\alpha > \pi/2$.

Chapter 3

The Lotka-Volterra Equations

3.1 Predator-Prey Model

In the 1920s year Vito Volterra was asked if it were possible to expalian the fluctuation which had been observed in the fish population of tha Adreatic-sea. Volterra (1926) constructed the model has become known as the Lotka-Volterra model because A. J. Lotka (1925) constructed a similar model in the different context.

Let $x(t)$ be the number of fish and $y(t)$ the number of sharks at time t. We assume that the plankton, which is the food supply for the fish, in unlimited, and thus that the per capita growth rate of the fish population in the absence of sharks would be constant. Thus, if there were no sharks the fish population would satisfy a different equation of the form

$$\frac{dx}{dt} = \lambda x$$

The shark on the other hand, defend on fish as their food supply, and we assumed that if there no wish the sharks would have a constant per capita death rate, thus, in the absence of fish, the shark population would a differential equation of the form

$$\frac{dy}{dt} = -\mu y$$

We assumed that the presence of fish increases the shark growth rate, changing the growth rate form $-\mu$ to $-\mu + cx$. The presence of sharks reduces

the fish population, changing the growth rate from λ to $\lambda - by$. This gives Lotka-Volterra equations

$$\frac{dx}{dt} = x(\lambda - by) \tag{3.1}$$

$$\frac{dy}{dt} = y(\mu + cx) \tag{3.2}$$

$$\tag{3.3}$$

We cannot solve this system of ordinary differential equations analytically, but we can obtain some information about the behavior of this solution. To solve for $x(t)$ and $y(t)$ as a function of t, we eliminate t and books for relation between x and y. We look for orbits, or trajectories of the solution-curve in the phase-plane representing the functional relation between x and y with the time t as the parameter. We may eliminate t from the equation in the following way

$$\frac{dy/dt}{dx/dt} = \frac{dy}{dx} = \frac{y(-\mu + cx)}{x(\lambda - by)}$$

We may solve this differential equations by separation of variables:

$$\begin{aligned} \int \frac{-\mu + cx}{x} &= \int \frac{\lambda - by}{y} dy \\ -\mu \log x + cx &= \lambda \log y - by + h \end{aligned}$$

where h is a constant of integration, or

$$-\mu \log x - \lambda \log y + cx + by = h$$

The minimum value of the function

$$V(x, y) = -\mu \log x - \lambda \log y + cx + by$$

is obtaining by setting

$$\frac{\partial V}{\partial x} = 0, \qquad \frac{\partial V}{\partial y} = 0$$

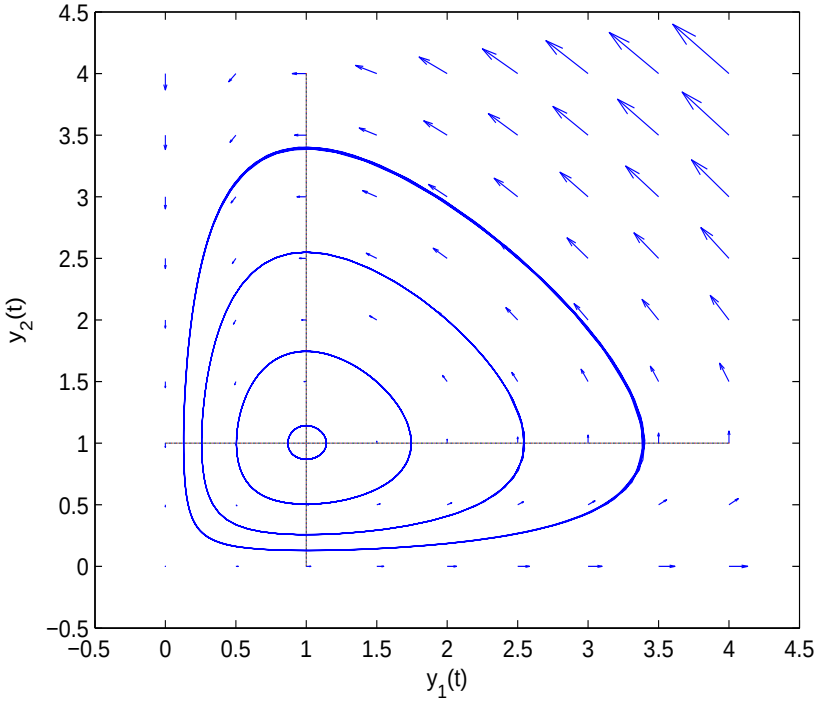

Figure 3.1: The slope field and trajectories of Lotka-Volterra equation

Then $\bar{x} = \frac{\mu}{c}$ and $\bar{y} = \frac{\lambda}{b}$, which is an *equilitrium* point of (3.1). Every orbit of the system is given implicitly by an equation $V(x(t), y(t)) = h$, for some constants h, which is determined by the initial conditions, i.e.

$$h = -\mu \log(x(0)) - \lambda \log(y(0)) + cx(0) + by(0)$$

The following $M - files$ will generate $Figure$ 3.1.

```
a=1.;b=1.;c=1.;d=1;
[y1,y2] = meshgrid(0:0.5:4,0:0.5:4)
Dy1Dt=y1.*(a-b.*y2);
Dy2Dt=y2.*(-d+c.*y1);
quiver(y1,y2,Dy1Dt,Dy2Dt);
hold on
```

```
z1=a/b;z2=d/c;
z=0:0.005:4;
plot(z,z1);
plot(z2,z);
tspan = [0,50]; yzero=[1.5,1.5];
options = odeset('AbsTol', 1e-7,'RelTol', 1e-4);
[t,y]=ode45(@LV,tspan,yzero,options,a,b,c,d);
plot(y(:,1),y(:,2)),title(''),grid
xlabel y_1(t),ylabel y_2(t)
tspan = [0,50]; yzero=[1.1,1.1];

[t,y]=ode45(@LV,tspan,yzero,options,a,b,c,d);
plot(y(:,1),y(:,2)),title(''),grid
xlabel y_1(t),ylabel y_2(t)
tspan = [0,50]; yzero=[2.5,2.5];

[t,y]=ode45(@LV,tspan,yzero,options,a,b,c,d);
plot(y(:,1),y(:,2)),title(''),grid
xlabel y_1(t),ylabel y_2(t)
tspan = [0,50]; yzero=[2,2];

[t,y]=ode45(@LV,tspan,yzero,options,a,b,c,d);
plot(y(:,1),y(:,2)),title(''),grid
xlabel y_1(t),ylabel y_2(t)
hold off

function yprime = LV(t,y,a,b,c,d)
%LV       LV predator-prey parammetrized
%         YPRIME = LV(T,Y,A,B,C)
yprime = [y(1)*(a-b*y(2)); y(2)*(c*y(1)-d)];
```

3.2 A competition equation

Let us return to ecology, and model the interaction of two *competing species*. If x and y denote their densities, then the rates of growth $\dot{x}\,/x$ and $\dot{y}\,/y$ will be decreasing functions of both x and y, since competition will act both

within and between the species. The most simpleminded assumption would be that this decrease is linear. This leads to

$$\begin{aligned} \dot{x} &= x(a - bx - cy) \\ \dot{y} &= y(d - ex - fy) \end{aligned} \tag{3.4}$$

with positive constants a to f. Again, since the boundary of R^2_+ is invariant, so is R^2_+ itself. In fact, if one population is absent, the other obeys the familiar logistic growth law.

The $x-$ and $y-$isoclines are given by

$$\begin{aligned} a - bx - cy &= 0 \\ d - ex - fy &= 0 \end{aligned}$$

in int R^2_+. These are straight with negative slopes.

There remains the case of unique intersection $\bar{F} = (\bar{x}, \bar{y})$ of the isoclines in int R^2_+ when

$$\bar{x} = \frac{af - cd}{bf - ce} \qquad \bar{y} = \frac{bd - ae}{bf - ce} \tag{3.5}$$

The Jacobian of (3.2) at F is

$$\mathbf{A} = \begin{bmatrix} -b\bar{x} & -c\bar{x} \\ -e\bar{y} & -f\bar{y} \end{bmatrix} \tag{3.6}$$

We have to distinguish two situations:
(a) If $bf > ce$ then the denominator in (3.3) is positive. This implies $af - cd > 0$, $bd - ae > 0$ and hence

$$\frac{b}{e} > \frac{a}{d} > \frac{c}{f}. \tag{3.7}$$

From the signs of $\dot{x}$ and $\dot{y}$ in the regions I, II, III, IV we infer that every orbit in int R^2_+ converges to $\bar{F}$. This agrees with the fact that the eigenvalues of (3.4) are negative and $\bar{x}$, consequently, is a sink. This is the case of *stable coexistence*, *Figure*3.2.

(b) otherwise

$$\frac{c}{f} > \frac{a}{d} > \frac{b}{e}. \tag{3.8}$$

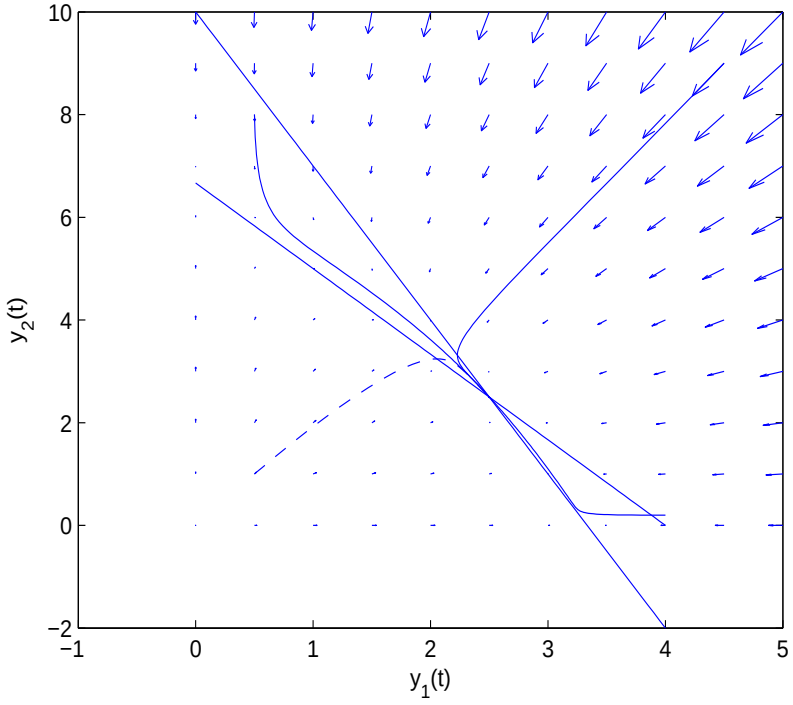

Figure 3.2: The slope field and trajectories of competition equation

As seen from *Figure*3.3,all orbits in region I converge to the y-axis and all those of region III to the x-axis. Since $detA = \overline{xy}(bf - ce) < 0$, $\bar{F}$ is a saddle. Its stable manifold consist of two orbits converging to $\bar{F}$. One of them lie in region II, the other on i region IV. Together, they divide int R^2_+ into two basins of attraction. All orbits from one basin converge to $\bar{F}_2 = (0, \frac{d}{f})$, all those from the other one to $\bar{F}_1 = (\frac{a}{e}, 0)$. This means that - depending on the initial conditions - one or the other species gets eliminated. This is the so-called *bistable case*.

The following M files will generate *Figure* 3.2, 3.3.

```
%interior equilibrium point a=10.;b=3.;c=1.;d=10;e1=2.5;f=1.5;
a=10.;b=2.5;c=1.5;d=10.;e1=3.;f=1.;
[y1,y2] = meshgrid(0:0.5:5,0:1:10);
Dy1Dt=y1.*(a-b.*y1-c.*y2);
```

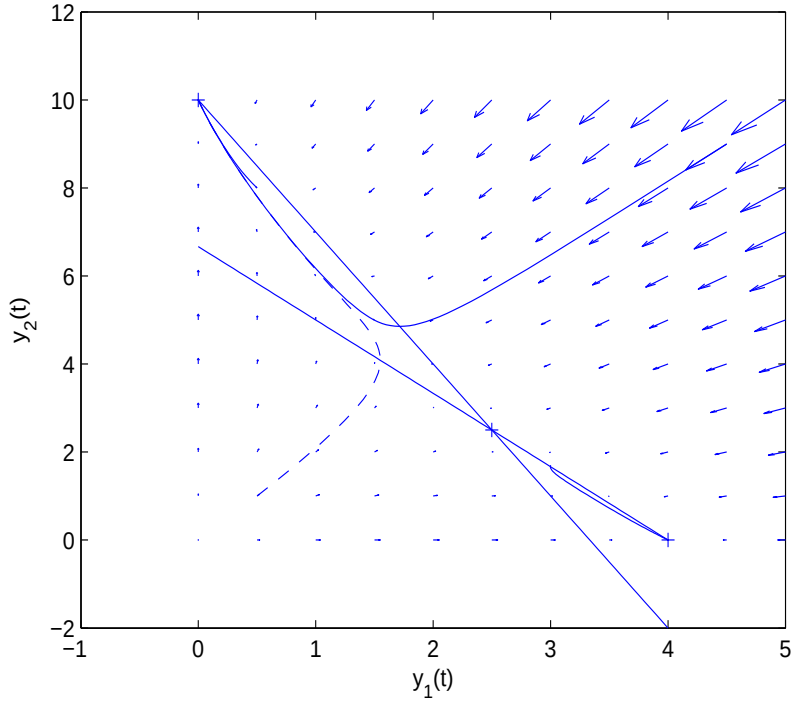

Figure 3.3: The slope field and trajectories of competition equation

```
Dy2Dt=y2.*(d-e1.*y1-f.*y2);
quiver(y1,y2,Dy1Dt,Dy2Dt);
hold on
z=0:0.05:4;
z1=(a-b*z)/c;z2=(d-e1*z)/f;
plot(z,z1,'r');
plot(z,z2,'c');
plot(a/b,0,'+');
plot(0,d/f,'+');
z3=(a*f-c*d)/(b*f-c*e1)
z4=(b*d-a*e1)/(b*f-c*e1)
plot(z3,z4,'+');
tspan = [0,50]; yzero=[0.5,1];
```

```
options = odeset('AbsTol', 1e-7,'RelTol', 1e-4);
[t,y]=ode45(@comp_equat,tspan,yzero,options,a,b,c,d,e1,f);
plot(y(:,1),y(:,2),'--'),title(''),grid
xlabel y_1(t),ylabel y_2(t)
tspan = [0,50]; yzero=[0.5,8];

[t,y]=ode45(@comp_equat,tspan,yzero,options,a,b,c,d,e1,f);
plot(y(:,1),y(:,2)),title(''),grid
xlabel y_1(t),ylabel y_2(t)
tspan = [0,50]; yzero=[4.5,9];

[t,y]=ode45(@comp_equat,tspan,yzero,options,a,b,c,d,e1,f);
plot(y(:,1),y(:,2)),title(''),grid
xlabel y_1(t),ylabel y_2(t)
tspan = [0,50]; yzero=[3.,1.7];

[t,y]=ode45(@comp_equat,tspan,yzero,options,a,b,c,d,e1,f);
plot(y(:,1),y(:,2)),title(''),grid
xlabel y_1(t),ylabel y_2(t)
hold off

function yprime = comp_equat(t,y,a,b,c,d,e1,f)
%comp_equat    competition equations
%         YPRIME = comp_equat(t,y,a,b,c,d,e,f)
yprime = [y(1)*(a-b*y(1)-c*y(2)); y(2)*(d-e1*y(1)-f*y(2))];
```

3.3 Lotka-Volterra Equations for More Than Two Populations

The general Lotka-Volterra equation for n populations is of the form

$$\dot{x}_i \;=\; x_i(r_i + \sum_{j=1}^{n} a_{ij}x_j) \qquad i = 1, \ldots, n \tag{3.9}$$

The x_i denote the densities; the r_i are intrinsic growth (or decay) rates, and the a_{ij} describes the effect of the j-th upon the i-th population, which is positive if it enhances and negative if it inhibites the growth. All sorts of

interactions can be modelled in the way, as long as one is prepared to assume that the influence of every species upon the growth rates is linear called the *interaction matrix*.

The state space is, of course, the positive orthant

$$\mathbf{R}^{\mathbf{n}}_{+} = \mathbf{x} = (x_1, \ldots, x_n) \in \mathbf{R}^{\mathbf{n}} : x_i \geq 0 \text{ for } i = 1, \ldots, n$$

The boundary points of $\mathbf{R}^{\mathbf{n}}_{+}$ lie on the coordinate planes $x_i = 0$, which correspond to the states where specifies i is absent. These "faces" are invariant, since $x_i(t) \equiv 0$ is the unique solution of the i-th equation of (3.7) satisfying $x_i(0) = 0$. In such a model, a missing species cannot "immigrate". Thus the boundary bd $\mathbf{R}^{\mathbf{n}}_{+}$ and consequently $\mathbf{R}^{\mathbf{n}}_{+}$ itself are invariant under (3.7). So is the interior int $\mathbf{R}^{\mathbf{n}}_{+}$, which means that if $x_i(0) > 0$ then $x_i(t) > 0$ for all t. The density $x_i(t)$ may approach 0, however, which means extinction.

The ecological equations of the last chapter where examples of (3.7) with $n = 2$. We shall see that all possible two dimensional cases can be classified. In higher dimensions, many open questions remain. In particular, numerical simulation shows that even the case of 3 populations may lead to some kind of *chaotic motion* the asymptotic behaviour of the solution consist of highly irregular oscillations and depends in a very sensitive way upon the initial conditions. The long term outcome, in such a case, in unpredictable.

In this section, we shall describe a few general results about (3.7) and then turn to some special cases of biological interest.

We will apply **LaSalle's extension theorem** of Lyapunov stability. We note the following definition and the theorem.

Let $\dot{x} = f(x)$ be a system of differential equations. The vector-valued function $f(x)$ is continuous in x for $x \in \bar{G}$ where G is an open set in R^n. Let V be a C^1 function on R^n to R.

Definition 3.1 *We say V is Lyapunov function in G for $\dot{x} = f(x)$ if $\dot{V} = gradV.f \leq 0$ on G.*

Let $E = x \in \bar{G} : \dot{V}(x) = 0$.

Theorem 3.1 *If V is a Lyapunov function in G for $\dot{x} = f(x)$, then each bounded solution $x(t) \subseteq G$ of $\dot{x} = f(x)$ approaches M where M is the largest invariant in set E.*

3.3.1 Interior equilibria

The equilibrium point of (3.7) in *int* $\mathbf{R}^{\mathbf{n}}_{+}$ are the solutions of the linear equations

$$r_i + \sum_{j=1}^{n} a_{ij} x_j = 0 \quad i = 1, \ldots, n \tag{3.10}$$

whose components are postivie. (The equilibria on the boundary faces of $\mathbf{R}^{\mathbf{n}}_{+}$ can be found in similar way: one has only to note that the restriction of (3.7) to any such face is again of Lotka-Volterra type.)

Theorem 3.2 *Int* $\mathbf{R}^{\mathbf{n}}_{+}$ *contains* α- *or* ω- *limit points if and only if (3.7) admits an interior equilibrium.*

One direction of this proposition is trivial. A rest point coincides with its own α- and ω- limit. It is a converse which is of interest, since it is (in principle) not hard check. If (3.8) admits positive solutions. If it does not, then every orbits has to converge to the boundary, or to infinity. In particular, if int $\mathbf{R}^{\mathbf{n}}_{+}$ contains a periodic orbit, it must also contains a rest point.

In order to prove the converse, let $L : \mathbf{x} \to \mathbf{y}$ be defined by

$$y_i = r_i + \sum_{j=1}^{n} a_{ij} x_j \qquad i = 1, \ldots, n$$

If (3.7) admits no interior equilibrium, the set $K = L(int\ \mathbf{R}^{\mathbf{n}}_{+})$ is disjoint from $\mathbf{0}$ A well known theorem from convex analysis implies that there exists a hyperplane H trough $\mathbf{0}$ which is disjoint from the convex set K. Thus there exists a vector $\mathbf{c} = (c_1, \ldots, c_n) \neq 0$ which is orthogonal to H ($\mathbf{c}.\mathbf{x} = 0$ for all $x \in H$) such that $\mathbf{c}.\mathbf{y}$ is positive for all $y \in K$. Setting

$$V(\mathbf{x}) = \sum c_i \log x_i, \tag{3.11}$$

we see that V is defined on int $\mathbf{R}^{\mathbf{n}}_{+}$. If $\mathbf{x}(t)$ is solution of (3.7) in int $\mathbf{R}^{\mathbf{n}}_{+}$, then the time derivative of $t \to V(\mathbf{x}(t))$ satisfies

$$\begin{aligned} \dot{V} &= \sum c_i \frac{\dot{x}_i}{x_i} \\ &= \sum c_i y_i = \mathbf{c}.\mathbf{y} > 0 \end{aligned}$$

Thus V is increasing along each orbit. But then no point $\mathbf{y} \in int\mathbf{R}^{\mathbf{n}}_{+}$ may belong to its ω- limit: indeed, by Lyapunov's theorem, the derivative $\dot{V}$ would have to vanish there. This contradiction completes the proof. It also shows: **Corollary**: *If (3.7) admits no interior equilibrium, then it is gradient-like in int* $\mathbf{R}^{\mathbf{n}}_{+}$.

In general (3.8) will admit one solution in int $\mathbf{R}^{\mathbf{n}}_{+}$, or none at all. It is only in the "degenerate" case $detA = 0$ that (3.7) can have more than one solution: these will form a continuum of rest points.

3.3.2 The Lotka-Volterra equation for food chains

Let us investigate food chains with n members (chains with up to six members are found in nature). The first population is the prey for second, which is the prey for the third etc. ... up to the n-th, which is at the top of the food pyramid. Taking competition within each species into account, and assuming constant interaction terms, we obtain

$$\begin{aligned} \dot{x}_1 &= x_1(r_1 - a_{11}x_1 - a_{12}x_2) \\ \dot{x}_j &= x_j(-r_j + a_{j,j-1}x_{j-1} - a_{jj}x_j - a_{j,j+1}x_{j+1}) \quad j = 2, \ldots, n-1 \\ \dot{x}_n &= x_n(-r_n + a_{n,n-1}x_{n-1} - a_{nn}x_n) \end{aligned} \tag{3.12}$$

with all $r_j, a_{ij} > 0$. The case $n = 2$ is just **vynechane**. We shall presently see that the general case leads to nothing new:

Theorem 3.3 *If (3.10) admits an interior equilibrium $\bar{x}$, then $\bar{x}$ is globally stable in the sense that all orbits in int* $\mathbf{R}^{\mathbf{n}}_{+}$ *converge to $\bar{x}$.*

In order to prove this we write (3.10) as $\dot{x_i} = x_i\omega_i$ and try

$$V(x) = \sum c_i(x_i - \bar{x}_i \log x_i) \tag{3.13}$$

for suitably chosen c_i, as a Ljapunov function in int $\mathbf{R}^{\mathbf{n}}_{+}$. Clearly

$$\dot{V}(x) = \sum c_i(\dot{x}_i - \bar{x}_i\frac{\dot{x}_i}{x_i}) = \sum c_i(x_i\omega_i - \bar{x}_i\omega_i) = \sum c_i(x_i - \bar{x}_i)\omega_i. \tag{3.14}$$

Since $\bar{x}$ is an equilibrium, we have

$$r_j = a_{j,j-1}\bar{x}_{j-1} - a_{jj}\bar{x}_j - a_{j,j+1}\bar{x}_{j+1}$$

for $j = 2, \ldots, n-1$, and similar equation for $j = 1$ or n. This implies

$$\omega_j = a_{j,j-1}(x_{j-1} - \bar{x}_{j-1}) - a_{jj}(x_j - \bar{x}_j) - a_{j,j+1}(x_{j+1} - \bar{x}_{j+1})$$

Writing $y_i = x_j - \bar{x}_j$, we obtain from (3.12)

$$\dot{V} = -\sum_{j=1}^{n} c_j a_{jj} y_j^2 + \sum_{j=1}^{n-1} y_j y_{j+1}(-c_j a_{j,j+1} + c_{j+1} a_{j+1,j}). \tag{3.15}$$

We are still free to choose the constants $c_j > 0$. Let us do it in such a way that

$$\frac{c_{j+1}}{c_j} = \frac{a_{j,j+1}}{a_{j+1,j}} \tag{3.16}$$

holds for $j = 1, \ldots, n$. (3.14) then implies

$$\dot{V} = -\sum c_j a_{jj}(x_j - \bar{x}_j)^2 \leq 0. \tag{3.17}$$

Let us consider the Volterra model for m species predator-prey systems in the form:

$$\dot{x}_i = x_i \left(b_i + \sum_{j=1}^{n} a_{ij} x_j \right), \qquad i, j = 1, \ldots, m \tag{3.18}$$

under the assumptions $a_{ij} a_{ji} \leq 0$, $a_{ii} \leq 0$. The following theorem holds.

Theorem 3.4 *If the nontrivial equilibrium* $(\bar{x_1}, \ldots, \bar{x_m})$ *of the model (3.16) is feasible and there exists a constant positive diagonal matrix* $\boldsymbol{C}$ *such that* $\mathbf{CA} + \mathbf{A^T C}$ *is negative definite, then the Lotka-Volterra model is globally stable in the feasible region.*

To prove this theorem Goh used the scalar Lyapunov function

$$V = \sum_{i=1}^{m} c_i(x_i - \bar{x}_i - \bar{x}_i \ln x_i/\bar{x}_i), \quad c_i > 0.$$

3.4 General mathematical model

In population dynamics and many other application of modelling, state space lies in the nonnegative orthant. Recall that the *positive orthant* of $n-$ *dimensional* state space contains all points $x = (x_1, x_2, ..., x_n)$ with each $x_i > 0$. The *nonnegative orthant* (R_+^n) refers to point $x_i \geq 0$.

For a given type of model, how can we be certain that embarrassing negative population do not arise? In other words, we want to be sure that solution or trajectories that start in the nonnegative orthant are trapped therein.

Suppose the system of differential equations in the form

$$\dot{x_i} = x_i g(x,t) + h_i(x,t)$$

where each $h_i(x,t)$ is nonnegative for $x \in R_+^n$.

The following is a simple theorem which has extensive fortunate implications for ecosystem modelling.

Theorem 3.5 *Let*

$$\dot{x_i} = x_i g(x,t) + h_i(x,t)$$

where: each $g_i(x,t)$ and each $h_i(x,t)$ is defined and continuous for all $x \in R_+^n$ and all t and $h_i(x,t) \geq 0$ for $i = 1, 2, \ldots, n$. Then all solutions with initial value $x_0 = (x_{01}, x_{02}, \ldots, x_{0n}) \in R_+^n$ are nonnegative for all $t \geq 0$.

Well-posed system: 1. there exists a solution, 2. the solution is unique, 3. the solution depends continuously on the initial data.

Let us consider a general differential equation.

$$\dot{x_i} = f_i(x,t) \quad for i \; = \; 1, 2, ..., n$$

Note 3.1 *A similar theorem holds for the following differential equations*

$$\dot{x_i} = f_i(x,t)$$

where $f_i(x_1, x_2, \ldots, x_{i-1}, 0, x_{i+1}, \ldots, x_n, t) \geq 0$ for all $x \in R_+^n$.

Definition 3.2 *For the differential equation of the form*

$$\frac{dx}{dt} = f(x) \tag{3.19}$$

the value $\bar{x}$ *is called an equilibrium if* $f(\bar{x}) = 0$.

Observe that if $\bar{x}$ is an equilibrium, then the constant function $x(t) = \bar{x}$ satisfies equation (2.10) and so $x(t) = \bar{x}$ is called an equilibrium solution of (3.17).

In order to describe the behaviour of the solution near an equilibrium we introduce the process of *linearization*. If $\bar{x}$ is an equilibrium of the differential equation $\dot{x} = f(x)$ so that $f(\bar{x}) = 0$, we make the change of variable $u(t) = x(t) - \bar{x}$. Substitution gives

$$\frac{dx}{dt} = f(u(t) + \bar{x})$$

The *linearization* of the differential equation at the equilibrium $\bar{x}$ is defined to be the linear homogeneous differential equation

$$\frac{dv}{dt} = \frac{df(\bar{x})}{dx} v \tag{3.20}$$

The importance of the linearization lies in the fact that the behaviour of its solution is easy to analyse.

Theorem 3.6 *If all solution of the linearization* (3.18) *at an equilibrium* $\bar{x}$ *tend to zero as* $t \to \infty$ *then all solution of* (3.17) *with x(0)sufficiently close to* $\bar{x}$ *tend to the equlibrium* $\bar{x}$ *as* $t \to \infty$.

Definition 3.3 *An equilibrium* $\bar{x}$ *is said to be stable if for every* $\epsilon > 0$ *there exists* $\delta >$*) such that* $|x(0) - \bar{x}| < \delta$ *implies* $|x(t) - \bar{x}| < \epsilon$ *for all* $t > 0$. *An equilibrium is said to be asymptotically stable if it is stable and if in addition* $|x(0) - \bar{x}| < \delta$ *implies* $\lim_{t\to\infty} x(t) = \bar{x}$.

We now examine a concept called asymptotic stability in the context of linear system of ODEs. The following fundamental result applies to constant coefficient systems.

Theorem 3.7 *Let A be a constant matrix with eigenvalues*

$$\lambda_1, \lambda_2, \ldots, \lambda_n.$$

Equilibrium $\bar{x} = 0$ of linear differential equation $\dot{x}(t) = Ax(t)$ is asymptotically stable if and only if all eigenvalues of the matrix has negative real part.

Now we recall some classic Hopf bifurcation theorem for the following system of ODDEs

$$\dot{x} = f(x, \mu),$$

where $f(0, \mu) = 0$ for μ in a neighborhood of 0.

Assume that $A(\mu) = \frac{df(0,\mu}{dx}$ has a pair of complex conjugate eigenvalues λ and $\bar{\lambda}$ such that $\lambda(\mu) = \alpha(\mu) + i\omega(\mu)$, where $\alpha(0) = 0$, $\omega(0) = \omega_0 > 0$, $\alpha'(0) \neq 0$, and the remaining $n - 2$ eigenvalues have strictly negative real parts. Then the system has a family of periodic solution.

3.4.1 Eigenvalues

Let $\mathbf{A}$ be a square matrix of dimension n x n and let $\mathbf{v}$ be a vector of dimension n. The product $\mathbf{Y} = \mathbf{Av}$ can be viewed as a linear transformation from n-dimensional space into itself. We want to find scalars λ for which there exists a nonzero vector $\mathbf{v}$ such that

$$\mathbf{Av} = \lambda\mathbf{v}; \tag{3.21}$$

that is, the linear transformation $T(\mathbf{v}) = \mathbf{Av}$ maps $\mathbf{v}$ onto the multiple $\lambda\mathbf{v}$. When this ocours, we call $\mathbf{v}$ an eigenvector that corresponds to the eigenvalue λ, and together they form the eigenpair $\lambda, \mathbf{v}$ for $\mathbf{v}$. In general, the scalar λ and vector $\mathbf{v}$ can involve complex numbers. For simplicity, most of our illustrations will involve real calculations. However, the techniques are easily extended to the complex case. The identity matrix $\mathbf{I}$ can be used to express equation (3.19) as

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{v} = 0. \tag{3.22}$$

The significance of equation (3.20) is that the product of the matrix $(\mathbf{A} - \lambda\mathbf{I})$ and the nonzero $\mathbf{v}$ is the zero vector! This linear system has nontrivial solutions if and only if the matrix $\mathbf{A} - \lambda\mathbf{I}$ is singular, that is,

$$det(\mathbf{A} - \lambda\mathbf{I}) = 0. \tag{3.23}$$

This determinant can be written in the form

$$\begin{vmatrix} a_{11} - \lambda & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} - \lambda & \dots & a_{2n} \\ \vdots & \vdots & \dots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} - \lambda \end{vmatrix} = 0. \tag{3.24}$$

When the determinant in (3.22) is expanded, it becomes a polynomial of degree n, which is called the characteristic polynomial

$$\begin{aligned} p(\lambda) &= det(\mathbf{A} - \lambda\mathbf{I}) \\ &= (-1)^n(\lambda^n + c_1\lambda^{n-1} + c_2\lambda^{n-2} + \ldots + c_{n-1}\lambda + c_n) \end{aligned} \tag{3.25}$$

There exists exactly n roots (not necessarily distinct) of a polynomial of degree n. Each root λ can be substituted into equation (5.31) to obtain an underdetermined system of equation that has a corresponding nontrivial solution vector $\mathbf{v}$. If λ is real, a real eigenvector $\mathbf{v}$ can be constructed. For emphasis, we state the following definitions.

Definition 3.4 ***Eigenvalue***. *If* $\mathbf{A}$ *is an n x n real matrix, then its n eigenvalues* $\lambda_1, \lambda_2, \ldots, \lambda_n$ *are the complex roots of the characteristic polynomial*

$$p(\lambda) = det(\mathbf{A} - \lambda\mathbf{I}). \tag{3.26}$$

Definition 3.5 ***Eigenvector***. *If* λ *is an eigenvalue of* $\mathbf{A}$ *and the nonzero vector* $\mathbf{A}$ *has the property that*

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}, \tag{3.27}$$

then $\mathbf{V}$ *is called an eigenvector of* $\mathbf{A}$ *corresponding to the eigenvalue* λ.

Consider the characteristic equation

$$|\lambda\mathbf{I} - \mathbf{A}| = \lambda^n + b_1\lambda^{n-1} + \ldots + b_{n-1}\lambda + b_n = 0$$

determining the n eigenvalues λ of each real n x n square matrix $\mathbf{A}$, where $\mathbf{I}$ is the identity matrix. Then the eigenvalues λ all have negative real parts if

$$\Delta_1 > 0, \Delta_2 > 0, \ldots, \Delta_n > 0,$$

where

$$\Delta_k = \begin{vmatrix} b_1 & 1 & 0 & 0 & 0 & 0 & \ldots & 0 \\ b_3 & b_2 & b_1 & 1 & 0 & 0 & \ldots & 0 \\ b_5 & b_4 & b_3 & b_2 & b_1 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ldots & \vdots \\ b_{2k-1} & b_{2k-2} & b_{2k-3} & b_{2k-4} & b_{2k-5} & b_{2k-6} & \ldots & b_k \end{vmatrix}$$

Particularly for a given n we have the following Routh-Hurwitz condition:
n=1
The polynomial $P(x) = x + a$ is stable if $a > 0$.
n=2
$P(x) = x^2 + ax + b$ is stable if $a > 0, b > 0$.
n=3
$P(x) = x^3 + ax^2 + bx + c$ is stable if $a > 0, b > 0, 0 < c < ab$.
n=4
$P(x) = x^4 + ax^3 + bx^2 + cx + d$ is stable if $a > 0, b > 0, 0 < c < ab, 0 < d < \frac{(abc-c^2)}{a^2}$.

3.5 Competition partial differential equation

Let us consider the following competition system with diffusion

$$\begin{aligned} \frac{\partial}{\partial t} y_1(x,t) &= D_1 \frac{\partial^2}{\partial t^2} y_1(x,t) + y_1(a_1 - a_2 y_2(x,t) - a_3 y_3(x,t)), \\ \frac{\partial}{\partial t} y_2(x,t) &= D_2 \frac{\partial^2}{\partial t^2} y_2(x,t) + y_2(a_4 - a_5 y_3(x,t)), \\ \frac{\partial}{\partial t} y_3(x,t) &= D_3 \frac{\partial^2}{\partial t^2} y_3(x,t) + y_3(-a_8 + a_6 y_1(x,t) + a_7 y_2(x,t)), \end{aligned}$$

with Neumann boundary condition

$$\frac{\partial}{\partial x} y_i(x,t) = 0, \ x = 0, \pi, \ t \geq 0, \tag{3.28}$$

and initial conditions

$$y_i(x,0) \ = \ \phi_i(x) \geq 0, \ 0 \leq x \leq \pi, \tag{3.29}$$

where D_i, a_i are all positive constant.
Let us denote $\bar{x} = \left(\bar{x}_3 = \frac{a_4}{a_5}, \bar{x}_2 = \frac{a_1 - a_3\bar{x}_3}{a_2}, \bar{x}_1 = \frac{a_8 - a_7\bar{x}_3}{a_6}\right)$.
If $x_i > 0$ then we have a positive spatially homogeneuos equilibrium and the linearisation around this equilibrium takes the form

$$\begin{aligned}
\frac{\partial}{\partial t} y_1(x,t) &= D_1 \frac{\partial^2}{\partial t^2} y_1(x,t) + \bar{y}_1(-a_2 y_2(x,t) - a_3 y_3(x,t)), \\
\frac{\partial}{\partial t} y_2(x,t) &= D_2 \frac{\partial^2}{\partial t^2} y_2(x,t) + \bar{y}_2(-a_5 y_3(x,t)), \\
\frac{\partial}{\partial t} y_3(x,t) &= D_3 \frac{\partial^2}{\partial t^2} y_3(x,t) + \bar{y}_3(a_6 y_1(x,t) + a_7 y_2(x,t)),
\end{aligned}$$

Let $X = C([0,\pi]; R^3)$ As the Laplace operator has eigennvalues $-k^2$, $k = 0, 1, ...$ with corresponding eigenfunctions $coskx$, λ is a characteristic value of the linearization if and only if for some $k = 0, 1, ...$ λ is a solution of characteristic equation

$$\lambda v \ = (-k^2 D + J)v \ , k = 0, 1, \ldots,$$

where J is a Jacobi matrix and D is a diagonal matrix, with $d_{ii} = d_i$.
The characteristic equation obtained from the linearization is given by:

$$\begin{aligned}
\lambda^3 + A_1(k)\lambda^2 + A_2(k)\lambda + A_3(k) = 0, \ where \\
A_1(n) = k^2(d_1 + d_2 + d_3) \\
A_2 = k^4(d_2 d_3 + d_1(d_1 + d_2)) + a_3 a_6 \bar{x}_1 \bar{x}_3 + a_5 a_7 \bar{x}_2 \bar{x}_3 \\
A_3 = k^6 d_1 d_2 d_3 + n^2(d_2 a_3 a_6 \bar{x}_1 \bar{x}_3 + d_1 a_5 a_7 \bar{x}_2 \bar{x}_3) - a_2 a_5 a_6 \bar{x}_1 \bar{x}_2 \bar{x}_3.
\end{aligned}$$

To test the stability we use Routh-Hurwitz criterion. For $k = 0$ we have $A_1(k) = 0$ which means the instability of the equilibrium point $\bar{x}$. The following $M - file$ gives a numerical solution of the system.

```
function  carasius
%Reaction-diffusion competition system
% Solves the PDE
global a1 a2 a3 a4 a5 a6 a7 a8 d1 d2 d3
a2=0.93; a3=0.1;
a4=0.19; a5=0.2;
a6=1; a7=0.05;
a8=0.2; d1=0.01;
d2=0.03; d3=0.009;
%a1=1.01;
a1=0.1
m=0;
xmesh = linspace(0,3.14,45);
tspan = linspace(0,100,250);
sol = pdepe(m,@mbpde,@mbic,@mbbc,xmesh,tspan);
u1 = sol(:,:,1);
u2 = sol(:,:,2);

subplot(121)
surf(xmesh,tspan,u1)
xlabel('x', 'Fontsize', 12)
ylabel('t','Fontsize', 12)
title('u_1','FontSize', 16)

subplot(122)
surf(xmesh,tspan,u2)
xlabel('x','Fontsize', 12)
ylabel('t','Fontsize', 12)
title('u_2','FontSize', 16)

% --------------------------------------------------------------
% Subfunction
% --------------------------------------------------------------
```

```
function [c,f,s] = mbpde(x,t,u,DuDx)
global a1 a2 a3 a4 a5 a6 a7 a8 d1 d2 d3
c=[1,1,1];
f = [d1;d2;d3].*DuDx;
s = [u(1)*(a1-a2*u(2)-a3*u(3)); u(2)*(a4-a5*u(3));
u(3)*(-a8+a6*u(1)+a7*u(2))];

% --------------------------------------------------------------------
function u0 = mbic(x);
u0 = [1; 1; 1];

% --------------------------------------------------------------------
function [pa,qa,pb,qb] = mbbc(xa,ua,xb,ub,t)
pa = [0,0,0];
qa = [1,1,1];
pb = [0,0,0];
qb = [1,1,1];
```

3.6 Predator-Prey partial functional differential equation

Let us consider the following predator-prey system with diffusion and a discrete time delay

$$\frac{\partial}{\partial t}M(x,t) = D_1\frac{\partial^2}{\partial t^2}M(x,t) + M(x,t)(a - bM(x,t) - cN(x,t)), \quad (3.30)$$
$$\frac{\partial}{\partial t}N(x,t) = D_2\frac{\partial^2}{\partial t^2}N(x,t) + lN(x,t)(M(x,t-\tau) - \beta),$$

with Neumann boundary condition

$$\frac{\partial}{\partial x}M(x,t) = \frac{\partial}{\partial x}N(x,t) = 0,\ x = 0,\pi,\ t \geq 0,$$

and initial conditions

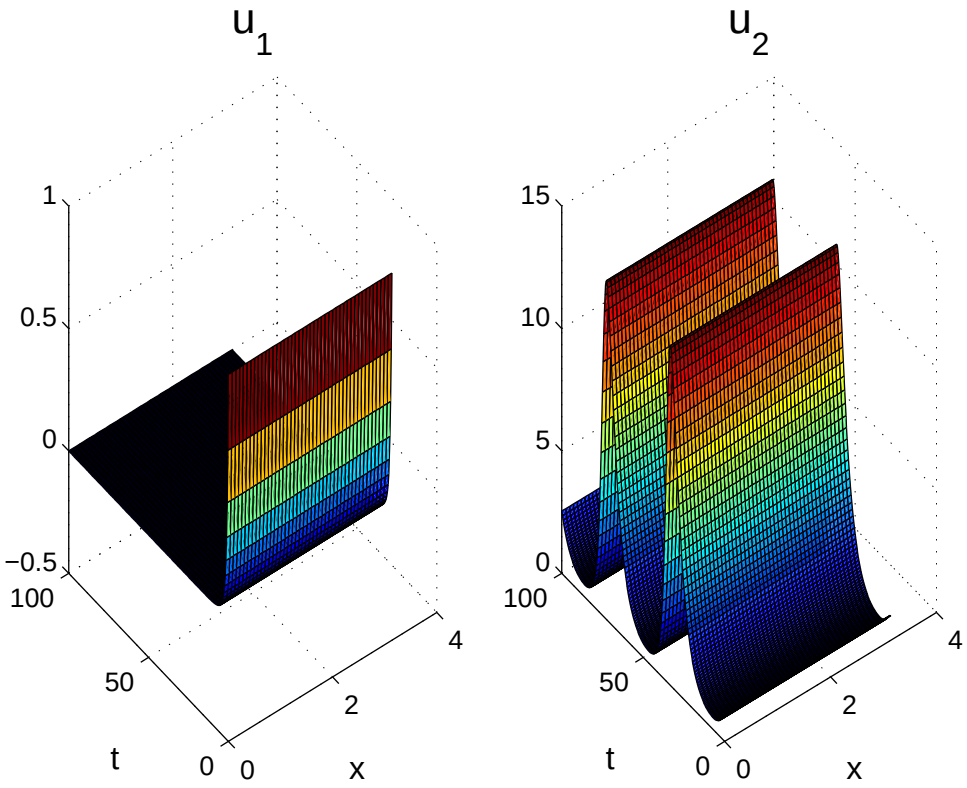

Figure 3.4: Numerical solution

$$N(x,t) \;=\; \phi(x,t) \geq 0,\ 0 \leq x \leq \pi,\ t \in \langle -\tau, 0 \rangle$$

where $D_1, D_2, a, b, c, l, \tau, \beta$ are all positive constant.
Let $u(x,t) = M(x,\tau t), v(x,t) = N(x,\tau t)$. We get

$$\frac{\partial}{\partial t}u(x,t) = \tau D_1 \frac{\partial^2}{\partial t^2}u(x,t) + \tau u(x,t)(a - bu(x,t) - cv(x,t)),$$
$$\frac{\partial}{\partial t}v(x,t) = \tau D_2 \frac{\partial^2}{\partial t^2}v(x,t) + \tau l v(x,t)(u(x,t-1) - \beta),$$

$$\frac{\partial}{\partial x}u(x,t) = \frac{\partial}{\partial x}v(x,t) = 0,\ x = 0,\pi,\ t \geq 0,$$

If $a > b\beta$ then we have a positive spatially homogeneuos equilibrium $(\beta, \frac{a-b\beta}{c})$ and the linearization around this equilibrium takes the form

$$\frac{\partial}{\partial t}y_1(x,t) = \tau D_1 \frac{\partial^2}{\partial t^2}y_1(x,t) + \tau b\beta y_1(x,t) - c\beta\tau y_2(x,t)),$$
$$\frac{\partial}{\partial t}y_2(x,t) = \tau D_2 \frac{\partial^2}{\partial t^2}y_2(x,t) + \tau l\frac{a-b\beta}{c}y_1(x,t-1),$$

Let $X = C([0,\pi]\,; R^2)$ As the Laplace operator has eigennvalues $-k^2,\ k = 0,1,...$ with corresponding eigenfunctions $coskx$, λ is a characteristic value of the linearization if and only if for some $k = 0,1,...$ λ is a solution of characteristic equation $H(\lambda) \equiv det\Delta(\lambda) = 0$, where

$$\Delta(\lambda) \ = \ -\lambda I - \begin{pmatrix} b\beta\tau + \tau D_1 k^2 & c\beta\tau \\ -l\frac{a-b\beta}{c}\tau e^{-\lambda)} & D_2\tau k^2 \end{pmatrix}.$$

That is λ solves

$$\lambda^2 + \tau(b\beta + D_1k^2 + D_2k^2)\lambda + \tau^2 D_2k^2(b\beta + D_1k^2) + l\beta\tau^2(a-b\beta)e^{-\lambda} \ = \ 0$$

We need the following result:

Theorem 3.8 *Consider the equation*

$$\lambda^2 + p\lambda + q(\gamma)e^{-\lambda} + v \ = \ 0,$$

where $p > 0,\ v \in \langle 0, \pi/2\rangle$ are given constants, $q(\gamma)$ is continuously differentiable and satisfies $q(\gamma) > 0$ and $q'(\gamma) > 0$ in a neighborhood of γ_0, $gamma_0$ is a real number such that

$$q(\gamma_0) \ = \ p\frac{\omega_0}{sin\omega_0},$$

$\omega_0 \in (0,\pi/2)$is the unique solution of

$$\frac{p\omega_0}{\omega^2 - v} = \tan\omega.$$

Then $\pm i\omega_0$ *are zeros of equation with* $\gamma = \gamma_0$ *and all others zeros with* $\gamma = \gamma_0$ *have negative real parts. Moreover, if* $\lambda(\gamma)$ *is the smooth curve of root such that* $\lambda(\gamma_0) = i\omega_0$, *then* $Re\frac{d}{d\gamma}\lambda(\gamma_0) > 0$.

By this theorem, we can see that if $k = 1$ and

$$\tau^2 D_2(b\beta + D_1) < \frac{\pi}{2}$$

then at $l = l_0$, where

$$l_0 = \frac{b\beta + D_1 + D_2}{\beta\tau(a - b\beta)} \frac{\omega_0}{\sin\omega_0}$$

and

$$\frac{(b\beta + D_1 + D_2)\omega_0}{\omega_0^2 - \tau^2 D_2(b\beta + D_1)} = \tan\omega_0,$$

equation has a pair of purely imaginnary zeros $\pm i\omega_0$ and all other zeros have negative real parts. moreover if $\lambda(l)$ is the smooth curve of root such that $\lambda(l_0) = i\omega_0$, then $Re\frac{d}{dl}\lambda(l_0) > 0$. Assume further that

$$\frac{l_0\beta\tau(a - b\beta)}{b\beta + 4(D_1 + D_2)} < 1.$$

By this assumption the following theorem holds.

Theorem 3.9 *If* τ, $D_1 + D_2$ *are sufficiently small,*

$$\frac{l_0\beta\tau(a - b\beta)}{b\beta + 4(D_1 + D_2)} < 1,$$

and

$$\tau^2 D_2(b\beta + D_1) < \frac{\pi}{2},$$

then system $(x.x)$ *has a family of periodic solutions bifurcating fom the spatially constant equilibrium* $(\beta, \frac{a - b\beta}{c})$, *when* l *is near* l_0.

Chapter 4

The Chemostat

4.1 Single Chemostat

A chemostat is a piece laboratory apparatus used to cultivate bacteria. It consists of a reservoir containing a nutrient, a culture vessel in which the bacteria are cultivated, and an output receptacle.

Nutrient is pumped from the reservoir to the culture vessel at a constant rate and bacteria are collected in receptacle by pumping the contents of the culture vessel out at the same constant rate. The process is called continuous culture of bacteria. We wish to describe the behavior of the chemostat by modeling the number of bacteria and nutrient concentration. We shall sketch the classical theory of the simple chemostat due to Novick and Szilard (1950) and Monod (1950). We will obtain a model for two interacting population that describes a laboratory realization of a very simple lake. More complicated chemostats, in which two or more cultures are introduced, give multispecies models representing more complicated real word situations. We let y present the number of bacteria and C the concentration of nutrient in the chemostat, both function of t. Let V be the volume of the chemostat and Q the rate of flow into the chemostat from the nutrient reservoir and also the rate of flow out from the chemostat. The fixed concentration of nutrient in the reservoir is a constant $C^{(0)}$.We assume that the average per capita bacterial birth rate is a function $b(C)$ of the nutrient concentration and that the rate of nutrient consumption of an individual bacterium is proportional to $b(C)$, say $\alpha b(C)$. Then the rate of charge of population is the birth rate $b(C)y$of bacteria minus the outflow rate $Q.y/V$. The rate of charge of nutri-

ent volume is the replenshment rate $QC^{(0)}$ minus outflow rate QC minus the consumption rate $\alpha b(C)$. This gives the pair off differential equations

$$\begin{aligned} \dot{y} &= b(C).y - q.y \\ \dot{C} &= q(C^{(0)} - C) - \beta b(C).y, \end{aligned}$$

where $q = Q/V$ and $\beta = \alpha/V$.
It is reasonable to assume that the function $b(C)$ is zero if $C = 0$ and that it saturates when C becomes large. The simplest function with these properties is

$$b(C) = \frac{aC}{C + A},$$

where a and A are constants, and this was the choise originally made by Monod. The explicit chemostat model is now

$$\begin{aligned} \dot{y} &= \frac{aCy}{A + C} - qy \\ \dot{C} &= q(C^{(0)} - C) - \frac{\beta aCy}{A + C}, \end{aligned}$$

4.2 Limiting behavior for competing species

Two competition models concerning n species consuming a single, limited resource are discussed. One in based on the Holing-type functional response and other on the Lotka-Valterra-type. The focus of the paper is on the asymptotic behavior of solutions. LaSalle's extension theorem of Lyapunov stability theory is the main tool.

1. Introduction. The section is concerned with the limiting behavior, as $t \to +\infty$, for the solutions of the system

$$\begin{aligned} \dot{S}(t) &= (S^{(0)} - S(t))D - \sum_{i=1}^{n} \frac{k_i x_i(t) S(t))}{a_i + S(t)} \\ \dot{x}_i(t) &= \frac{m_i x_i(t) S(t)}{a_i + S(t)} - D_i x_i(t), \qquad i = 1, \ldots, n \end{aligned} \tag{4.1}$$

where $S^{(0)}, D, k_i, a_i, m_i, D_i$ are positive. Only the positive solutions are analyzed, because they are of realistic interest.

The system (4.2) describes n species, with populations x_i, $i = 1, \ldots, n$, and death rates D_i competing for a single, limited resource S. This generalizes the model (4.1) by allowing species-specific death rates. The species are

assumed to feed on the resource with a saturating functional response to the resource density. Specifically we assume that Michaelis-Menten kinetics or the Holling "disc" model describe how feeding rates and birth rates change in increasing resource density. Close parallels of this model in future are e.g. the plantkonics communities of unicellular algae in lake and oceans.

The mathematical future of this section is to apply LaSalle's extension theorem of Lyapunov stability theory. This technique allows us to generalize the results and to give simple, elegant proof. In this section, we will discuss the limiting behavior of solution of the system (4.2). First we note the following lemmas, omitting the proofs.

Lemma 4.1 *The solutions* $S(t), x(t), i = 1, \ldots, n$ *of* (4.1) *are positive and bounded.*

Lemma 4.2 *Let* $b_i = m_i/D_i$, $\lambda_i = a_i/(b_i - 1), i = 1, \ldots, n$. *If*

$$(i) \qquad b_i \leq 1$$

or

$$(ii) \qquad \lambda_i > S^{(0)},$$

then $\lim_{t\to\infty} x_i(t) = 0$.

Our basic hypothesis is (H_n)

$$0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n, \qquad \lambda_1 < S^{(0)}.$$

The equations in (4.2) may be relabeled without loss of generality, so that the parameters λ_i are nondecreasing in i.

Theorem 4.1 *Let* (H_n) *hold.*
(i) If $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$, *then the solutions of (4.1) satisfy*

$$\begin{aligned} \lim_{t\to\infty} S(t) &= \lambda_1, \\ \lim_{t\to\infty} x_1(t) &= x_1^* = \frac{(S^{(0)} - \lambda_1)(a_1 + \lambda_1)D}{k_1\lambda_1}, \\ \lim_{t\to\infty} x_i(t) &= 0 \qquad i = 2, 3, \ldots, n. \end{aligned} \tag{4.2}$$

(ii) If $0 < \lambda_1 = \ldots = \lambda_j < \lambda_{j+1} \leq \ldots \leq \lambda_n$, *for some* $j, 2 \leq j \leq n$, *then the trajectory of (4.1) approaches* M, *where*

$$M = \left\{(\lambda_1, x_1, \ldots, x_j, 0, \ldots, 0) : (S^{(0)} - \lambda_1)D = \sum_{i=1}^{j} \frac{k_i \lambda_i}{\lambda_i + a_i} x_i, x_i \geq 0, \quad i = 1, \ldots, j\right\}$$

Proof. A rearrangement of (4.2) yields

$$\begin{aligned} \dot{S}(t) &= (S^{(0)} - S(t))D - \sum_{i=1}^{n} \frac{k_i x_i(t) S(t)}{a_i + S(t)}, \\ \dot{x}(t) &= (m_i = D_i)\frac{S(t) - \lambda_i}{a_i + S(t)} x_i(t). \end{aligned}$$

Let

$$V(S, x_1, \ldots, x_n) = S - \lambda_1 - \lambda_1 . \ln\left(\frac{S}{\lambda_1}\right) + c_1\left[(x_1 - x_1^*) - x_1^* . \ln\left(\frac{x_1}{x_1^*}\right)\right] + \sum_{i=2}^{n} c_i x_i,$$

and $G = \{(S, x_1, \ldots, x_n) : S > 0, \ x_i > 0, \ i = 1, \ldots, n\}$. Choose $c_i = k_i/(m_i - D_i), \ i = 1, \ldots, n$. Then time derivative of V computed along solution of the differential equation is

$$\dot{V} = (S - \lambda_1)\left[\frac{(S^{(0)} - S)}{S} D - \frac{k_1 x_1^*}{a_1 + S}\right] + \sum_{i=2}^{n} k_i(\lambda_1 - \lambda_i)\frac{x_i}{a_i + S}$$

or

$$\dot{V} = \frac{(S - \lambda_1)^2 D}{(a_1 + S) S \lambda_1}(-\lambda_1 S - a_1 S^{(0)}) + \sum_{i=2}^{n} k_i(\lambda_1 - \lambda_i)\frac{x_i}{a_i + S} \leq 0 \text{ on } G. \quad (4.3)$$

If $0 < \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n$, then

$$E = \{(\lambda_1, x_1, \ldots, x_j, 0, \ldots, 0) : x_1 \geq 0\}$$

and the largest invariant set M in E is $\{(\lambda_1, x_1^*, 0, \ldots, 0)\}$. Hence (4.4) follows directly from Lemma4.1 and LaSalle's theorem.

If $0 < \lambda_1 = \ldots = \lambda_j < \lambda_{j+1} \leq \ldots \leq \lambda_n$ for some $j, \ 2 \leq j \leq n$, then from (4.4) we have

$$E = \{(\lambda_1, x_1, \ldots, x_j, 0, \ldots, 0) : x_1, \ldots, x_j \geq 0\}$$

and

$$M = \left\{(\lambda_1, x_1, \ldots, x_j, 0, \ldots, 0) : (S^{(0)} - \lambda_1)D = \sum_{i=1}^{j} \frac{k_i \lambda_1}{a_1 + \lambda_1} x_i, x_i \geq 0, \quad i = 1, \ldots, j\right\}$$

Hence the trajectory approaches M.

4.3 Asymptotic behavior of a chemostat with delayed response in growth

Let us consider the asymptotic behavior of solutions of a model of two species of microorganisms in a chemostat. The derivation of our model is as follows. The parameters are the folow rate of the chemostat denoted by $D > 0$ and the concentration of growth-limiting nutrient in the fresh infolowing medium denoted by $S^{(0)}$ The concenttration of nutrient external to cells at time t is assumed to be a continuous function $S(t)$. For $i = 1, 2$, species-specific per capacita nutrient uptake function is assumed to be a known continuous function $p_i : \langle 0, \infty \rangle$ with $p_i(0) = 0$, and the species-sfecific time delay in nutrient conversion is denoted by τ_i.

$$\begin{aligned} \dot{S}(t) &= (S^{(0)} - S(t))D - \sum_{i=1}^{2} p_i(S(t))x_i(t) \\ \dot{x_1}(t) &= -x_1(t))D + e^{D\tau_1} p_1(S(t))x_1(t - \tau_1) \qquad (4.4) \\ \dot{x_2}(t) &= -x_2(t))D + e^{D\tau_2} p_2(S(t))x_2(t - \tau_2) \end{aligned}$$

$$(4.5)$$

in the unknowns $S(t), x_1(t)$ and $x_2(t)$ with continuous nonnegative initial data $S(t) = \phi_0(t), x_i(t) = \phi_i(t), t \in \langle -\tau, 0 \rangle$. Throughout our analysis of chemostat we assume that D and $S^{(0)}$ are positive constant, that τ_1, τ_2 are positive constant with $\tau = max\{\tau_1, \tau_2\}$ and the function $p_i : \langle 0, \infty \rangle$ are continuously differentiable and bounded with $p_i(0) = 0$ and $p_i'(\xi) > 0$ for $\xi \geq 0$. The equilibruim points of (4.6) depend on the parameters of the model. Let a_i and b_i for $i = 1, 2$, be defined by

$$a_i = \begin{cases} S^{(0)} & p_i(S^{(0)}) \leq De^{D\tau_i}, \\ p_i^{-1}(De^{D\tau_i}) & p_i(S^{(0)}) > De^{D\tau_i}, \end{cases}$$

$$b_i = e^{-D\tau_i}(S^{(0)}) - a_i)$$

The only possible eqilibrium points are

$$E_0 = (S^{(0)}, 0, 0), \ E_1 = (a_1, b_1, 0), \ E_2 = (a_2, 0, b_2).$$

Equilibrium points $E_1,\ E_2$ exist if and onlly if $a_i < S^{(0)}$. The stability of E_1 is determined by the stability of the trivial solution of the linearization, which can also be written as

$$\begin{aligned}
\dot{v}_0 &= -(D + p_1'(a_1)b_1)v_0(t) - De^{D\tau_i}v_1(t) - p_2(a_1)v_2(t), \\
\dot{v}_1 &= p_1'(a_1)b_1e^{-\tau_1 D}v_0(t-\tau) - Dv_1(t) - Dv_1(t-\tau_1) \\
\dot{v}_2 &= -Dv_2(t) + p_2(a_1)e^{-\tau_2 D}v_2(t-\tau_2).
\end{aligned}$$

Linearization has nontrivial solutions of the form

$$(v_0(t), v_1(t), v_2(t)) = (k_0e^{\lambda t}, k_1e^{\lambda t}, k_2e^{\lambda t})$$

if and only if λ is a root of the characteristic equation $H(\lambda) \equiv det\Delta(\lambda) = 0$, where

$$\Delta(\lambda) = \lambda I - \begin{pmatrix} -(D + p_1'(a_1)b_1 & -De^{D\tau_i} & -p_2(a_1) \\ p_1'(a_1)b_1e^{-\tau_1(D+\lambda)} & -D + De^{\lambda\tau_1} & 0 \\ 0 & 0 & -D + p_2(a_1)e^{-\tau_2(D+\lambda)} \end{pmatrix}.$$

Upon simplification, the charasteristic equation becomes

$$H(\lambda) = (\lambda + D)(\lambda + D + p_1'(a_1)b_1 - De^{-\tau_1\lambda})(\lambda + D - p_2(a_1)e^{-\tau_2(\lambda+D)}).$$

Theorem 4.2 *If A,B are real number, then all roots z of*

$$Ae^z + B - ze^z = 0$$

have negative real parts if and only if $A < 1$ *and* $A < -B < \sqrt{\alpha^2 + A^2}$, *where* α *is a root of* $\alpha = A\tan\alpha$, *such that* $0 < \alpha < \pi/2$. *If* $A = 0$, *then take* $\alpha = \pi/2$.

We conclude that E_1 is asymptotically stable if and only if $a_1 < a_2$.

4.4 Diffusive mathematical model of chemostat

Another alternative is empty to use one vessel and remove the the "well-stirred" hypothesis of the basic chemostat yielding a system of reaction-diffusion equations of the following form assuming equal diffucion rates:

$$\begin{aligned}
\frac{\partial S}{\partial t} &= d\frac{\partial^2 S}{\partial x^2} - \frac{m_1 S u}{a_1 + S} - \frac{m_2 S v}{a_2 + S}, \\
\frac{\partial u}{\partial t} &= d\frac{\partial^2 u}{\partial x^2} + \frac{m_1 S u}{a_1 + S}, \\
\frac{\partial v}{\partial t} &= d\frac{\partial^2 v}{\partial x^2} + \frac{m_2 S v}{a_2 + S}, \quad 0 < x < \pi,
\end{aligned} \tag{4.6}$$

with boundary conditions

$$\begin{aligned}
\frac{\partial S}{\partial x}(t,0) &= -S^{(0)}, \\
\frac{\partial u}{\partial x}(t,0) &= \frac{\partial v}{\partial x}(t,0) = 0,
\end{aligned}$$

$$\begin{aligned}
\frac{\partial S}{\partial x}(t,\pi) + rS(t,\pi) &= 0, \\
\frac{\partial u}{\partial x}(t,\pi) + ru(t,\pi) &= 0, \\
\frac{\partial v}{\partial x}(t,\pi) + rv(t,\pi) &= 0
\end{aligned} \tag{4.7}$$

and initial conditions

$$\begin{aligned}
S(0,x) &= S_0(x) \geq 0, \\
u(0,x) &= u_0(x) \geq 0, \qquad u_0(x) \neq 0, \\
v(0,x) &= v_0(x) \geq 0, \qquad v_0(x) \neq 0,
\end{aligned}$$

```
function  chemostat
% Reaction-diffusion chemostat system
```

```
% Solves the PDE
global a1 a2 m1 m2 d1 d2 d3 s0
d1=1;d2=1; d3=1;s0=1.;
a1=1; a2=1; m1=4; m2=1;
m=0;
xmesh = linspace(0,3.14,45);
tspan = linspace(0,10,50);
sol = pdepe(m,@mbpde,@mbic,@mbbc,xmesh,tspan);
u1 = sol(:,:,1);
u2 = sol(:,:,2);
u3 = sol(:,:,3);

subplot(131)
surf(xmesh,tspan,u1)
xlabel('x', 'Fontsize', 12)
ylabel('t','Fontsize', 12)
title('u_1','FontSize', 16)

subplot(132)
surf(xmesh,tspan,u2)
xlabel('x','Fontsize', 12)
ylabel('t','Fontsize', 12)
title('u_2','FontSize', 16)

subplot(133)
surf(xmesh,tspan,u3)
xlabel('x','Fontsize', 12)
ylabel('t','Fontsize', 12)
title('u_3','FontSize', 16)

% --------------------------------------------------------------
% Subfunction
% --------------------------------------------------------------

function [c,f,s] = mbpde(x,t,u,DuDx)
global a1 a2 m1 m2 d1 d2 d3 s0
c=[1,1,1];
f = [d1;d2;d3].*DuDx;
```

```
s = [-m1*u(1)*u(2)/(a1+u(1))-m2*u(1)*u(3)/(a2+u(1));
m1*u(1)*u(2)/(a1+u(1)); m2*u(1)*u(3)/(a2+u(1))];

% ------------------------------------------------------------------
function u0 = mbic(x);
u0 = [1; 1; 1];

% ------------------------------------------------------------------
function [pa,qa,pb,qb] = mbbc(xa,ua,xb,ub,t)
global a1 a2 m1 m2 d1 d2 d3 s0
pa = [s0,0,0];
qa = [1,1,1];
pb = [ub(1),ub(2),ub(3)];
qb = [1,1,1];
```

Chapter 5

Application of Optimal Control Theory

5.1 Nonlinear optimal problem

The Pontriagin maximum principle deals with the general control problem of maximizing an objective function

$$J(u) = \int_0^T g(t, y, u(t))dt, \tag{5.1}$$

where $u(t)$ is chosen from some class of admissible controlllers u on $0 \leq t \leq T$, with a state equation

$$\dot{y} = f(t, y(t, u(t))), \ y(0) = y_0 \tag{5.2}$$

terminal condition $y(t) = y_T$.

We define the Hamiltonian

$$H(t, y(t), u(t), \lambda(t)) = g(t, y, u) + \lambda f(t, y, u), \tag{5.3}$$

where Λ is an unknown function called the adjoint variable. The maximum principle says that if "u" is the optimal control and y the corresponding solution, then there is an adjoint variable λ such that

$$\frac{d\lambda}{dt} = -\frac{\partial g}{\partial y} - \lambda \frac{\partial f}{\partial y} \tag{5.4}$$

and the optimal control maximizes the value of the Hamiltonian over all admissiblle controllers for each t, that is

$$H(t, \hat{y}, \hat{u}, \lambda) = max_{u \in \Omega} H(t, \hat{y}, u, \lambda)$$

In general, we have three functions $y(t)$, $u(t)$, $\lambda(t)$ to determine, and three equations can be used for their determination.

We now give a interpretation of the maximum principle. The computations which lead to this interpretation actually can be redefined to give a proof of the maximum principle under the assumption that all functions invaloved are sufficiently smooth (twice differentiable). For a full proof, we refer the reader to the books of Pontriagin or Lee and Markus (1968).

We consider the problem of maximizing

$$J(u) = \int_{t_0}^{T} g(s, y(s), u(s))ds$$

subject to a state equation

$$\dot{y} = f(t, y, u)$$

with initial and terminal condition

$$y(t_0) = y_0 \; and \; y(t_1) = y_1.$$

The admissiable controllers "u(t)" on a specified finite interval $t_0 \leq t \leq T$ will constitute a certain family "F" of measmable m-vector functions.

Let we consider the initial point (t_0, y_0) as variable, assuming that an optimal control $\hat{u}(t)$ exists for all initial points (t_0, y_0) under consideration. For each initial point we define the function

$$w(t_0, y_0) = J[\hat{u}] = max J[\hat{u}] \tag{5.5}$$

Because the optimal policy must be optimal at each point of the interval $t_0 \leq t \leq T$, we must have

$$w(t_0, y_0) = \int_{t_0}^{t} g(s, \hat{y}(s), \hat{u}(s))ds + w(t, \hat{y}(t))$$

for every "t", where

$$w(t, \hat{y}(t)) = \int_{t}^{t_1} g(s, \hat{y}(s), \hat{u}(s))ds = max \int_{t}^{t1} g(s, y(s), u(s))ds$$

Differentiation of (5.8) with respect to "t" gives

$$\frac{d}{dt}w(t,\hat{y}(t)) = \frac{\partial w(t,\hat{y}(t))}{\partial t} + \frac{\partial w(t,\hat{y}(t))}{\partial y} f(t,\hat{y}(t),\hat{u}(t)) = -g(t,\hat{y}(t),\hat{u}(t))$$

If we define $\lambda(t) = \frac{\partial w}{\partial y}(t,\hat{y}(t))$ and the Hamiltonian

$$H(t,y,u,\lambda) = g(t,y,u) + \lambda f(t,y,u)$$

the maximum principle implies that

$$H(t,\hat{y},\hat{u},\lambda) = maxH(t,\hat{y},u,\lambda).$$

The Function $G(t,y,u)$ defined by

$$G(t,y,u) = \frac{\partial w}{\partial t}(t,y) + \frac{\partial w}{\partial y} f(t,y,u) + g(t,y,u)$$

has the property that

$G(t,y(t),\hat{u}(t)) = 0$. (*necessary condition of optimality of* $w(t,y)$)

It is possible to show, that

$G(t,\hat{y}(t),u) \leq 0$ (*noninereasing in the neighbourhood of* $(\hat{y}(t),\hat{u}(t))$)

$G(t,y,u)$ is maximized by the choise $y = \hat{y}(t)$, $u = \hat{u}(t)$. In particular, if we fix $y = \hat{y}(t)$ then $G(t,\hat{y}(t),u)$ is maximized by the choise $u = \hat{u}(t)$ and if we fix $u = \hat{u}(t)$ then $G(t,y,\hat{u})$ is maximized by the choise $y = \hat{y}(t)$ as.

$$\begin{aligned} H(t,\hat{y}(t),u,\lambda) &= g(t,\hat{y},u) + \lambda f(t,\hat{y}(t),u) \\ &= g(t,\hat{y},u) + \frac{\partial w(t,\hat{y}(t))}{\partial y} f(t,\hat{y}(t),u) \\ &= G(t,\hat{y},u) - \frac{\partial w(t,\hat{y}(t))}{\partial t}; \end{aligned}$$

maximazition of $G(t,\hat{y},u)$ equivalent to maximization of $H(t,\hat{y}(t),u,\lambda)$.

Derivative $\frac{\partial G(t,y,u)}{\partial y}$ at $y = \hat{y}(t)$ and $u = \hat{u}(t)$ is equal to 0, i. e.

$$\frac{\partial G(t,y,u)}{\partial y} = \frac{\partial^2 w}{\partial t \partial y} + \frac{\partial^2 w}{\partial y} f(t,y,u) + \frac{\partial w}{\partial y}\frac{\partial f}{\partial y} + \frac{\partial g}{\partial y} = 0$$

and we get the adjoint equation

$$\frac{d\lambda(t)}{dt} = \frac{d}{dt}\left(\frac{\partial w(t,y)}{\partial y}\right) = \frac{\partial^2 w}{\partial y \partial t} + \frac{\partial^2 w}{\partial y^2} f(t,y,u) =$$
$$= -\frac{\partial w}{\partial y}\frac{\partial f}{\partial y} - \frac{\partial g}{\partial y} = -\lambda \frac{\partial f}{\partial y} - \frac{\partial g}{\partial y}.$$

5.2 The steepest Descent Algorithm

The procedure we use to solve optimal control problems by the method of steepest descent is

1. Select a discrete approximation to the nominal control history $\mathbf{u}^{(0)}(t)$, $t \in [t_0, t_f]$, and store this in the memory of the digital computer. This can be done, for example, by subdiving the interval $[t_o, t_f]$ into N subinterval (generally of equal duration) and considering the control $\mathbf{u}^{(0)}$ as being piecewise-constant during each of these subintervals; that is,

   $$\mathbf{u}^{(0)}(t) = \mathbf{u}^{(0)}(t_k), \quad t \in [t_k, t_{k+1}), \quad k = 0, 1, \ldots, N-1.$$

   Let the iteration index i be zero.

2. Using the nominal control history $\mathbf{u}^{(i)}$, integrate the state equations (5.2) from t_0 to t_f with initial conditions $\mathbf{x}(t_0) = \mathbf{x}_0$ and store the resulting state trajectory $\mathbf{x}^{(i)}$ as a piecewise-constant vector function.

3. Calculate $\lambda^{(i)}(t_f)$ by substituting $\mathbf{x}^{(i)}(t_f)$ from step 2 into Eq. (5.4). Using this value of $\lambda^{(i)}(t_f)$ as the "initial condition" and the piecewise-constant values of $\mathbf{x}^{(i)}$ stored in step 2, integrate the adjoint equations from t_f to t_0, evaluate $\partial \mathbf{H}^{(i)}(t)/\partial \mathbf{u}$, $t \in [t_0, t_f]$, and store this function in piecewise-constant fashion. The trajectory of adjoiny equation does not need to be stored.

4. If

$$\left\| \frac{\partial \mathbf{H}^{(i)}}{\partial \mathbf{u}} \right\| \leq \gamma, \tag{5.6}$$

where γ is a preselected positive constant and

$$\left\| \frac{\partial \mathbf{H}^{(i)}}{\partial \mathbf{u}} \right\|^2 \triangleq \int_{t_0}^{t_f} \left[\frac{\partial \mathbf{H}^{(i)}}{\partial \mathbf{u}}(t) \right]^T \left[\frac{\partial \mathbf{H}^{(i)}}{\partial \mathbf{u}}(t) \right] dt,$$

terminate the iterative procedure, and output the external state and control. If the stopping criterion (5.6) is not satisfied, generate a new piecewise-constant control given by

$$\mathbf{u}^{(i+1)}(t_k) = \mathbf{u}^{(i)}(t_k) + \tau \frac{\partial \mathbf{H}^{(i)}}{\partial \mathbf{u}}(t_k), \quad k = 0, \ldots, N-1, \tag{5.7}$$

where

$$\mathbf{u}^{(i)}(t) = \mathbf{u}^{(i)}(t_k), \qquad for\ t \in [t_k, t_{k+1}), \qquad k = 0, \ldots, N-1.$$

Replace $\mathbf{u}^{(i)}(t_k)$ by $\mathbf{u}^{(i+1)}(t_k), k = 0, \ldots, N-1$, and return to step 2.

5.3 Optimization of Harvesting Returns

Let us suppose that we try to regulate the fishery by reducing the harvesting effort in order to increase the field. In order to do this we must take into a account the time value of money because of interest. As the quantity which we shall is the present value of all future harvest rents, we shall do this by using a discount rate δ, and as we are studying a continuous model we shall assume that this discount rate is compounded continuously.

When we speak of a discount rate δ, we mean that the present value of an amount which would have value 1 at a time t units in the future is $(1-\delta)^t$. If the discount is compounded K times per year, we use discount rate $\frac{\delta}{K}$ per discount period. Then "t" years would be t K discount period and the percent value of an amount 1 at a time t units in the future would be $\left(1 - \frac{\delta}{K}\right)^{tK}$. By continuous compounding we obtain

$$\lim_{K \to \infty} \left(1 - \frac{\delta}{K}\right)^{tK}.$$

Let us assume that the harvest at time "t" has the form

$$h(t) = E.G(y(t)),$$

where E - effort, $G(y)$ - non-negative, non-decreasing function of "y". We continue to assume a constant price "p" and constant cost "c" of unit effect. Then the unit harvest cost when the population level is y is a function $c(y)$ given by $c(y) = \frac{c}{G(y)}$.

That the net evenue is

$$pEG(y)\Delta t - cE\Delta t = (p - c(y))h(t)\Delta t.$$

The presente value of all future harvesting effect is thus

$$J(h(t)) = \int_0^\infty e^{-\delta t}(p - c(y))h(t)dt.$$

If we choose a finit time horison

$$J(h(t)) = \int_0^T e^{-\delta t}(p - c(y))h(t)dt.$$

The optimal control problem which we wish to solve is to choose the harvest rate function which will maximize the integral $J(h(t))$ subject to the state equations

$$\dot{y} = F(y) - h(t)$$

and the constraints $y(t) \geq 0$ and $0 \leq h(t) \leq h_{max}$

We will show that

$$\hat{h}(t) = \begin{cases} 0 & if\ y < y^* \\ F(y^*) & if\ y = y^* \\ h_{max} & if\ y > y^*. \end{cases}$$

We have

$$g(t, y, h) = e^{-\delta t}(p - c(y))h$$
$$f(t, y, h) = F(y) - h(t)$$

The Hamiltonian has the form

$$H(t, y, h, \lambda) = e^{-\delta t}(p - c(y))h(t) + \lambda(t)(F(y) - h(t))$$

and the adjoint equation

$$\frac{d\lambda}{dt} = -c'(y)h(t)e^{-\delta t} + \lambda F'(y)$$

The maximum principle gives

$$H = h(t)\left(e^{-\delta t}(p - c(y)) - \lambda(t)\right) + \lambda(t)F(y)$$

If $\lambda(t) > e^{-\delta t}(p - c(y))$ then $h(t) = 0$
If $\lambda(t) < e^{-\delta t}(p - c(y))$ then $h(t) = h_{max}$

When $\lambda(t) = e^{-\delta t}(p - c(y))$, we have

$$\begin{aligned} -\delta e^{-\delta t}(p - c(y)) &= -c'(y)he^{-\delta t} + \lambda F'(y) \\ &= -c'(y)F(y)e^{-\delta t} + e^{-\delta t}(p - c(y))F'(y) \\ &\qquad (F(y) = h) \\ &= e^{-\delta t}\left(-c'(y)F(y) + (p - c(y))F'(y)\right) \end{aligned}$$

We get

$$\begin{aligned} -\delta(p - c(y)) &= \frac{d}{dy}(F(y).(p - c(y)) \\ F'(y) - \frac{c'(y)F(y)}{(p - c(y))} &= \delta \end{aligned}$$

Let y^* is a solution of the equation then $h(t) = F(y^*)$. $c(y)$ is non-increasing function of y

For $y > y^*$ is $c(y) \leq c(y^*)$ and $\lambda < e^{-\delta t}(p - c(y))$

If $y < y^*$ then $c(y) \geq c(y^*)$ and $\lambda > e^{-\delta t}(p - c(y))$ and we get

$$\hat{h}(t) = \begin{cases} 0 & if\ y < y^* \\ F(y^*) & if\ y = y^* \\ h_{max} & if\ y > y^*. \end{cases}$$

Note that we have in effect set an equilibrium value terminal condition when we replaced h by $F(y)$, e.i. $F(y(T) = EG(y(T))$ to reach *optimal equilibrium population level* y^*.

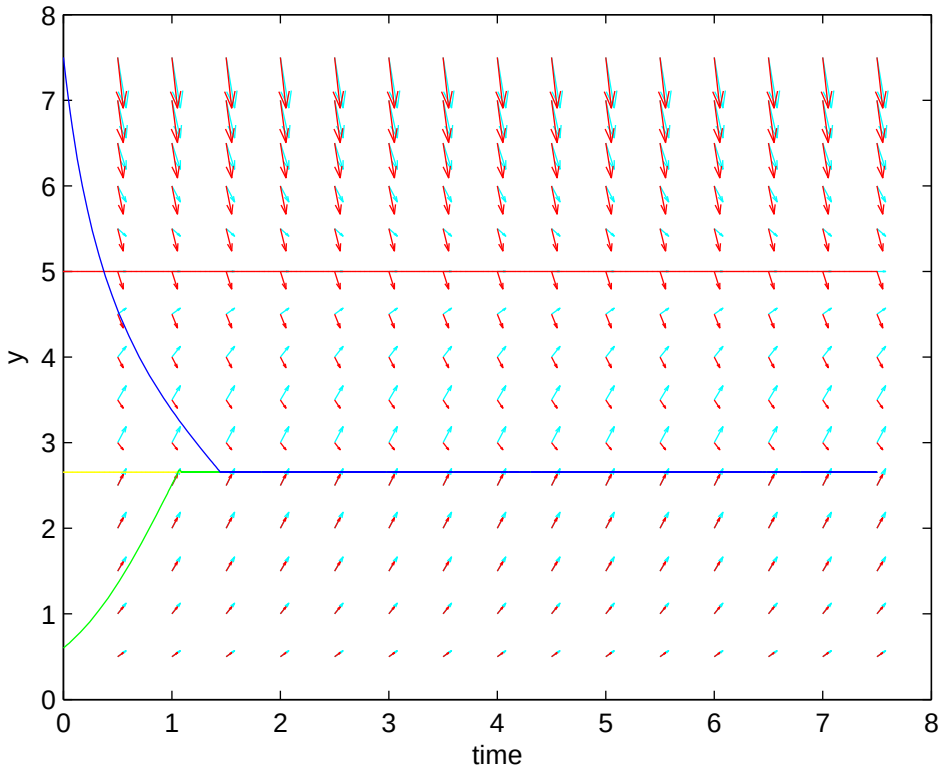

Figure 5.1: Optimal harvesting

```
function optimal_control
global a1 a2 K r p c be
a1=1;a2=0.5;K=5;r=2;p=5;c=2;
contmax=4;be=0.01;
[y1,y2] = meshgrid(0.5:0.5:7.5,0.5:0.5:7.5);
Dt=ones(15,15);
DyDt=r*y2.*(1-y2/K);
quiver(y1,y2,Dt,DyDt,'c');
ocl=fzero(@OCF,10)
D=fz(y2,r,K,ocl,contmax);
for i=1:15
```

```
    for j=1:15
        Dy2Dt(i,j)=D(i);
    end
end
hold on
quiver(y1,y2,Dt,Dy2Dt,'r');
z1=K;
z2=ocl;
z=0:0.005:7.5;
plot(z,z1,'r');
plot(z,z2,'y')
tspan = [0,7.5]; yzero=[0.6];
options = odeset('AbsTol', 1e-7,'RelTol', 1e-4);
[t,y]=ode45(@FY,tspan,yzero,options,r,K,ocl,contmax);
plot(t,y,'g'),title(''),
xlabel 'time',ylabel y
tspan = [0,7.5]; yzero=[7.5];
[t,y]=ode45(@FY,tspan,yzero,options,r,K,ocl,contmax);
plot(t,y,'b')
hold off
%---------------------------------------
function harvest = FY(t,y,r,K,ocl,contmax)
%FY       F(y) parammetrized
%         HARVEST = FY(t,y,r,k)
if y>ocl cont=contmax;
elseif y == ocl cont=y*r*(1-y/K);
    else cont=0;
end
harvest = [y*r*(1-y/K)-cont];
end
%-----------------------------------
function fopl = OCF(y)
%OCF     Function of optimal population level
%        OCF(y,a1,a2,p,c,r,K)
global a1 a2 K r p c be
fy=y*r*(1-y/K);
cy=c*(a2+y)/a1/y;
dfy=-2*r/K*y+r;
```

```
dcy=-c*a2/a1/y^2;
fopl = dfy*(p-cy)-dcy*fy-be*(p-cy);
end
%------------------------------
function [z] = fz(y,r,K,ocl,contmax)
%FZ       F(y) parammetrized
%         HARVEST = FY(y,r,K,ocl,contmax)
for i=1:15
 if y(i) > ocl cont(i)=contmax;
end
if y(i) == ocl cont(i)=y(i)*r*(1-y(i)/K);
end
if y(i)<ocl cont(i)=0;
end
end
for j=1:15
z(j)=r*y(j)*(1-y(j)/K)-cont(j);
end
end
end
```

5.4 The growth model of microorganisms

One of the important tracks of biotechnology is to examine the capability of microorganisms to degrade harmful substances which are the result of industrial production. In this section we start from a simple mathematical model describing the growth of mmiicroorganisms on two substitutable nutrients x_1 and x_2,, assuming that substrate x_1 inhibits the assimilation of the other.

The model is based on the folloving assumptions:

1. A single microbial population grows, which is fed with a medium containing two substitutable nutrients (x_1, x_2) as limiting factors.

2. An organism exhibits the preference of nutrient x_1 over nutrient x_2.

3. The uptake rates of nutrients x_1 and x_2 are those of the Monod and the 'Double Monod' type, respectively.

Based on the above assumption, we can write equation of specific growth

rates of the organism on each substrate:

$$\mu 1 = \frac{\mu_{1max} x_1}{K_1 + x_1}, \tag{5.8}$$

$$\mu 2 = \frac{\mu_{2max} x_2}{K_2 + x_2} . \frac{K_3}{K_3 + x_1} \tag{5.9}$$

where μ_{imax} is the maximum specific growth rate of the organisms on substrate 'i'. The second factor in equation (5.2) represents the inhibition effect of x_1 on the assimilation of substrate x_2 with the inhibitor constant K_3.

The rate of the cell growth depends on the combined contributions from the growth on x_1 and x_2 and on the cell concentration x_3. The kinetics of a multiple substitutable substrate utilization has been modelled by using an additive growth rate equation that incorporates separate functions to describe the growth and the utilization of the individual components of a mixture. The balance equation of the biomass in the chemostat is

$$\dot{x_3} = x_3 \left(\mu 1 / y_1 + \mu 2 / y_2 - D - b \right) \tag{5.10}$$

The substrate utilization kinetics is given by the following equations

$$\dot{x_1} = -\mu 1 x_3 + D(x_{1_F} - x_1) \tag{5.11}$$

$$\dot{x_2} = -\mu 1 x_3 + D(x_{2_F} - x_2) \tag{5.12}$$

where D is the dilution rate of the chemostat, x_{if} is the concentration of x_i in the feed and y_i are the yield coefficients of the nutrients.

In the terms of our second assumption, substrate x_1 has been preferentially used, i. e. it inhibited the initial rate of the substrate x_2 utilization. We show that in spite of this it accelerates the degradiation of this substrate. This phenomenon may be studied in the continuous flow system.

In the continuous flow system the concentration of x_1 in the inflow water can be regulated by the addition of the preferred substrate. The question is how to add the preferred substrate to the inflow water so as make the x_2 concentration drop beyond a define limiting value within the shortest time T.

Let us denote $u(t) = x_{1_f}(t)$. The task is to find a function $u(t)$ for which the objective function:

$$J(u, T) = \int_0^T dt$$

attains its minimum, where the terminal time T is defined by the inequality

$$x_2(T) \leq \varepsilon. \tag{5.13}$$

Hence we are led to the following optimal control problems: to find $u(t)$ satisfying the constraints

$$u(t) \in \langle 0; U_{max} \rangle ,$$

which minimize $J(u,T)$ with T defined by the inequality (5.6). We solve the problem by using Pontryagin's maximum principle (Pontryagin et al., 1983) which involves the definition of the Hamiltonian and a set of adjoint differential equations corresponding to the state variable. For this problem, the Hamiltonian is linear in u and can be represented as

$$H = \sigma u + \gamma,$$

where σ is referred as the switching function, and depending on its value we have following optimal solution

$$\hat{u}(t) = \begin{cases} 0 & if\ \sigma < 0, \\ \mu_{1max} & if\ \sigma > 0. \end{cases}$$

Terminal time T is determined by equality $x_2(T) = \varepsilon$.
Let we consider the following penalty function

$$J_k(u,T) = \int_0^T dt + \beta_k \int_0^T \left(min(0, x_2 - \varepsilon)\right)^2 dt$$

where β_k is an increasing sequence of positive number.

$$J_k(u,T) = \int_0^T \left(1 + \beta_k \left(min(0, x_2 - \varepsilon)\right)^2\right) dt$$

$$T^{m+1} = T^m - \lambda_k \frac{\partial J_k(n,T)}{\partial T} =$$

$$= T^m - \lambda_k \left(1 + \beta_k \left(min(0, x_2 - \varepsilon)\right)^2\right)$$

Chapter 6

Numerical solution

6.1 Numerical solution of ordinary diferential equations

Differential equations are commonly used for mathematical modelling in science. Many mathematical models of biological problems result in the formulation of a first order ordinary differential equation of the form

$$\dot{y} = f(y, t).$$

Here f is a given function of two real variables and y is unknown function of the independent variable "t". In order to determine the solution uniquely, it is necessary to improve an additional condition on y. This usually takes the form.

$$y(t_0) = y_0$$

Definition 6.1 *A solution to the initial value problem (I.V.P.)*

$$\dot{y} = f(y, t) \text{ with } y(t_0) = y_0$$

on an interval $\langle t_0; b\rangle$ *is a differentiable function* $y = y(t)$ *such that*

$$y(t_0) = y_0 \text{ and } \dot{y}(t) = f(y(t), t)$$

for all $t \in \langle t_0; b\rangle$

Definition 6.2 *Given the rectangle*

$$R = \{(y,t) : c \leq y \leq d,\ a \leq t \leq b\},$$

assume that $f(y,t)$ is continuous on R. The function is said to satisfy a Lipschitz condition in the variable y on R provided that a constant $L > 0$ exists with the property that

$$|f(y_1,t) - f(y_2,t)| \leq L\,|y_2 - y_1|$$

for all (y_1,t), $(y_2,t) \in R$. The constant L is called a Lipschitz constant for f.

Theorem 6.1 *(Existence and Uniqueness)*
assume that $f(y,t)$ is continuous in a region

$$R = \{(y,t) : c \leq y \leq d,\ a \leq t \leq b\}.$$

If f satisfied a Lipschitz condition on R in the variable y and $(t_0,y_0) \in R$, then the initial value problem

$$\dot{y} = f(y,t), y(t_0) = y_0$$

has a unique solution $y = y(t)$ on some subinterval $t_0 \leq t \leq t_0 + \delta$

The aim of this charter is to derive numerical techniques for solution of I.V.P. at a sequence of points $t_k = t_0 + kh$. We shall let y_i demote the numerical value obtained as an approximation to the exact solution $y(t_k)$. The size of the interval h is usually called the step length.(size)

6.1.1 Euler's Methods

We now show how the differential equation and given initial condition can be used to calculate values $y_1, y_2, y_3, \ldots$ in a step-by-step manner. First of all we choose the absissas (mesh point) for the points. We subdivide the interval $\langle t_0; b\rangle$ into M subintervals and select the mesh points $t_k = t_0 + kh$ for $k = 0, 1, \ldots, n$, where $h = \frac{b-a}{M}$. We now proceed to solve approximately

$$\dot{y} = f(y,t) \text{ over } \langle t_0; t_n\rangle \text{ with } y(t_0) = y_0.$$

The simplest way of approximating this equation is to replace the derivative $\dot{y}(t_0)$ by approximation $\frac{y_1-y_0}{h}$. This gives

$$\frac{y_1 - y_0}{h} = f(y_0, t_0)$$

which can be rearranged as

$$y_1 = y_0 + hf(y_0, t_0)$$

The process is repeated and generates a sequence of points that approximates the solution curve $y = y(t)$. The general step for Euler's methods is

$$t_{k+1} = t_k + h,\ y_{k+1} = y_k + hf(y_k, t_k)$$

for $k = 0, 1, \ldots, M-1$

```
function E = euler (f, a, b, ya, M)
% Input - f is the function entered as a string 'f'
% - a and b are the left and right end points
% - ya is the initial condition y(a)
% - M is the number of steps
%Output- E = [T' Y'] where T is the vector of abscissas and
% Y is the vector of ordinates
h = (b-a)/M;
T = zeros(1, M+1);
Y = zeros(1, M+1);
T = a:h:b;
Y(1) = ya;
for j = 1:M
Y(j+1) = Y(j)+h*feval(f, T(j), Y(j));
end
E = [T' Y'];
```

6.1.2 Predictor-Corrector Methods

Trapezoidal Formula

The next approach introduced a new idea for constructing an algorithm to solve the I.V.P

$$\dot{y}(t) = f(y(t), t)\ over\ \langle t_0; b\rangle \qquad y(t_0) = y_0.$$

to obtain the solution point (t_1, y_1), we can use the fundamental theorem of calculus and integrate $\dot{y}(t)$ over $\langle t_0, t_1 \rangle$ to get

$$\int_{t_0}^{t_1} f(y,(t),t)dt = \int_{t_0}^{t_1} \dot{y}(t)dt = y(t_1) - y(t_0)$$

When equation is solved for $y(t_1)$, the result is

$$y(t_1) = y(t_0) + \int_{t_0}^{t_1} f(y(t),t)dt.$$

Now a numerical integration method can be used to approximate the definit integral. If the trapezoidal rule is used with the step $h = t_1 - t_0$, then the result is

$$y(t_1) = y(t_0) + \frac{h}{2}\left(f(y_0,t_0) + f(y_1,t_1)\right)$$

Notice that the formula on the right-hand side involves the yet to be determined value $y(t_1)$. To proceed, we use an estimate for $y(t_1)$. Euler's method will suffice for this purpose. At each step, Euler's method is used as a prediction, and then the trapezoidal rule is used to make a correction to obtain the final value.
The general step for method is

$$\begin{aligned} p_{k+1} &= y_k + hf(y_k,t_k), \qquad t_{k+1} + h \\ y_{k+1} &= y_k + \frac{h}{2}(f(y_k,t_k) + f(p_{k+1},t_{k+1})) \end{aligned}$$

```
function H = heun (f, a, b, ya, M)
% Input - f is the function entered as a string 'f'
% - a and b are the left and right end points
% - ya is the initial condition y(a)
% - M is the number of steps
%Output- H = [T' Y'] where T is the vector of abscissas and
% Y is the vector of ordinates
h = (b-a)/M;
T = zeros (1, M+1);
Y = zeros (1, M+1);
T = a:h:b;
```

```
Y(1) = ya;
for j = 1:M
k1 = feval(f, T(j), Y(j));
k2 = feval(f, T(j+1), Y(j)+h*k1);
Y(j+1) = Y(j)+(h/2)*(k1+k2);
end
H = [T' Y'];
```

6.1.3 Runge-Kutta Methods

The fourth-order Runge-Kutta methods is based on computing y_{k+1} as follows:

$$y_{k+1} = y_k \frac{h}{6}(f_1 + 2f_2 + 2f_3 + f_4)$$

where

$$\begin{aligned} f_1 &= f(y_k, t_k) \\ f_2 &= f(y_k + \frac{h}{2} f_1, t_k = \frac{h}{2}) \\ f_3 &= f(y_k + \frac{h}{2} f_2, t_k + \frac{h}{2}) \\ f_4 &= f(y_k + h f_3, t_k + h) \end{aligned}$$

This method is started as follows.Start with the initial point (t_0, y_0) and generate the sequence of approximation using

$$y_{k+1} = y_k \frac{h}{6}(f_1 + 2f_2 + 2f_3 + f_4)$$

```
function R = rk4 (f, a, b, ya, M)
% Input - f is the function entered as a string 'f'
% - a and b are the left and right end points
% - ya is the initial condition y(a)
% - M is the number of steps
%Output- R = [T' Y'] where T is the vector of abscissas and
```

```
% Y is the vector of ordinates
h = (b-a)/M;
T = zeros(1, M+1);
Y = zeros(1, M+1);
T = a:h:b;
Y(1) = ya;
for j = 1:M
k1 = h*feval(f, T(j), Y(j));
k2 = h*feval(f, T(j)+h/2, Y(j)+k1/2);
k3 = h*feval(f, T(j)+h/2, Y(j)+k2/2);
k4 = h*feval(f, T(j)+h, Y(j)+k3);
Y(j+1) = Y(j)+(k1+2*k2+2*k3+k4)/6;
end
R = [T' Y'];
```

6.1.4 System of differentiable equations

This section is an introduction to systems of differential equations. To illustrate the concepts, we consider the initial value problem

$$\begin{aligned} \dot{x} = &\quad f(t,x,y) \qquad x(t_0) = x_0 \\ \dot{y} = &\quad g(t,x,y) \qquad y(t_0) = y_0 \end{aligned}$$

over $\langle t_0, b\rangle$

Euler's method for solving the system is easy to formulate. The interval $\langle t_0, b\rangle$ is devided into M subintervals, $h = \frac{b-t_0}{M}$ and the mesh points are $t_{k+1} = t_k + h$. This is used to get the recursive formulas for Euler's method:

$$\begin{aligned} t_{k+1} &= t_k + h \\ x_{k+1} &= x_k + hf(t_k, x_k, y_k) \\ y_{k+1} &= hg(t_k, x_k, y_k) \quad k = 0, 1, \ldots, M-1 \end{aligned}$$

Runge-Kutta method of order 4 are

$$x_{k+1} = x_k + \frac{h}{6}(f_1 + 2f_2 + 2f_3 + f_4)$$

$$y_{k+1} = y_k + \frac{h}{6}(g_1 + 2g_2 + 2g_3 + g_4),$$

where

$$\begin{aligned} f_1 &= f(t_k, x_k, y_k) \\ f_2 &= f\left(t_k + \frac{h}{2}, x_k + \frac{h}{2}f_1, y_k + \frac{h}{2}g_1\right) \\ f_3 &= f\left(t_k + \frac{h}{2}, x_k + \frac{h}{2}f_2, y_k + \frac{h}{2}g_2\right) \\ f_4 &= f\left(t_k + h, x_k + hf_3, y_k + hg_3\right) \end{aligned}$$

$$\begin{aligned} g_1 &= g(t_k, x_k, y_k) \\ g_2 &= g\left(t_k + \frac{h}{2}, x_k + \frac{h}{2}f_1, y_k + \frac{h}{2}g_1\right) \\ g_3 &= g\left(t_k + \frac{h}{2}, x_k + \frac{h}{2}f_2, y_k + \frac{h}{2}g_2\right) \\ g_4 &= g\left(t_k + h, x_k + hf_3, y_k + hg_3\right) \end{aligned}$$

Runge-Kutta methods to approximate the solution of the system of differential equations.

```
function [T, Z] = rks4 (F, a, b, Za, M)
% Input - F is the system input as a string 'F'
% - a and b are the end points of the interval
% - Za = [x(a) y(a)] are the initial conditions
% - M is the number of steps
%Output- T is the vector of steps
% - Z = [x1(t)  xn(t)]; where xk(t) is the approximation
% to the kth dependent variable
h = (b-a)/M;
T = zeros(1, M+1);
Z = zeros(M+1, length(Za));
T = a:h:b;
```

```
Z(1,: ) = Za;
for j = 1:M
k1 = h*feval(F, T(j), Z(j,: ));
k2 = h*feval(F, T(j)+h/2, Z(j,: )+k1/2);
k3 = h*feval(F, T(j)+h/2, Z(j,: )+k2/2);
k4 = h*feval(F, T(j)+h, Z(j,: )+k3);
Z(j+1,: ) = Z(j,: )+(k1+2*k2+2*k3+k4)/6;
end
```

6.2 Numerical solution of delay differential equation - Linear spline approximation

We introduce a useful technique for approximating of differential-difference equations of the form

$$\dot{x}(t) = f(x(t), x(t-\tau))$$

with a goal solving them numerically. The idea is to take the delay interval of length τ and divide it up into N interval. At each point of the partition, say t_j, we define $x(t_j)$ to be a node of a *linear spline*. We will approximate the function $x(t)$ over this interval by taking a piecewice linear function. The approximating function is described by the function $(y_0, ..., y_N)$. Let

$$y_j(t) = x(t - j\tau/N)$$

for the $N+1$ nodes $j = 0, ..., N$. In partiicular $y_N(t) = x(t-\tau)$. Between nodes y_j is a linear function. We see that the derivation of $y_j(t)$ is approximately

$$\dot{y}_j(t) = \frac{y_{j-1} - y_j}{\tau/N}$$

Using the linear spline approximation, we obtain the system of ordinary differential equations (containing no time delay)

$$\begin{aligned} \dot{y}_0(t) &= f(y_0, y_N) \\ \dot{y}_j(t) &= \frac{N}{\tau}(y_{j-1} - y_j) \end{aligned}$$

for $j = 1, ..., N$. With this notation, we have the following theorem.

Theorem 6.2 *Under the condition listed above*

$$x(t - \tau) = y_N(t) + O(1/N)$$

as $N \to \infty$, uniformy for t on any finite set over which $x(t)$ exists.

6.2.1 DDE problems - Numerical solution with dde25

The DDE solver can solve systems of ordinary differential equations

$$\dot{y}(t) = f(t, y(t), y(t - \tau_1), \ldots, y(t - \tau_k))$$

where t is the independent variable, y is the dependent variable, and $\dot{y}$ represents dy/dt. The delays (lags) $\tau_1, \ldots, \tau_k$ are positive constants.

In an *initial value problem*, we seek the solution on an interval $[t_0, t_f]$ with $t_0 < t_f$. The DDE shows that $\dot{y}(t)$ depends on values of the solution at times prior to t. In particular, $\dot{y}(t_0)$ depends on its values for $t \leq t_0$, i.e., its *history* $S(t)$.

The function dde23 solves initial value problems for delay differential equations (DDEs) with constant delays. It integrates a system of first-order differential equations

$$\dot{y}(t) = f(t, y(t), y(t - \tau_1), \ldots, y(t - \tau_k))$$

on the interval $[t_0, t_f]$ with $t_0 < t_f$ and given history $y(t) = S(t)$ for $t \leq t_0$. dde23 produces a solution that is continuous on $[t_0, t_f]$. You can use the function deval and the output of dde23 to evaluate the solution at specific points on the interval of integration.

dde23 tracks discontinuities and integrates the differential equations with the explicit Runge-Kutta (2,3) pair and interpolant used by ode23. The Runge-Kutta formulas are implicit for step size longer than the delays. When the solution is smooth enough that steps this big are justified, the implicit formulas are evaluated by a predictor-corrector iteration.

DDE Solver Basic Syntax

The basic syntax of the DDE solver is

```
sol = dde23(ddefun,lags,history,tspan)
```

The input arguments are

ddefun A function that evaluates the right side of the differential equations. The function must have the form
`dydt = ddefun(t,y,z)`
where the scalar `t` is the independent variable, the column vector `y` is the depend variable, and `Z(:,j)` is $y(t-\tau_j)$ for τ_j=`lags(j)`.

lags A vector constant positive delays $\tau_1, \ldots, \tau_k$.

history Funstion of t that evaluates the solution $y(t)$ for $t \leq t_0$. The function must be of the form
`S = history(t)`
where `S` is a column vector. Alternatively, if $y(t)$ is constant, you can specify `history` as this constant vector.
If the current call to `dde23` continues a previous integration to `t0`, use the solution `sol` from that call as the history.

tspan The interval of integration as a two-element vector `[t0,tf]` with `t0<tf`.

The output arguments `sol` is a structure created by the solver. It has fields:

`sol.x`	Nodes of the mesh selected by `dde23`
`sol.y`	Approximation to $y(t)$ at the mesh points of `sol.x`
`sol.yp`	Approximation to $\dot{y}(t)$ at the mesh points of `sol.x`
`sol.solver`	`'dde23'`

The evaluate the numerical solution at any point from `[t0,tf]`, use `deval` with the output structure `sol` as its input.

Additional DDE Solver Arguments

For more advanced applications, you can also specify as input arguments solver options and additional parameters

options Structure of optional parameters that change the default integration properties. This is the fifth input argument.
sol = dde23(ddefun,lags,history,tspan,options)
"Creating and Maintaining a DDE Options Structure" on page 5-17 tells you how to create the structure and describes the properties you can specify.

p1,p2,... Parameters that the solver passes to ddefun and the history function, and all functions specified in options.
sol = dde23(ddefun,lags,history,tspan,options,p1,p2,...)
The solver passes any input parameters that follow the options argument to the functions every time it calls them. Use options=[] as a placeholder if you set no options. In the ddefun arguments list, parameters follow the other arguments.
dydt = ddefun(t,y,Z,p1,p2,...)
Similarly, if history is a function, then
S = history(t,p1,p2,...).

Solving DDE Problems

The section uses an example to describe:

- Using dde23 to solve initial value problems (IVPs) for delay differential equations (DDEs)
- Evaluatong the solution at specific points

Example: A Straightforvard Problem

This example illustrate the straightforward formulation, computation, and display of the solution of a system of DDEs with constant delay. The history is constant, which is often the case. The differential equation are

$$\begin{aligned} y_1'(t) &= y_1(t-1) \\ y_2'(t) &= y_1(t-1) + y_2(t-0.2) \\ y_3'(t) &= y_2(t) \end{aligned}$$

The example solves the equations on [0,5] with history

$$y_1(t) = 1$$

$$y_2(t) = 1 \; for \; t \leq 0$$
$$y_3(t) = 1$$

```
function ddex1
%DDEX1  Example 1 for DDE23.
%   This is a simple example of Wille' and Baker
%   that illustrates the
%   straightforward formulation, computation, and
%   plotting of the solution
%   of a system of delay differential equations (DDEs).
%
%   The lags are specified as a vector [1, 0.2], the
%   delay differentialequations are coded in the
%   subfunction DDEX1DE, and the history is
%   evaluated by the function DDEX1HIST.
%   Because the history is constant it
%   could be supplied as a vector:
%       sol = dde23(@ddex1de,[1, 0.2],ones(3,1),[0, 5]);
%
%   See also DDE23, @.

%   Jacek Kierzenka, Lawrence F. Shampine and Skip Thompson
%   Copyright 1984-2002 The MathWorks, Inc.
%   $Revision: 1.2 $  $Date: 2002/04/15 03:35:26 $

sol = dde23(@ddex1de,[1, 0.2],@ddex1hist,[0, 5]);
figure;
plot(sol.x,sol.y)
title('An example of Wille'' and Baker.');
xlabel('time t');
ylabel('solution y');

% ----------------------------------------

function s = ddex1hist(t)
% Constant history function for DDEX1.
s = ones(3,1);
```

```
% --------------------------------------

function dydt = ddex1de(t,y,Z)
% Differential equations function for DDEX1.
ylag1 = Z(:,1);
ylag2 = Z(:,2);
dydt = [ ylag1(1)
         ylag1(1) + ylag2(2)
         y(2)               ];
```

6.3 Numerical solution of partial differential equations

Let us consider the one-dimensional parabolic differential equation

$$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2} + s\left(x, t, u\right), \tag{6.1}$$

where $a \leq x \leq b$ and $t_0 \leq t \leq t_f$. Initial and boundary condition must be supplied in the following form. For $a \leq x \leq b$ and $t = t_0$ the solution must satisfy $u(x, t_0) = u_0(x)$ for a special function u_0. For $x = a$ and $t_0 \leq t \leq t_f$ the solution must satisfy

$$u(a, 0) = g_1(t)\ and u(b, 0) = g_2(t)$$

Assume that the rectangle $R = \{(x, t) : 0 \leq x \leq a, 0 \leq t \leq b\}$ is subdivided into $n - 1$ by $m - 1$ rectangles with sides $\Delta x = h$ and $\Delta t = k$. Start at the bottom row, where $t = t_0$, and the solution is $u(x_i, t_i) = u_0(x_i)$. A method for computing the approximations to $u(x, t)$ at grid points in successive rows $\{u(x_i, t_j) : i = 1, 2, \ldots, n\}$, for $j = 1, 2, \ldots, m$, will be developed.

The difference formulas for $u_t(x, t)$ and $u_{xx}(x, t)$ are

$$u_t(x, t) = \frac{u(x, t + k) - u(x, t)}{k} + \mathbf{O}(k) \tag{6.2}$$

and

$$u_{xx}(x,t) = \frac{u(x-h,t) - 2u(x,t) + u(x+h,t)}{h^2} + \mathbf{O}(h^2) \tag{6.3}$$

The grid spacing is uniform in every row: $x_{i+1} = x_i + h$ (and $x_{i-1} = x_i - h$), and it is uniform in every column: $t_{j+1} = t_j + k$. Next, we drop the terms $\mathbf{O}(k)$ and $\mathbf{O}(k^2)$ and use the approximation $u_{i,j}$ in equations (6.2) and (6.3), which are in turn substituted into equation (6.1) to obtain

$$\frac{u_{i,j+1} - u_{i,j}}{k} = c^2 \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} + ks_{i,j}, \tag{6.4}$$

which approximates the solution to (6.1). For convenience, the substitution $r = c^2k/h^2$ is introduced in (6.4), and the result is the explicit forward-difference equation

$$u_{i,j+1} = (1-2r)u_{i,j} + r(u_{i-1,j} + u_{i+1,j}) + ks_{i,j}. \tag{6.5}$$

Equation (6.5) is employed to create the $(j+1)$th row across the grid, assuming that approximations in the jth row are known. Notice that this formula explicitly gives the value $u_{i,j+1}$ in terms of $u_{i-1,j}, u_{i,j}$ and $u_{i+1,j}$.

The simplicity of formula (6.5) makes it appealing to use. However, it is important to use numerical techniques that are stable. If any error made at stage of the calculations is eventually dampened out, the method is called stable. The explicit forward-difference equation (6.5) is stable if and only if r is restricted to the interval $0 \leq r \leq \frac{1}{2}$. This means that step size k must satisfy $k \leq h^2/(2c^2)$.

```
function U = forwdif (f, c1, c2, a, b, c, n, m)
% Input - u0 =u(x, 0) as a string 'u0'
% - a and b right end points of [0,a] and [0, b]
% - c the constant in the heat equation
% - n and m number of grid points over [0, a] and [0, b]
%Output- U solution matrix
% Initialize parameters and U
h = a/(n-1);
k = b/(m-1);
r = c^2*k/h^2;
s = 1-2*r;
```

```
U = zeros (n, m);
% Boundary conditions
U(1, 1:m) = c1;
U(n, 1:m) = c2;
% Generate first row
U(2:n-1, 1) = feval(f, h:h:(n-2)*h)';
% Generate remaining rows of U
for j = 2:m
for i = 2:n-1
U(i, j) = s*U(i, j-1)+r*(U(i-1, j-1)+U(i+1, j-1));
end
end
U = U';
```

6.3.1 The Crank-Nicholson Method

An implicit scheme, invented by Jon Crank and Phyllis Nicholson, is based on numerical approximations for solution of equation (6.1) at the point $(x, t+k/2)$ that lies between the rows in the grid. Specifically, the approximation used for $u_t(x, t+k/2)$ is obtained from the central-difference formula,

$$u_t\left(x, t+\frac{k}{2}\right) = \frac{u(x,t+k)-u(x,t)}{k} + \mathbf{O}(k^2). \tag{6.6}$$

The approximation used for $u_{xx}(x, t+k/2)$ is the average of the approximations $u_{xx}(x,t)$ and $u_{xx}(x,t+k)$, which has an accuracy of the order $\mathbf{O}(h^2)$:

$$\begin{aligned} u_{xx}\left(x, t+\frac{k}{2}\right) = \frac{1}{2h^2}(&u(x-h,t+k) - 2u(x,t+k) \\ &+u(x+h,t+k) + u(x-h,t) - 2u(x,t) + u(x+h,t)) + \mathbf{O}(h^2) \end{aligned} \tag{6.7}$$

In a fashion similar to the previous derivation, we substitute (6.6) and (6.7) into (6.1) and neglect the error terms $\mathbf{O}(h^2)$ and $\mathbf{O}(k^2)$. The employing the notation $u_{i,j} = u(x_j, t_j)$ will produce the difference equation

$$\frac{u_{i,j+1}-u_{i,j}}{k} = c^2\frac{u_{i-1,j+1} - 2u_{i,j+1} + u_{i+1,j+1} + u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{2h^2} + ks_{i,j} \tag{6.8}$$

Also, the substitution $r = c^2k/h^2$ is used in (6.8). But this time we must solve for the three 'yet to be computed' values $u_{i-1,j+1}, u_{i,j+1}$ and $u_{i+1,j+1}$.

This is accomplished by placing them all on the left side of the equation. Then rearrangement of the terms in equation (6.8) results in the implicit difference formula

$$\begin{aligned} -ru_{i-1,j+1} + (2+2r)u_{i,j+1} - ru_{i+1,j+1} \\ = (2-2r)u_{i,j} + r(u_{i-1,j} + u_{i+1,j}) + ks_{i,j}. \end{aligned} \tag{6.9}$$

for $i = 2, 3, \ldots, n-1$. The terms on the right-hand side of equation (6.8) are all known. Hence the equations in (6.8) form a tridiagonal linear system $A\mathbf{X} = \mathbf{B}$. The six point used in the Crank-Nicholson formula (6.8), together with the intermediate grid point where the numerical approximations are based.

Implementation of formula (6.8) is sometimes done by using the ratio $r = 1$. In this case the increment along the t-axis is $\Delta t = k = h^2/c^2$, and the equations in (6.8) simplify and become

$$-u_{i-1,j+1} + 4u_{i,j+1} - u_{i+1,j+1} = u_{i-1,j} + u_{i+1,j} + ks_{i,j}, \tag{6.10}$$

for $i = 2, 3, \ldots, n-1$. The boundary conditions are used in the first and last equations (i.e. $u_{1,j} + u_{1,j+1} = c_1$ and $u_{n,j} = u_{n,j+1} = c_2$, respectively). Equation (6.9) are especially pleasing to view in their tridiagonal matrix from $\mathbf{AX} = \mathbf{B}$.

$$\begin{bmatrix} 4 & -1 & & & & & \\ -1 & 4 & -1 & & & \mathbf{O} & \\ & & \ddots & & & & \\ & & -1 & 4 & -1 & & \\ & & & & \ddots & & \\ & \mathbf{O} & & & -1 & 4 & -1 \\ & & & & & -1 & 4 \end{bmatrix} \begin{bmatrix} u_{2,j+1} \\ u_{3,j+1} \\ \vdots \\ u_{p,j+1} \\ \vdots \\ u_{n-2,j+1} \\ u_{n-1,j+1} \end{bmatrix} = \begin{bmatrix} 2c_1 + u_{3,j} + ks_{2,j} \\ u_{2,j} + u_{4,j} + ks_{3,j} \\ \vdots \\ u_{p-1,j} + u_{p+1,j} + ks_{p,j} \\ \vdots \\ u_{n-3,j} + u_{n-1,j} + ks_{n-2,j} \\ u_{n-2,j} + 2c_2 + ks_{n-1,j} \end{bmatrix}.$$

When the Crank-Nicholson method is implemented with a computer, the linear system $\mathbf{AX} = \mathbf{B}$ can be solved by their direct means or by iteration.

```
function U = crnich (f, c1, c2, a, b, c, n, m)
% Input - f = u(x, 0) as a string 'f'
% - c1 = u(0, t) and c2 = u(a, t)
% - a and b right end points of [0, a] and [0, b]
% - c the constant in the heat equation
```

```
% - n and m number of grid points over [0, a] and [0, b]
%Output- U solution matrix; analogous to Table 10.5
% Initialize parameters and U
h = a/(n-1);
k = b/(m-1);
r = c^2*k/h^2;
s1 = 2+2/r;
s2 = 2/r-2;
U = zeros (n, m);
% Boundary conditions
U(1, 1:m) = c1;
U(n, 1:m) = c2;
% Generate first row
U(2:n-1, 1) = feval(f, h:h:(n-2)*h)';
% Form the diagonal and off-diagonal elements of A and
% the constant vector B and solve tridiagonal system AX = B
Vd(1, 1:n) = s1*ones(1, n);
Vd(1) = 1;
Vd(n) = 1;
Va = -ones(1, n-1);
Va(n-1) = 0;
Vc = -ones(1, n-1);
Vc(1) = 0;
Vb(1) = c1;
Vb(n) = c2;
for j = 2:m
for i = 2:n-1
Vb(i) = U(i-1, j-1)+U(i+1, j-1)+s2*U(i, j-1);
end
X = trisys(Va, Vd, Vc, Vb);
U(1:n, j) = X';
end
U = U';
```

6.3.2 Semi-discretize methods for partial differential equation

Let us consider the system of ODEs

$$\dot{y}(t) \;=\; Ay(t) + y(t).*(1 - y(t)) + v$$

where A is $N - by - N$ and v is $N - by - 1$ with

$$A \;=\; r_1 \begin{bmatrix} 0 & 1 & & & & & \\ -1 & 0 & 1 & & & \mathbf{O} & \\ & & \ddots & & & & \\ & & -1 & 0 & 1 & & \\ & & & & \ddots & & \\ & \mathbf{O} & & & -1 & 0 & 1 \\ & & & & & -1 & 0 \end{bmatrix}$$

$$+r_2 \begin{bmatrix} -2 & 1 & & & & & \\ 1 & -2 & 1 & & & \mathbf{O} & \\ & & \ddots & & & & \\ & & 1 & -2 & 1 & & \\ & & & & \ddots & & \\ & \mathbf{O} & & & 1 & -2 & 1 \\ & & & & & 1 & -2 \end{bmatrix},$$

where $r_1 = -a/(2h)$, $r_2 = b/h^2$ and $v = (r_2 - r_1, 0, \ldots, 0, r_2 + r_1)$. Here, $a,\ b\ and\ h = 1/(N+1)$ are parameters. This ODE system arises when the method of lines based on centrel differences is used to semi-discretize the partial differential equation (PDE).

$$\frac{\partial}{\partial t}u(x,t) + a\frac{\partial}{\partial x}u(x,t) \;=\; b\frac{\partial^2}{\partial x^2}u(x,t) + u(x,t)(1 - u(x,t)),\ 0 \le x \le 1,$$

with Dirichlet boundary conditions $u(0,t) = u(1,t) = 0$ and initial data $u(x,0) = (1 + \cos(2\pi x))/2$

```
function rcd
%RCD Stiff ODE from method of lines
%on reaction-convection-diffusion problem.

N = 38; a = 1; b = 5e-2;
tspan = [0 2]; space = [1:N]/(N+1);

y0 = 0.5*(1+cos(2*pi*space));
y0 = y0(:);
options = odeset('Jacobian',@jacobian);
options = odeset(options,'RelTol',1e-3,'AbsTol',1e-3);

[t,y] = ode15s(@f,tspan,y0,options);
e = ones(size(t)); U = [e y e];
waterfall([0:1/(N+1):1],t,U)
xlabel('space','FontSize',16), ylabel('time','FontSize',16)

    % --------------------------- Nested functions --------
    function dydt = f(t,y)
    %F         Differential equation.

    r1 = -a*(N+1)/2;
    r2 = b*(N+1)^2;
    up = [y(2:N);0]; down = [0;y(1:N-1)];
    e1 = [1;zeros(N-1,1)]; eN = [zeros(N-1,1);1];

    dydt = r1*(up-down) + r2*(-2*y+up+down) + (r2-r1)*e1 + ...
           (r2+r1)*eN + y.*(1-y);
    end

    function dfdy = jacobian(t,y)
    %JACOBIAN  Jacobian matrix.

    r1 = -a*(N+1)/2;
    r2 = b*(N+1)^2;
    u = (r2-r1)*ones(N,1);
    v = (-2*r2+1)*ones(N,1) - 2*y;
    w = (r2+r1)*ones(N,1);
```

```
    dfdy = spdiags([u v w],[-1 0 1],N,N);
    end

end
```

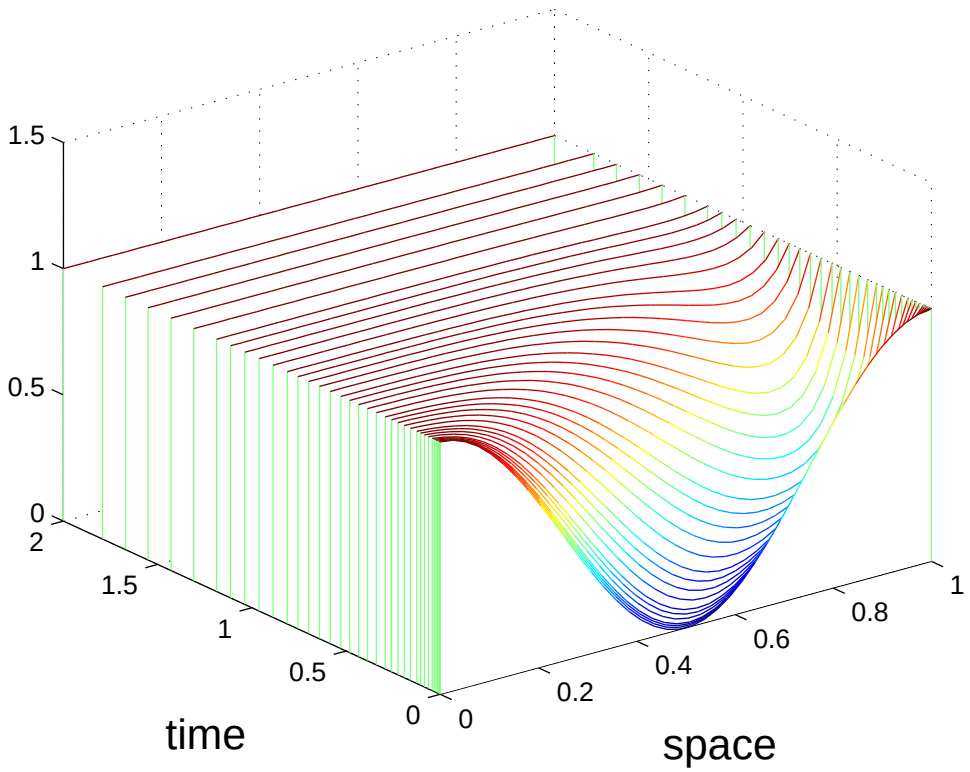

Figure 6.1: Numerical solution

6.3.3 Partial Differential Equations with **pdepe**

MATLAB's pdepe a class of parabolic/elliptic differential equation (PDE) systems. These systems involve a vector- valued unknown function u that

depends on scalar space variable, x, and a scalar time variable, t. The general class to with pdepe applies has the form

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t}=x^{-m}\frac{\partial}{\partial x}\left(x^m f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right)+s\left(x,t,u,\frac{\partial u}{\partial x}\right),$$

where $a \le x \le b$ and $t_0 \le t \le t_f$. The integer m can be 0, 1 or 2, corresponding to slab, cylindrical and spherical symmetry, respectively. The function c is a diagonal matrix and the flux and source function f and s are vector valued. Initial and boundary conditions must be supplied in the following form. For $a \le x \le b$ and $t = t_0$ the solution must satisfy $u(x, t_0) = u_0(x)$ for a specified function u_0. For $x = a$ and $t_0 \le t \le t_f$ the solution must satisfy

$$p_a(x,t,u)+q_a(x,t)f\left(x,t,u,\frac{\partial u}{\partial x}\right)=0,$$

for specified functions p_a and q_a. Similarly, for $x = b$ and $t_0 \le t \le t_f$,

$$p_b(x,t,u)+q_b(x,t)f\left(x,t,u,\frac{\partial u}{\partial x}\right)=0$$

must hold for specified functions p_b and q_b. Certain other restrictions are placed on the class of problems that can be solved by pdepe; see doc pdepe for details.

A call to pdepe has the general form

```
sol=pdepe(m,@pdefun,@pdeic,@pdebc,xmesh,tspan,options,p1,p2,...);
```

which is similar to the syntax for bvp4c. The input argument m can take the values 0,1 or 2, as describe above. The function pdefun hast the form

```
function[c,f,s] = pdefun(x,t,u,DuDx,p1,p2,...)
```

It accepts the space and time variables together with vectors u and DuDx that approximate the solution u and the partial derivative $\partial u/\partial x$, and returns vectors containing the diagonal of the matrix c and the flux and source functions f and s. Initial conditions are encoded in the function pdeic, which takes the form

```
function u0 = pdeic(x,p1,p2,...)
```

The function pdebc of the form

function [pa,qa,pb,qb] = pdebc(xa,ua,xb,ub,t,p1,p2,...)

evaluates p_a, q_b, p_b and q_b for the boundary conditions at xa $= a$ and xb $= b$. The vector xmesh in the argument list of pdepe is a set of points in $[a, b]$ with xmesh(1) $= a$ and xmesh(end) $= b$, ordered so that xmesh(i) ¡ xmesh(i+1). This defines the x values at which the numerical solution is computed. The algorithm uses a second-order spatial discretization method based on the xmesh values. Hence the choice of xmesh has a strong influence on the accuracy and cost of the numerical solution. Closely spaced xmesh points should be used in regions where the solutions is likely to vary rapidly with respect to x. The vector tspan specifies the time points in $[t_0, t_f]$ where the solution is to be returned, with tspan(1)=t_0, tspan(end) =t_f and tspan(i)¡tspan(i+1). The time integration in pdepe is performed by ode15s and the actual timesteps values are chosen dynamically–the tspan points simply determine where the solution is returned and have little impact on the cost or accuracy.

Chapter 7

More complex mathematical models

7.1 A Mechanistical Model of the Adaptation of Phytoplankton Photosynthesis

7.1.1 Description of the Model

Modelling phytoplankton photosynthesis in aquatic ecology is mostly based on an empirical approximation of the photosynthesis-light (P - I) curves. However, because different types of curves seem to fit better particular situations and parameters of these curves vary widely from observation to observation, the prediction obtained are limited in scope. One of the reasons is that the process of photo-adaptation is not taken into account. Therefore, more recently attempts have been made to use algal physiological information for building for ecological purposes somewhat more elaborate mechanistic models of the process and to cover photo-adaptation (Crill 1977, Liou and vanEybergen 1982, Geider and Platt 1986, Eilers and Peeters 1988). It is clear that no equivalence between detailed physiological models of the biochemical mechanisms of photosynthesis and ecological models is useful. The purposes are different and therefore also the models. Nevertheless, without covering at least the principal physiological mechanisms no major progress of ecological models can be expected. In this respect models with a few parameters having some physical meaning are to be recommended. The present paper is based on one of such models.

Basic for the following consideration is the mechanistic model of phytoplankton photosynthesis by Eilers and Peeters (1988). It is based on unit processes concerning the cellular reaction centres called $photo-syntheticfactories-PSF$. It is known from algal physiology (e.g. Steward 1974) that three states of a PSF are possible: x_i - resting, x_2 - activated and x_3 - inhibited. Transitions between states depend both on light intensity and time. The probabilities of the PSF being in the state x_1, x_2 or x_3, are given as p_1, p_2 and p_3, respectively. Transitions between states can be expressed as follows:

$$\begin{aligned} \dot{p}_1 &= -\alpha I p_i + \gamma p_2 + \delta p_3 \\ \dot{p}_2 &= \alpha I p_1 - (\beta I + \gamma) p_2 \\ \dot{p}_3 &= \beta I p_2 - \delta p_3 \end{aligned} \tag{7.1}$$

The parameters α, β, γ and δ occurring in this model are positive constants.

Let $p(t, p^0)$ be a solution of (1) with the initial condition $p(0, p^0) = p^0$, where $p_1^0 + p_2^0 + p_3^0 = 1$. Note that solutions of the system (1) exist for all $t \geq 0$. By adding up the right-hand side of (1) we get

$$\dot{p}_1 + \dot{p}_2 + \dot{p}_3 = 0,$$

i.e. $\sum p_i(t, p^0) = 1$ for all $t \geq 0$. Of course these equations are considered in $S = \{p \in R_+^3 : p_1 + p_2 + p_3 = 1\}$. The simplex S is positively invariant.

7.1.2 Global behaviour under constant condition

Theorem 7.1 *Let $\alpha, \beta, \gamma, \delta$ and I be positive, then there exists an unique positive equilibrium $\bar{p}$ which is globally asymptotically stable on S.*

Proof 7.1 *Vector $\bar{p}$ is the solution of the following linear equation system :*

$$\begin{aligned} -\alpha I p_i + \gamma p_2 + \delta p_3 &= 0 \\ \alpha I p_i - (\beta I + \gamma) p_2 &= 0 \\ \beta I p_2 - \delta p_3 &= 0 \end{aligned} \tag{7.2}$$

Let us consider the matrix $D = P + \rho E$, where $\rho \max P_{ii}$, E is the unit matrix. D is an irreducible nonnegative matrix and so the apparatus of the

Perron-Frobenius theory of a nonnegative matrix applies. Since $1P = 0$, *also* $1D = \rho 1$, *where 1 denotes the unit vector. By the Perron-Frobenius theory there is a unique positive right eigenvector* r *associated with the eigenvalue* ρ *and we can normalize to get*

$\bar{p}_i = r_i / \sum r_i$.

Since $(P + \rho E)\bar{p} = \rho p$, *then* $P\bar{p} = 0$ *and* $\bar{p} > 0$. *By the Perron-Frobenius theorem we get (see Akin, 1979 for proof) that the matrix* P *is a stable matrix on* S, *i.e.* P *has one zero eigenvalue and the other eigenvalues have negative real parts. This proves the statement of the proposition. From Proposition 2 it follows that system (1) has a unique positive equilibrium* $\bar{p}$ *with entries*

$$\begin{aligned} \bar{p}_1 &= \frac{\beta\delta I + \gamma\delta}{F} \\ \bar{p}_2 &= \frac{\alpha\delta I}{F} \\ \bar{p}_3 &= \frac{\alpha\beta I^2}{F}, \end{aligned} \tag{7.3}$$

where $F = \alpha\beta I^2 + (\alpha + \beta)\delta I + \gamma\delta$.

7.1.3 Optimization of photosynthetic production

Let us assume that phytoplankton regulates its photosynthetic production rate (FP) with a certain strategy which maximizes production. The rate of the photosynthetic production FP is proportional to the number of transitions from x_2 to x_1 (Eilers and Peeters 1988). In this section we investigate for a fixed value of light intensity I the optimal values of $\alpha^*, \beta^*, \gamma^*$ and δ^*,i.e. values α, β, γ and δ for which the photosynthetic production FP is under the given environmental condition expressed by I is maximal under constraints

$$\begin{aligned} \alpha^* &\in [\alpha_{min}, \alpha_{max}] \\ \beta^* &\in [\beta_{min}, \beta_{max}] \\ \gamma^* &\in [\gamma_{min}, \gamma_{max}] \\ \delta^* &\in [\delta_{min}, \delta_{max}]. \end{aligned}$$

We will examine two strategies:

1. instantaneous maximal photosynthetic production with respect to α, β, γ

and δ i.e. $FP = \gamma p_2^* \rightarrow \max$,

2. integral maximal photosynthetic production as a goal function

$$J(\alpha, \beta, \gamma, \delta) = \int_0^T \gamma p_2(t) dt \rightarrow \max$$

.

Local optimality

In the case 1, we examine the following function

$$FP = \frac{\alpha \delta I \gamma}{\delta\gamma + (\beta\delta + \alpha\delta)I + \alpha\beta I^2}.$$

By straightforward calculation we get

$$\alpha^* = \alpha_{max} \tag{7.4}$$
$$\beta^* = \beta_{min}$$
$$\gamma^* = \gamma_{max} \tag{7.5}$$
$$\delta^* = \delta_{max}.$$

Global optimality

The optimization problem consists in finding the functions $\alpha_{min} \leq \alpha^*(t) \leq \alpha_{max}$, $\beta_{min} \leq \beta^*(t) \leq \beta_{max}$, $\gamma_{min} \leq \gamma^*(t) \geq \gamma_{max}$ and $\delta_{min} \leq \delta^*(t) \leq \delta_{max}$, which maximize the functional

$$J(\alpha, \beta, \gamma, \delta) = \int_0^T \gamma p_2(t) dt,$$

where T is constant. To find an optimal solution and test its uniqueness we use the Pontryagin maximum principle (Pontryagin et al. 1983), which gives a necessary condition for optimal control. For the problem considered the Hamiltonian has the form :

$$H(\alpha, \beta, \gamma, \delta, p, z) = \alpha I p_1(z_2 - z_1) + \gamma p_2(1 + z_1 - z_2) + \delta p_3(z_1 - z_3) + \beta I p_2(z_3 - z_2)$$

and the adjoint equation is

$$\dot{z} = -zP + b \quad b = (0, -\gamma, 0)$$

with terminal condition $z(T) = 0$.

By routine calculation we get that for all $t < T, z_3(t) < z_1(t) < z_2(t)$ and $1 + z_1(t) > z_2(t)$, (see Appendix). It means that an optimal solution which maximizes the Hamiltonian has the form

$$\alpha^*(t) = \alpha_{max} \tag{7.6}$$
$$\beta^*(t) = \beta_{min}$$
$$\gamma^*(t) = \gamma_{max} \tag{7.7}$$
$$\delta^*(t) = \delta_{max}$$

and we get the following proposition.

Theorem 7.2 *The optimal control $\alpha^*, \beta^*, \gamma^*$ and δ^* which maximizes the goal function*

$$J(\alpha, \beta, \gamma, \delta) = \int_0^T \gamma p_2(t) dt,$$

using

$$\dot{p} = Pp$$

is determined by (8) uniquely and is independent of $T > 0$.

7.1.4 APPENDIX

The adjoint equation of system (1) has the form :

$$\dot{z}_1 = \alpha I(z_1 - z_2)$$
$$\dot{z}_2 = \gamma(z_2 - z_1 - 1) + \beta I(z_2 - z_3)$$
$$\dot{z}_3 = \delta(z_3 - z_1).$$

We now prove the following lemma:

Lemma 7.1 *Let $z(t)$ be a solution of (14) with initial condition for $t \to -\infty$, $z(T) = 0$, then for all $t, 0 \leq t < T$ holds:*

$$1 + z_1(t) > z_2(t) > z_1(t) > z_3(t).$$

Proof 7.2 *$z(T) = 0$, therefore*

$$\dot{z}_1(T) = \alpha I(z_1(T) - z_2(T)) = 0$$
$$\dot{z}_2(T) = \gamma(z_2(T) - z_1(T) - 1) + \beta I(z_2(T) - z_3(T)) = -\gamma$$
$$\dot{z}_3 = \delta(z_3 - z_1) = 0.$$

For the second derivative of z_1 and z_3 there hold

$$\ddot{z}_1(T) = \alpha I(\dot{z}_1(T) - \dot{z}_2(T)) = -\alpha I\gamma$$
$$\ddot{z}_3(T) = \delta(\dot{z}_3(T) - \dot{z}_1(T)) = 0.$$

$z(t)$ is continuous therefore there exists $t < T$ such that for all t, $t_1 < t < T$ the following inequality holds

$$1 + z_1(t) > z_2(t) > z_1(t) > z_3(t).$$

Let $t_2 > 0$ to be the smallest time for which our statement holds for all $t \in (t_2, T)$. We can distinguish three cases

1. *$z_1(t_2) = z_2(t_2) = z_3(t_2)$*
2. *$1 + z_1(t_2) = z_2(t_2)$ or $z_1(t_2) = z_3(t_2)$*
3. *$z_3(t_2) = z_2(t_2)$,*

which contradict the statement of lemma.

Suppose that $z_1(t_2) = z_2(t_2) = z_3(t_2)$. In this case for derivative of z_1, z_2 and z_3 there holds $\dot{z}_1 = 0$, $\dot{z}_2 = -\gamma$ and $\dot{z}_3 = 0$. It means that near the point $z_1 = z_2 = z_3$ solution $z_2(t)$ is decreasing more slowly than $z_1(t)$ and $z_2(t)$. This contradicts the fact that for all t, $t_2 < t < T$ $z_2(t) > z_1(t) > z_3(t)$.

In the second case we get for $1 + z_1(t_2) = z_2(t_2)$ or $z_1(t_2) = z_3(t_2)$ similarly as above

$$\dot{z}_1 = \alpha I(z_1 - z_2) < 0$$
$$\dot{z}_2 = \beta I(z_2 - z_3) > 0$$
$$\dot{z}_3 = \delta(z_3 - z_1) = 0.$$

This contradicts the fact that for all t, $t_2 < t < T$

$$1 + z_1(t) > z_2(t) > z_1(t) > z_3(t).$$

In the last case for $z_1(t_2) = z_2(t_2)$ *we get*

$$\begin{aligned} \dot{z}_1 &= \alpha I(z_1 - z_2) = 0 \\ \dot{z}_2 &= -\gamma + \beta I(z_2 - z_3) \\ \dot{z}_3 &= \delta(z_3 - z_1) < 0 \end{aligned}$$

We show that for all $t, t_2 < t < T$ *holds* $z_2 < z_3 + \gamma/\beta/I$. *Near the point* $z_2 = z_3 + \gamma/\beta/I$ *solution* $z_2(t)$ *is increasing and* $z_3(t)$ *decreasing that means* $z_2(t) < z_3(t) + \gamma/\beta/I$ *for all* t, $t_2 < t < T$. *As it follows from this proposition* $\dot{z}_2(t_2) < 0$ *and* $\dot{z}_1(t_2) = 0$. *For this reason there exists a* $t_3 > 0$ *such that for all* $t \in (t_2, t_3)$, $z_2(t) < z_1(t)$. *This contradicts the fact that for all* t, $t_2 < t < T$, $z_2(t) > z_1(t)$. *If* $\dot{z}_2(t_2) = 0$ *then* $\ddot{z}_2(t_2) = -\delta\gamma < 0$ *and* $\ddot{z}_1(t_2) = 0$. *Similarly as above we get a contradiction.*

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