Finite Difference Schemes for the McKendrick-von Foerster Equation

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Abstract

While the mechanics of fish populations and the mathematical models that govern them are extremely well studied, there is still large effort needed before numerical methods for those models can be accurately evaluated. This project researches the underlying models of fish predation as well as the numerical theory the implementation of those models.

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Chapter 1

Introduction

The study of partial differential equations (PDEs) has always been of interest due to their close relation with the real world systems. In particular a class of PDEs called transport equations relate real world convection-diffusion systems to analytic equations and are studied extremely widely. In this project we study the details around one particular transport equation: the McKendrick-von Foerster equation.

$$\frac{\partial u(t,w)}{\partial t} = -\frac{\partial}{\partial w}\left(g(w)\cdot u(t,w)\right) - \mu(w)\cdot u(t,w) \tag{1.1}$$

1.1 Marine System Populations

The current study of marine systems when related back to the original work of McKendrick (1925) and Foerster (1959) has, on the face of it, changed remarkably. The work of Silvert and Platt (1978) who developed the "standard" equation for modeling marine population, Equation 1.1, has become central to the principles of modeling population. The work of Silvert and Platt (1980) later coupled growth at one size to death at another and developed equations which constructed the growth and mortality of organisms based upon their weight.

Issues however begin to arise when developing even more sophisticated and accurate population models. The work of Datta et al. (2010) introduced the Jump-Growth Equation and showed that the McKendrick-von Foerster equation can be taken as a good approximation. However the Jump-Growth equation suffers because of it is complexity. The non-linear equation is impossible to solve analytically currently, and thus research relies heavily on numerical methods for solutions.

1.2 Project Outline

This project investigats the current methods used in research around Equation 1.1. In Chapter 2 we highlight the historical context of the equation and it is derivation and then examine more recent research into a new equation, the Jump Growth Equation. Before examining the current numerical methods in Chapter 5 we review the mathematical theory behind the method of finite differences in Chapter 4.

Chapter 2

Size Spectrum Theory

In this chapter we consider the models in McKendrick (1925) and Foerster (1959) who describe a system indexed by age. We consider the advances in Silvert and Platt (1978) who describe new equations indexed by weight and derive the standard McKendrick-von Foerster Equation for weight indexed systems.

This work serves as the basis for Datta et al. (2010), who construct a stochastic model for the dynamics of population which they call the "Deterministic Jump-Growth Equation". We consider the similarities between this equation and the McKendrick-von Foerster Equation.

2.1 Age Indexed Models

McKendrick (1925) first posed the idea of modelling biological processes for medicinal science by a single characteristic. In a process if individuals meet they transfer information within the system, and if we considers these individuals as particles in a system moving according to a dimension indexed by this single characteristic then their movement becomes a study in kinetics.

Foerster (1959) extended the principle equations derived in McKendrick (1925). Trucco (1965) gives a full rigorous discussion of the advancements made in Foerster (1959) and further considers the steady state solutions of what he calls "The Von Foerster Equation".

2.1.1 The Von Foerster Equation

The Von Foerster Equation was a major extension to the work of McKendrick (1925). It defines the standard in age indexed population models and reads

$$\frac{\partial n}{\partial t} + \frac{\partial n}{\partial a} = -m(a)n, \tag{2.1}$$

for a mortality function dependent on age $m(a)$. We now derive Equation 2.1 following the method discussed in Trucco (1965) based upon the discussion in Foerster (1959). Suppose that $n(t, a)$ represents the density of individuals at time t in the age category $[a, a + \Delta a)$, then

$$\begin{aligned} \frac{\partial}{\partial t}\left(n(a,t)\Delta a\right) \quad = \quad & + \text{rate of entry of } a \\ & - \text{rate of departure at } (a + \Delta a) \\ & - \text{deaths in } [a, a + \Delta a). \end{aligned} \tag{2.2}$$

We can express Equation 2.2 in mathematical terms for some flux, $J(t, a)$, which describes the rate of movement of individuals in $[a, a + \Delta a)$ as

$$\frac{\partial n}{\partial t} = \frac{J(t,a) - J(t, a + \Delta a)}{\Delta a} - M \cdot n(a, t), \tag{2.3}$$

for some per capita mortality rate $M([a, a + \Delta a))$. We take the flux, J, to define the movements of individuals within the system. As individuals become older the flux can be assumed the be proportional to the density of individuals with some velocity $v(t, a)$. If the ageing corresponds to the passing of time then

$$v(t, a) = \frac{\partial a}{\partial t} = 1$$

and so $J(t, a) = n(t, a)$. Substituting this in to Equation 2.3 it is clear that in the limit as $\Delta a \to 0$, Equation 2.3 tends to Equation 2.1.

2.2 The Transport Equation

After considering Equation 2.1 we consider a more general form of equation. Transport equations, or convection-diffusion equations, take the general form

$$\frac{\partial u}{\partial t} = \nabla \cdot (D \nabla u) - \nabla \cdot (\vec{v} u) + R. \tag{2.4}$$

They describe particles undergoing diffusion and convection. In one dimension Equation 2.4

reduces to

$$\frac{\partial u}{\partial t} = -vu_x + R + (Du_x)_x. \tag{2.5}$$

Comparing the coefficient definitions from Stocker (2011) to the ideas from the derivation of Equation 2.1 we take u as the quantity of interest (population or population density) then we can interpret each term in Equation 2.5.

The first term $-vu_x$ describes the convection (movement due to mass) in the system. v describes the velocity the particles in the system are moving at. This is analogous to the growth of the individuals in the population the rate at which they grow and move through the weight range.

The second term R describes the creation or destruction of u. Thus in Equation 2.1 this becomes the death (naturally or predatorily) of the population.

Lastly we have the diffusion term $(Du_x)_x$. Imagine that c is the concentration of a chemical. When concentration is low somewhere compared to the surrounding areas (e.g. a local minimum of concentration), the substance will diffuse in from the surroundings, so the concentration will increase. Conversely, if concentration is high compared to the surroundings (e.g. a local maximum of concentration), then the substance will diffuse out and the concentration will decrease. This is analogous to phenomenon that are exhibited in the Jump-Growth Equation which we talk about in the next section.

2.3 Weight Indexed Models

2.3.1 McKendrick-von Foerster Equation

Silvert and Platt (1978) introduced a more general construction of the McKendrick-von Foerster Equation, notwithstanding a change from age indexed populations to sized based populations, in a model which allowed growth and mortality to be functions of body mass. Their changes are widely used in mathematical biology and a full derivation can be found in Silvert and Platt (1978). However a simple argument is that the flux described in Equation 2.3 is changed for a flux that depends on the growth of individuals

$$J(t, w) = g(t, w)n(t, w) \tag{2.6}$$

and $m(a)$ becomes a mortality function in weight rather than age $\mu(w)$. Thus the

McKendrick-von Foerster Equation reads

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial w}(g \cdot n) = -\mu \cdot n. \tag{2.7}$$

Considering this equation in the context of Section 2.2 we can see that the Equation 2.7 is a transport equation with no diffusion term. While a transport equation is defined on the region of $\mathbb{R}^+ \times \mathbb{R}$, simply requiring an initial condition, the Von Foerster Equation is only defined on $\mathbb{R}^+ \times \mathbb{R}^+$, thus requiring a left boundary condition along the line $(t, 0)$. Generally this boundary condition is defined as the births across the population which could simply be defined with

$$u(t, 0) = 0. \tag{2.8}$$

This would be an uninteresting problem since the system would only include growth and death, but no birth. Thus instead of Equation 2.8 we introduce a birth rate $b(w)$ and integrate over the population to give a boundary condition

$$u(t, 0) = \int_0^\infty b(w)u(t, w)\, \mathrm{d}t. \tag{2.9}$$

Numerical methods cannot handle the domain $[0, \infty]$ and thus we need to introduce a right hand boundary condition at some weight W. This will be dealt with in due course.

2.3.2 Jump Growth Equation

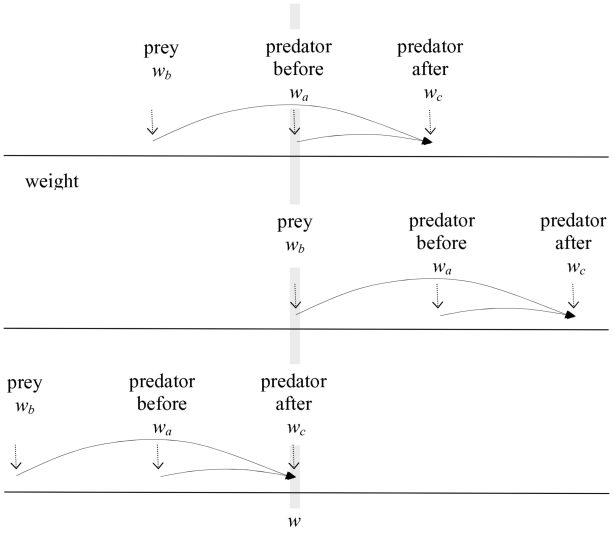
While the mathematical framework presented in Silvert and Platt (1978), Datta et al. (2010) presents a different method of describing weight indexed population under the assumption that predation is a Markov process. The predation event extends the ideas of Silvert and Platt (1980) where predation is modelled by coupling the death of an individual in one weight interval $[w, w + \Delta w)$ with the growth of an individual in a different weight interval $[w', w' + \Delta w)$. This is illustrated in Figure 2.1 where we see there are three types of predation to yield 'new' individuals.

Resolving the macroscopic behaviour of these predation events yields the deterministic equation

$$\frac{\partial \varphi_i}{\partial t} = \sum_j \left(-k_{ij}\varphi_i\varphi_j - k_{ji}\varphi_j\varphi_i + k_{mj}\varphi_m\varphi_j\right), \tag{2.10}$$

where m is the index satisfying the weight bracket $w_m \leq w_i - Kw_j < w_{m+1}$ and k_{xy} is the rate of predation events, indexed predator before prey. Datta et al. (2010) explains that these three

Figure 2.1: The death of an individual with weight w_b is attributed to the growth of another individual with weight w_a who dies to yield a new individual with weight $w_c = w_a + Kw_b$ for some predation efficiency K. Taken from from Datta et al. (2010).



terms correspond to the three types of predation event seen in Figure 2.1: losses from bracket i (negative terms) occur because individuals in this bracket eat prey and become heavier, and because these individuals are themselves eaten. Gains into weight bracket i (the positive term) occur through smaller predators growing into this bracket by eating prey.

We can create an analytic equation for use in calculations by taking the continuum limit of Equation 2.10 and using a continuous feeding rate function $k(w, w')$ to replace the rate constants k_{xy}. Thus Equation 2.10 becomes

$$\begin{aligned}\frac{\partial \phi(w)}{\partial t} = \int (& - k(w', w)\phi(w)\phi(w') \\ & - k(w, w')\phi(w')\phi(w) \\ & + k(w - Kw', w')\phi(w - Kw')\phi(w')) \, \mathrm{d}w'. \end{aligned} \tag{2.11}$$

Datta et al. (2010) defines Equation 2.11 as the "Deterministic Jump-Growth Equation" and again the three terms represent the methods of transferring weight within in the system through predation corresponding to the methods in Figure 2.1: Predation on prey to become larger, being predated upon and being fed with the correct weight to increase.

2.3.3 McKendrick-von Foerster Equation with Diffusion

The McKendrick-von Foerster Equation can be shown to be an approximation to the Jump-Growth Equation, but only to first order. A second order approximation can be yielded by including a diffusion term. If we consider the third term in the Jump-Growth Equation as a Taylor Series, then

$$\begin{aligned} k(w - Kw', w')\phi(w - Kw') =& k(w, w')\varphi(w) \\ &+ (-Kw')\frac{\partial}{\partial w}\left(k(w, w')\varphi(w')\varphi(w)\right) \\ &+ \frac{1}{2}(-Kw')^2\frac{\partial^2}{\partial w^2}\left(k(w, w')\varphi(w)\right) + \ldots \end{aligned} \tag{2.12}$$

Once this is substituted back in to Equation 2.11

$$\begin{aligned} \frac{\partial\phi(w)}{\partial t} =& \int -k(w', w)\phi(w)\phi(w')\,\mathrm{d}w' \\ &- \frac{\partial}{\partial w}\int Kw'k(w, w')\varphi(w)\varphi(w')\,\mathrm{d}w' \\ &+ \frac{1}{2}\frac{\partial^2}{\partial w^2}\int (Kw')^2k(w, w')\varphi(w)\varphi(w')\,\mathrm{d}w' + \ldots \end{aligned} \tag{2.13}$$

which can be seen as an approximation to the McKendrick-von Foerster Equation, with a diffusion term added. Thus for an appropriate choice of coefficients we can restrict our attention to equations in a Transport Equation form

$$\frac{\partial u}{\partial t} = -(g \cdot u)_w - \mu \cdot u + \frac{1}{2}(Du)_{xx}. \tag{2.14}$$

2.4 Summary

In this chapter we have introduced the mathematical framework that will be used to model populations and shown that the macroscopic stochastic Jump-Growth equation is comparable to the Transport Equation form of the McKendrick-von Foerster Equation. In Chapter 3 we introduce a numerical construction of the coefficients giving rise to the true models that will be solved in Chapter 5.

Chapter 3

Model Equations

In this chapter we build on Chapter 2 to construct a fully derived equation to model in Chapter 5. We begin by considering numerical interpretations of "feeding kernels" and prey selection, then construct the various predation coefficients for Equation 2.13.

3.1 Feeding Kernels

Central to the models that we are studying is the idea of a feeding kernel which is the rate at which a predator eats prey of a different size. While there are many interpretations of feeding kernels we use an interpretation centralised around the idea that 'big fish eat smaller fish'. We assume that the likelihood a predators of weight w feeds upon prey with weight w' is based upon both theses weights.

Based upon this key idea Benoıt and Rochet (2004) showed that the feeding kernel for an individual takes the form

$$k(w, w') = sw^{\alpha} S\left(\frac{w}{w'}\right) \tag{3.1}$$

for some parameters s, α to be determined and for the size selection function s. This states the rate at which a predator of weight w feeds is a product of the volumetric search rate sw^{α} and the feeding preference function S. In this thesis we make the assumption that $s = 1$ for convenience.

3.1.1 Prey Selection

As discussed the prey selection will peak around some fixed ratio w/w' for predator / prey, which we call β. Assuming there is some spread for which individuals will vary from this ratio, taken as σ, then we can say that the prey selection function S will take the form

$$S(z) = \kappa \exp\left(-\frac{(z-\beta)^2}{2\sigma^2}\right) \tag{3.2}$$

for some κ that we discuss later.

3.1.2 Coefficient Functions

When we consider the transport equation form of the McKendrick-von Foerster we can extract coefficients. Taking Equation 2.13 in the form of Equation 2.14 it reads

$$\begin{aligned}\frac{\partial u}{\partial t} = &-\left(\left(\int (Kw')k(w,w')u(w')\,\mathrm{d}w'\right)\cdot u\right)_w \\ &-\left(\int k(w',w)u(w')\,\mathrm{d}w'\right)\cdot u \\ &+\frac{1}{2}\left(\left(\int (Kw')^2 k(w,w')u(w')\,\mathrm{d}w'\right)\cdot u\right)_{xx}.\end{aligned} \tag{3.3}$$

Consider the growth term in Equation 3.3,

$$g(w) = \int (Kw')k(w,w')u(w'), \tag{3.4}$$

we can think of this as the expected value of the mass eaten by individuals of weight w. Thus the prey selection function can be thought of as a probability distribution and so we take

$$\kappa = \frac{1}{\sigma\sqrt{2\pi}}.$$

If we take Equation 3.4 and let $v = g$, and define

$$R = \mu(w) = \int k(w',w)u(w')\,\mathrm{d}w', \tag{3.5}$$

$$D(w) = \int (Kw')^2 k(w,w')w(w')\,\mathrm{d}w' \tag{3.6}$$

we have Equation 2.13 in the form of Equation 2.5.

3.2 Steady State Solutions

In marine ecosystems it is been found that the abundance of organisms within weight classes is roughly constant (Sheldon et al. (1972)) if these weight classes are distributed logarithmically. Further, averaged over time, Datta et al. (2011) observes that this abundance changes little suggesting the system is near steady state.

Benoıt and Rochet (2004) found that the McKendrick-von Foerster Equation has a power law steady state of the form $\phi(w) \propto w^{\gamma}$, for $\gamma \in \mathbb{R}^{-}$. We note that in the real world such a power law steady state must break down since it predicts an infinite number of individuals with weight $w = 0$.

Combining this research to show that Equation 3.3 can be transformed using the logarithmic change of variables and appropriate change of function to have a constant solution as Benoıt and Rochet (2004) discusses.

3.2.1 Logarithmic Scale

Sheldon and Parsons (1967), who first introduced the idea of a size spectrum to organise counts of particles in the ocean, stipulates the fundamental conjecture that the total mass within logarithmically spaced size groups was constant over the size range from bacteria to whales.

Interpreting this conjecture biologically Silvert and Platt (1980) poses that the total mass of prey is the same as the mass of their predators, but can be written in terms of the number spectrum, where the number of individuals with size m per volume is described by a density function $N(w) \propto w^{-\gamma}$. Which has later been confirmed by Benoıt and Rochet (2004).

Since these conjectures assume a logarithmic weight scale, we perform a change of variables from Equation 3.3 using the dimensionless variable $x = \log w$ assuming that $\phi(x)\mathrm{d}x = u(w)\mathrm{d}w$. Following Equation 2.14 we have

$$u_t = -(g \cdot u)_w - \mu \cdot u + \frac{1}{2}(D \cdot u)_{ww} \tag{3.7}$$

then after changing variables using a logarithmic weight scale we gain a new equation for ϕ reading

$$\phi_t = -(\hat{g}\cdot\phi)_x - \hat{\mu}\cdot\phi + \frac{\mathrm{e}^{-x}}{2}\left(\left(\hat{D}\cdot\phi\right)_{xx} - \left(\hat{D}\cdot\phi\right)_x\right). \tag{3.8}$$

However, if we are to maintain a constant steady state as stipulated by Sheldon and Parsons (1967), we must perform a simple change of variables. The steady state $u(w) \propto w^\gamma$ reduces to $\phi(x) \propto \mathrm{e}^{x(\gamma+1)}$, which is clearly not constant. If we reduce to a constant by taking $\mathrm{e}^{\gamma x}\,\rho(x) = \phi(x)$ then we have our constant but ρ is governed by the more complicated equation

$$\mathrm{e}^{\gamma x}\,\rho_t = -(\bar{g}\cdot\rho)_x - \bar{\mu}\,\mathrm{e}^{\gamma x}\,\rho + \frac{\mathrm{e}^{-x}}{2}\left(\left(\bar{D}\cdot\rho\right)_{xx} - \left(\bar{D}\cdot\rho\right)_x\right). \tag{3.9}$$

for transformed coefficients $\bar{g}, \bar{\mu}, \bar{D}$.

3.2.2 Constant Steady State

Following the change of variables $\mathrm{e}^{\gamma x}\,\rho(x)\mathrm{d}x = u(w)\mathrm{d}w$ we find that the coefficients of Equation 3.9 read

$$\bar{g}(x) = \int K\,\mathrm{e}^{x'+(\alpha+\gamma-1)x}\,S(\mathrm{e}^{x-x'})\,\mathrm{e}^{\gamma x'}\,\rho(x')\,\mathrm{d}x' \tag{3.10}$$

$$\bar{d}(x) = \int K^2\,\mathrm{e}^{2x'+(\alpha+\gamma-1)x}\,S(\mathrm{e}^{x-x'})\,\mathrm{e}^{\gamma x'}\,\rho(x')\,\mathrm{d}x' \tag{3.11}$$

$$\bar{\mu}(x) = \int \mathrm{e}^{\alpha x'}\,S(\mathrm{e}^{x'-x})\,\mathrm{e}^{\gamma x'}\,\rho(x')\,\mathrm{d}x'. \tag{3.12}$$

Taking the same assumption as Datta et al. (2011) that $\alpha+\gamma-1=0$ and substituting $\rho(x) = C$ as the steady state, we can find an equation for α which will guarantee a constant steady state. Cancelling some factors and taking the convention that $r = x - w'$ the steady state condition for the McKendrick-von Foerster Equation with diffusion reads

$$0 = \int S(\mathrm{e}^r)\left(-1 + \alpha K\,\mathrm{e}^{(\alpha+1)r} + + \alpha(\alpha+1)\frac{K}{2}\,\mathrm{e}^{(\alpha+2)r}\right)\,\mathrm{d}r \tag{3.13}$$

while if we do not include the diffusion term, we can ignore the K^2 terms in Equation 3.13.

3.3 Summary

In this chapter we have outlined the realised equations that will be used in Chapter 5. Next we will discuss some of the methods that we can use to approach these equations analytically and numerically.

Chapter 4

Mathematics of Discretization

The major benefit of studying equations which hold the form of a Transport equation is the large body of research of their solutions and behaviour. We begin this chapter by considering the most basic transport equation, the Advection Equation, which will allow the introduction of finite difference techniques.

Following this we discuss the theory of errors for finite difference equations and how these determine the convergence and stability of the solutions when difference approximations are used with in the equations.

4.1 Advection Equation

The Advection Equation is a simple hyperbolic partial differential equation, in one dimension we take

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = du, \tag{4.1}$$

for some transfer velocity v and destruction rate d on the domain $\mathbb{R}^+ \times R$ for some $R \subseteq \mathbb{R}$. The linear advection has been studied extensively and thus we can gain some insight into potential issues that might occur in more complicated equations such as Equation 3.8.

4.1.1 Analytic Solution

As with ordinary differential equations, partial differential equations can be solved with the "method of characteristics" (or method of lines). Consider Equation 4.1 on the domain $\mathbb{R}^+ \times \mathbb{R}^+$ so that when the correct boundary conditions are applied the problem aligns with the

McKendrick-von Foerster Equation. Then we define some boundary value and initial value problem (BVP and IVP):

$$\begin{aligned} u_t + v\,u_x &= +d\,u \\ u(0,x) &= I(x) \\ u(t,0) &= B(t) \end{aligned} \tag{4.2}$$

Using the method of characteristics we consider a point in the domain $\{(t,x) : t,x > 0\}$ and solve the equation along some characteristic line $(t(s),x(s)) = y(s)$ stemming from an $y_0 \in \Gamma = \{(0,x) : x \in \mathbb{R}^+\} \cup \{(t,0) : t \in \mathbb{R}^+\}$. The full details of the method are left to the reader, or can be found in Chapter 4 of Holmes (2006). The solution of Equation 4.2 is defined by

$$u(t,x) = \begin{cases} I(x-vt)\,\mathrm{e}^{-d\,t} & x - vt > 0 \\ B(x-vt)\,\mathrm{e}^{-d\,t} & x - vt \leq 0 \end{cases} \tag{4.3}$$

along the characteristics $x - vt = C$. We note that the McKendrick-von Foerster equation will take a form similar to this if the growth and death terms are constants, but the problem will become more complicated if the coefficients are functions of t,x or non-linear. However this problem does allow us to introduce the idea of domain of dependence.

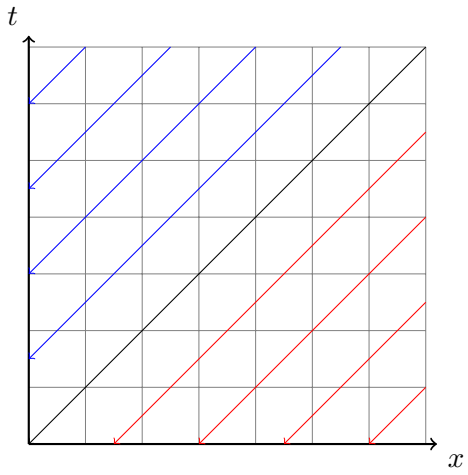


Figure 4.1: The characteristic lines for the solution of Equation 4.3 with constant coefficients. There is no overlap between the lines which means that the solution can be smooth if the boundary conditions along Γ are smooth. The analytic domain of dependence traverses the direction of each arrowhead line.

Given any BVP and/or IVP on $U \subseteq \mathbb{R}^n$ with solution φ, the domain of dependence for for any

$x \in U$ is the set $V \subseteq U$ that $\varphi(x)$ depends on to be calculated. Figure 4.1 shows the characteristic lines for Equation 4.3; the blue lines represent characteristics which depend on the time axis boundary condition. The red arrows depend on the spatial axis initial condition. Looking at the analytic solution to Equation 4.2 we see that the initial condition is carried along the characteristic.

While it is not obvious how this definition will be useful now, it will become extremely important in the analysis of stability of the numerical methods that we discuss in the Subsection 5.1.1.

4.1.2 Numerical Solutions to the Advection Equation

When constructing a numerical method for solving the advection equation we can first consider writing the equation using limits.

$$\lim_{\Delta t \to 0} \frac{u(t+\Delta t, x) - u(t,x)}{\Delta t} + v \lim_{\Delta x \to 0} \frac{u(t, x+\Delta x) - u(t,x)}{\Delta t} = du(t,x). \tag{4.4}$$

If we simply ignore the limits and substituted Newtonian infinitesimals $\Delta t, \Delta x$ we find

$$\frac{u(t+\Delta t, x) - u(t,x)}{\Delta t} + v \frac{u(t, x+\Delta x) - u(t,x)}{\Delta x} = du(t,x) \tag{4.5}$$

which can be rearranged to solve for $u(t+\Delta t, x)$. This yields a explicit disctrize algorithm for calculating u at a point forward in time. This method of constructing algorithms for solving discrete steps of the solution forms the fundamental idea for finite difference equations. These equations approximate a problem by considering a discrete mesh on the domain and then solving the equation using suitable difference approximations.

4.2 Difference Equations

In general, most partial differential equations do not have explicit analytic solutions. Consequently we must find accurate numerical approximations and methods for solving these problems. In this section we introduce the required mathematics for understanding the numerical methods used to solve problems in partial differential equation theory.

Boole and Moulton (1880) writes "Differential Calculus is occupied about the limits to which such ratios approach as the increments are indefinitely diminished." However, "The Calculus of Finite Differences may be strictly defined as the science which is occupied about the ratios of the simultaneous increments of quantities mutually dependent." In simple terms, the calculus

of finite differences is only concerned about ratios of infinitesimals, in line with the ideas of Newtonian calculus.

In Equation 4.4 we broke down the limits in the derivitives by simply ignoring the limit, in this section we reconstruct this equation using difference equations derived from Boole and Moulton (1880) and Hildebrand (1987).

Definition 4.1 (First Forward Difference)**.** For a function $u : U \to \mathbb{R}$ the first forwards difference of u is

$$\Delta_f[u](x) = u(x + \delta x) - u(x). \tag{4.6}$$

Definition 4.2 (First Backwards Difference)**.** For a function $u : U \to \mathbb{R}$ the first backwards difference of u is

$$\Delta_b[u](x) = u(x) - u(x - \delta x). \tag{4.7}$$

These two definitions form the basis for finite difference theory. We can take any difference $\Delta[u](x)$ as a combination of forward and backward differences. Just as with the differential operator, the difference operator is linear and satisfies the Leibniz rule. The proof of this is left to the reader, but follows exactly the same method as for derivatives. It is easy to construct the n^{th} difference ($\Delta^n[f](x)$) by simply considering $\Delta[\Delta^{n-1}[f]](x)$.

When we consider the partial derivative of $u : \mathbb{R} \to \mathbb{R}$ we have that

$$u'(x) = \lim_{\delta x \to 0} \frac{\Delta[u](x)}{\delta x} \tag{4.8}$$

which can easily be extended to higher dimensions.

4.2.1 Taylor's Theorem, Big & little O Notation

When calculating an equation we can replace terms by their approximate sizes if the exact size is not required. In such cases we generally replace terms by their big (or little) O size. If $f, g : \mathbb{R} \to \mathbb{R}$, the informal assertions that $f(x)$ is big-O (or little-O) of $g(x)$ can be defined rigorously by comparing their sizes in limits around a point.

Definition 4.3 (Big O)**.** We define formally that

$$f(x) = O(g(x)) \tag{4.9}$$

as $x \to a$ if and only if

$$\limsup_{x \to a} \left| \frac{f(x)}{g(x)} \right| < \infty \tag{4.10}$$

Definition 4.4 (Little O)**.** We define

$$f(x) = o(g(x)) \tag{4.11}$$

as $x \to a$ if

$$\lim_{x \to a} \left| \frac{f(x)}{g(x)} \right| = 0 \tag{4.12}$$

Intuitively calling $f(x)$ big-O of $g(x)$ states that $f(x)$ is "about as big" as $g(x)$, while if $f(x)$ is little-o of $g(x)$ then it is "much smaller" in size that $g(x)$. A very classical theorem in calculus is Taylor's theorem, which is used to construct finite difference approximations.

Theorem 4.1 (Taylor)**.** If $u : \mathbb{R} \to \mathbb{R}$ is k times differentiable in a region around $x \in \mathbb{R}$ then $u(x + \delta x)$ can be written as

$$u(x + \delta x) = u(x) + (\delta x)\, u'(x) + \ldots + \frac{(\delta x)^k}{k!} u^{(k)}(x) + h_k(x + \delta x)(\delta x)^k \tag{4.13}$$

for some function $h_k(x)$ such that $\lim_{\delta x \to 0} h_k(x + \delta x) = 0$.

If Equation 4.13 is reformulated to give a polynomial estimation $P(x)$ for $u(x)$ then the approximation error for a Taylor polynomial $R_k(x) = u(x) - P_k(x)$ can be estimated as $o((\delta x)^k)$. Using this theorem we know that if u is a differentiable function then by taking $k = 1$

$$u(x + \delta x) = u(x) + \delta x u'(x) + o(\delta x) \tag{4.14}$$

and so we can take the difference equation

$$\frac{\Delta[u](x)}{\delta x} = u(x) + O(\delta x) \tag{4.15}$$

an approximation to a first derivative of u. Given a difference equation $d_k(x)$ that depends on $k = \delta x$ that represents the left hand side of Equation 4.15 that approximates an n^{th} derivative of u we define the order of the approximation to be the integer N that satisfies

$$d_k(x) - u^{(n)}(x) = O(k^N). \tag{4.16}$$

4.3 Finite Difference Equation Errors

Since finite difference equations have become a staple in numerical analysis there are many texts that supply the different coefficients required to approximate derivatives accurately. By combining n^{th} forward and backward differences we can construct higher order approximations to derivatives at higher orders and higher orders of accuracy. Fornberg (1988) provides a details derivation as well as a set of tables for almost all derivatives required for general partial differential equation problems up to high orders in both accuracy and order. We define a finite difference scheme as a particular choice of approximation for a collection of derivatives.

However, as with all numerical problems, issues arise when constructing approximations due to errors that occur with the generation of those approximations themselves. In this section we begin to outline the two main types of error that occur in approximations and introduce the idea of consistency and convergence.

4.3.1 Notation

Before we move forward to discuss the rigorous theory of finite difference equations, their errors and use to approximate partial differential equations, we introduce some general theory. As we saw in Chapter 2 we deal with equations with the form

$$L(u) = \frac{\partial u(t,x)}{\partial t} - \mathcal{L}(u(t,x)), \tag{4.17}$$

where $\mathcal{L}$ is an m times differential operator in x (with most cases satisfying $m < 3$). Given this we have that if u is in the set of real valued functions, C^m, which are one times differentiable in t and m times differentiable in x on some region in the plane $\Omega = \mathbb{R}^+ \times U$ for some $U \subset \mathbb{R}^+$ then $L : C^M \to C$. We aim to solve the partial differential equation $L(u) = 0$ with for specified boundary conditions on $\partial\Omega$.

To do this we first discretise our domain into a mesh grid. In Figure 4.2 we discretise an area of the plane $[0,T] \times [0,X]$ into a grid spaced with $\delta x = k$ and $\delta t = h$. We index the time axis by n and the spatial axis by j, thus for any function $u : [0,T] \times [0,X] \to \mathbb{R}$ we write $u(t,x) = u(nh, jk) = u_j^n$.

With this numerical realisation of the domain for a partial differential equation, and a choice of finite difference approximation, we construct a finite difference equation D_j^n which takes a C^m function, u, and returns a combination of u_i^m for relative values of m and i to n and j.

Example 4.1. Consider the advection equation with a first order approximation for the time and

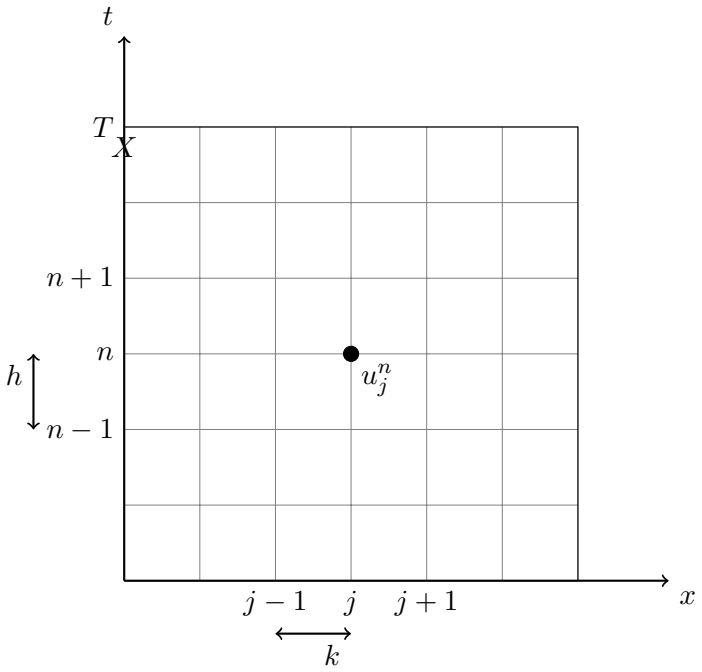


Figure 4.2: An example mesh-grid for the region $[0, T] \times [0, X]$ with an illustration of a grid on the central region of the domain.

spatial derivatives. Then our finite difference equation states that

$$D_j^n(u) = \frac{1}{h} u_j^{n+1} + \left(\frac{\upsilon}{k}\right) u_{j+1}^n + \left(\frac{-1}{h} - \frac{\upsilon}{k}\right) u_j^n. \tag{4.18}$$

4.3.2 Consistency

When considering how appropriate a choice of finite difference equation is to model a particular partial differential equation there are three issues that may arise. The most easy of these to understand is consistency. The broad definition of consistency is that a finite difference equation D is consistent with a partial differential equation L if the truncation error of D from L tends to 0 for smaller mesh grid approximations.

To introduce formally consistency consider a partial differential equation in the form of Equation 4.17 with a true solution Φ. Suppose we take any finite difference equation D_j^n to approximate Equation 4.17 and let ϕ be a non-zero solution to $D(u) = 0$.

Definition 4.5 (Truncation Error). For any problem described above, the Truncation error for a function $\psi : \Omega \to \mathbb{R}$ at any grid point (n, j) is given as

$$T_j^n(\psi) = D_j^n(\psi) - L_j^n(\psi) \tag{4.19}$$

where L_j^n represents $L(u)$ evaluated at $(t, x) = (nh, jk)$.

While we can consider the global truncation of a finite difference approximation by considering D acting upon arbitrary functions v, if $v = \Phi$ is the true solution of L and is known, then the local truncation error τ_j^n is defined as $T_j^n(\Phi)$. If $\tau_j^n = O(h^p)$, then D is said to be an approximation order p method. In reality most finite difference equations are of order p for some $p \in \mathbb{N}$. However this is not always the case and this is why we rely on consistency in a numerical calculation. T_j^n gives an estimate of the error of replacing $L_j^n(v)$ by $D_j^n(v)$. This gives arise to a formal definition of consistency.

Definition 4.6 (Consistency). A finite difference approximation D_j^n is consistent to a partial differential equation L described above. If v is any function, with a sufficient number of continuous derivatives such that $L_j^n(v)$ can be evaluated, D_j^n is considered consistent with L if

$$\lim_{k,h\to 0} T_j^n(v) = \lim_{k,h\to 0} D_j^n(v) - L_j^n(v) = 0. \tag{4.20}$$

If $v = \Phi$, then $T_j^n(v) = \tau_j^n$, so another definition of consistency is that the limiting value of the local truncation error is 0. Suppose that we review Equation 4.5 as an approximation to Equation 4.1, having engineered the scheme using Fornberg (1988) seen in Equation 4.18, we know that rearranging to gain an equation in the form $D(u) = 0$ the truncation error can be written as

$$T(v) = D(v) - L(v) = O(h) + vO(k) - dO(1) = O(h) + O(k) \tag{4.21}$$

and thus as $h, k \to 0$ then $T(v) \to 0$ and we have a consistent difference equation of order $p = 1$.

4.3.3 Stability

Numerical stability theory stems directly from analytical stability theory. Suppose that $L(u)$ is a partial differential equation problem with two analytic solutions Ψ_1 and Ψ_2, we can analyse how likely a perturbation in the initial condition is to affect the system as it tends to one of the two analytic solutions. This principle applies to numerical methods. The essential idea defining stability is that the numerical process should not cause any small perturbations introduced through rounding at any stage to grow and ultimately dominate the solution, similar to the study of whether a small perturbation introduced into an analytic solution will cause the solution to tend to a dominant solution.

For mathematical analysis a definition of stability is given with relation to the growth of the exact solution to the finite difference equation. Therefore, if rounding errors of perturbations to the solution are introduced at any stage in time, these will be bounded if the exact solution is bounded.

Definition 4.7 (Numerical Stability). A numerical method is stable if, for a fixed spatial domain $[0, X]$, for every $T > 0$ there exists a constant $c(T) > 0$ such that

$$||\boldsymbol{\phi}^n||_k < c(T) \tag{4.22}$$

for all $n = 0, 1, .., T/h$ and $h \to 0$, $k \to 0$.

The norm $|| \cdot ||_k$ is a grid dependent Euclidean Norm for the space, for example

$$||\mathbf{u}||_k = \left(k \sum |u_j|^2\right)^{1/2},$$

acting on the vector $\boldsymbol{\phi}^n = (\phi_j^n : j = 0, .., X/k) \in \mathbb{R}^{(X/k)+1}$.

Eigenvalue Method

If a finite difference approximation can be written in matrix form $u^{n+1} = S^{n+1}u^0$, where u^n represents a vector of the values of u_j^n for all j and S^{n+1} is an invertible matrix which consolidates the finite difference approximation. Then we can determine the stability of that approximation by considering the eigenvalues of the matrix S. If all the eigenvalues, λ_S, of S satisfy $|\lambda_S| \leq 1$, then we have that

$$|S^n z| < \infty \tag{4.23}$$

as $n \to \infty$ for all vectors z. Thus, if we consider the eigenvalues for this matrix, we can determine the stability of the system.

Example 4.2. Suppose that we consider the approximation for the advection equation seen in Equation 4.18, this can be written with S in the tridiagonal form

$$\begin{pmatrix} a & b & & & \\ c & a & b & & \\ & c & \ddots & \ddots & \\ & & \ddots & a & b \\ & & & c & a \end{pmatrix} \tag{4.24}$$

and thus has eigenvalues $\lambda_j = a + 2\sqrt{bc}\cos\left(\frac{j\pi}{J}\right)$ for $j = 1, ..., J-1$ if there are J points in the mesh grid along the x axis. Considering the worst case for this eigenvalue spectrum will yield a relation between h and k that must be satisfied for the method to be stable.

This way of analysing the stability of a scheme is not easily generalised since it involves finding the eigenvalues of the corresponding S-matrix. Therefore, we look at a different way of determining stability - the Fourier method or von Neumann method.

Fourier Method

The Fourier method is one of the most common methods for analyzing the stability of a finite difference equation. If the spatial differential operator $\mathcal{L}$, in L, is linear then in the limit as $h, k \to 0$ the numerical error for a finite difference equation also satisfies L since

$$L(\phi - \Phi) = (\phi - \Phi)_t - \mathcal{L}(\phi - \Phi) = (\phi_t - \mathcal{L}(\phi)) - (\Phi_t - \mathcal{L}(\Phi)).$$

We assume that the scheme admits a solution in the form

$$v_j^n = \lambda^n(\omega)\, \mathrm{e}^{ij\omega\Delta x} \tag{4.25}$$

and define

$$G(\omega) = \frac{\lambda^{n+1}(\omega)}{\lambda^n(\omega)} \tag{4.26}$$

to give the amplification factor which governs the growth of the solution at each time step. The von Neumann stability condition is given by

$$|G(w)| \leq 1 \tag{4.27}$$

for all $0 \leq \omega \Delta x \leq \pi$. If a finite difference equation is stable then it is said to be conditionally stable if there is dependence on $G(\omega)$ for the stability condition to hold, otherwise the scheme is unconditionally stable. The Fourier method is the most widely used but can break down for non-linear methods since it can be more difficult to solve for $G(\omega)$.

4.4 Convergence Theory

In Subsection 4.3.2 we defined the Truncation Error of a finite difference equation as the approximation error for a partial differential equation. In this section we deal with the numerical error.

Definition 4.8 (Numerical Error). Given a BVP/IVP problem with true solution $\Phi(t, x)$ and a finite difference equation $D(u)$ with true solution ϕ the numerical error of ϕ is defined as

$$e_j^n(u) = \phi_j^n - \Phi_j^n. \tag{4.28}$$

Broadly speaking, we define convergence of a problem in a simple way. Does our numerical solution accurately model the real solution? However the numerical error and true solution, and thus convergence, of a general problem is quite difficult to calculate since it relies on the knowledge of the solution. Thus more theory is needed to deal with this issue. Before we move on to this theory we give the rigorous definition of convergence.

Definition 4.9 (Convergence). Given a BVP/IVP problem with true solution $\Phi(t, x)$ and a finite difference equation $D(u)$, with $\Delta t = h$ and $\Delta x = k$. The solution D, ϕ, is said to converge to Φ if

$$\lim_{k \to 0} \left(\max_{n=0,1,\ldots,T/k} ||\boldsymbol{\phi}_j - \boldsymbol{\Phi}_j||_k \right) = 0 \tag{4.29}$$

for every initial condition and for every $T > 0$.

The most major result in the theory of linear finite difference equations is the Lax-Richtmyer Equivalence theorem.

Theorem 4.2 (Lax-Richtmyer). For a uniformly solvable linear finite difference scheme which is consistent with a well-posed linear evolution problem, stability is a necessary and sufficient condition for its convergence.

In plain terms, the theorem states that **Consistency + Stability implies convergence**. This is an extremely useful result which allows numerical mathematicians to ignore issues with finding

the true solution of a partial differential equation to calculate the convergence of finite difference equations.

The issue that arises from this theorem is that it only holds for linear problems. Thus in our research on Equation 3.8 with non-linear coefficients the theorem will break down. Luckily Theorem 4.2 has been extended by the work of Rosinger (2008) who classes a more general set of partial differential equations using nonlinear semigroup theory. This allows us to continue with the problem for non-linear equations assuming that we can treat our coefficients in finite difference approximations for the McKendrick-von Foerster Equation with diffusion as if they were linear for stability and consistency calculations.

Chapter 5

Method

In this chapter we review the current methods for numerically solving partial-integro differential equations. We begin by considering the simplest model for the McKendrick-von Foerster equation with constant coefficients, and a simple first order approximation to solve it.

To further this, we consider the work of Hartvig et al. (2011) who discusses a stable first order method for the McKendrick-von Foerster Equation when integral coefficients are used, but works equally well for constant coefficients. Finally we discuss the boundary conditions for the problem and adding the diffusion term to the problem.

5.1 First Order Upwind / Downwind Scheme

We first consider the McKendrick-von Foerster Equation with constant coefficients

$$L(u) = \frac{\partial u}{\partial t} + g\frac{\partial u}{\partial x} + \mu \cdot u \tag{5.1}$$

on the discretised domain $[0, T] \times [0, W]$. By simply replacing the time derivative with a forward difference, and the spatial derivative with a backwards difference we can get a first order approximation and yields a finite difference equation

$$D_j^n(u) = \frac{u_j^{n+1} - u^n}{h} + g\frac{u_j^n - u_{j-1}^n}{k} + \mu u_j^n \tag{5.2}$$

as an approximation to $L(u)$.

5.1.1 Courant Condition

At this point one might question of the choice of the downwind scheme (backwards difference) as a choice for the spatial derivative. This is is ultimately for stability of the overall scheme. As discussed in Chapter 4 solutions to partial differential equations have an analytic domain of dependence. We saw the domain of dependence for the advection equation in Figure 4.1 and the McKendrick-von Foerster Equation has the same domain of dependence.

The work of Courant et al. (1928) researched the idea of a Courant Number, which in a simple terms says that the numerical domain of dependence - the region on which the numerical solution depends for information about it's solution - must contain the analytic domain of dependence.

Formally Courant et al. (1928) stated that if the Courant Number

$$C = \frac{\upsilon \delta t}{\delta x} > C_{\text{max}}, \tag{5.3}$$

where υ is the largest magnitude of velocity that information travels in the system and C_{max} is a constant that depends on the approximations used (but is normally 1), then the finite difference approximation is unstable.

5.1.2 Stability of the Scheme

If we are to to solve the problem $L(u) = 0$ then we can rearrange D_j^n to solve for u_j^{n+1}, which gives a recursive formula for $\mathbf{u}^n$:

$$u_j^{n+1} = \left(1 + h \cdot \mu - \frac{gh}{k}\right) u_j^n + \frac{gh}{k} u_{j-1}^n \tag{5.4}$$

This gives us a matrix problem in the form $\mathbf{u}^{n+1} = A\mathbf{u}^n$ where

$$A = \begin{pmatrix} 1 + h \cdot \mu - \lambda & 0 & & & \\ \lambda & 1 + h \cdot \mu - \lambda & 0 & & \\ & \lambda & \ddots & \ddots & \\ & & \ddots & 1 + h \cdot \mu - \lambda & 0 \\ & & & \lambda & 1 + h \cdot \mu - \lambda \end{pmatrix} \tag{5.5}$$

which, using the eigenvalue method gives us a stability condition of

$$k \leq \frac{g}{\mu}. \tag{5.6}$$

5.1.3 Solution

To numerically solve the problems described in this chapter we will create a iPython notebook for each problem and produce a contour plot for each solution.

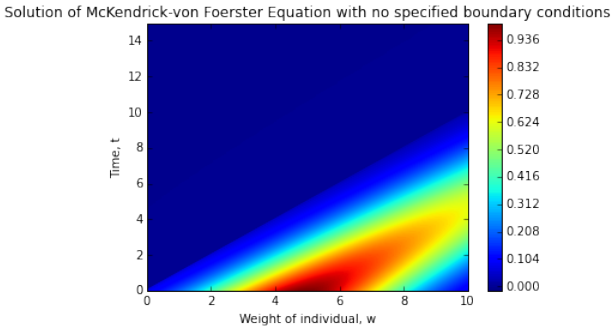


Figure 5.1: A simulation of the advection equation with no left boundary conditions specified.

Using Equation 5.4 as a model for iterating through each time step and a gauassian distribution as the initial condition we produce Figure 5.1, which clearly shows a decreasing solution through time. However we note that above the line $w = gt$ the solution is zero, since there has been no specified left boundary condition. This is becasue the matrix A in Equation 5.5 does not appropriately deal with the derivatives in the boundary. On the left boundary for $x = 0$ we find that

$$u_0^{n+1} = (1 + h \cdot \mu - \lambda)\, u_0^n, \tag{5.7}$$

which is clearly not an accurate approximation for $L(u)$. While a plotting the numerical solution for this would, without further inspection shows that the left boundary is decreasing exponentially, which can be seen in Figure 5.2.

To solve this issue, and throughout the problems here after, we imposed periodic boundary conditions on the domain so that

$$u(t, X_{\text{Low}}) = u(t, X_{\text{Hight}}) \tag{5.8}$$

for our choice of spatial domain $[X_{\text{Low}}, X_{\text{High}}]$. Biologically we can interpret this in terms of birth and death, as on the boundary $x = 0$ we have that the the approximation looks to the oldest

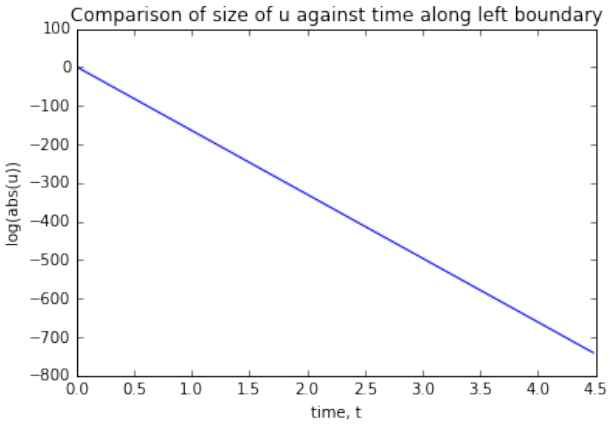


Figure 5.2: Size absolute value of the solution along the of left boundary.

individuals and the growth rate g to determine the number of individuals who are born and have a weight less than the lower boundary on the domain. By taking $X_{\text{low}} = k$ then we have that $u^n_{-1} = 0$ which is a suitable birth weight. When we add this condition the matrix A is rewritten to include the extra term in the top right and

$$A = \begin{pmatrix} 1+h\cdot\mu-\lambda & 0 & & & \lambda \\ \lambda & 1+h\cdot\mu-\lambda & 0 & & \\ & \lambda & \ddots & \ddots & \\ & & \ddots & 1+h\cdot\mu-\lambda & 0 \\ & & & \lambda & 1+h\cdot\mu-\lambda \end{pmatrix}. \tag{5.9}$$

A simulation confirms that the boundary conditions work as we see the solution decaying further over time and continuing the move to the right through the spatial domain for weight.

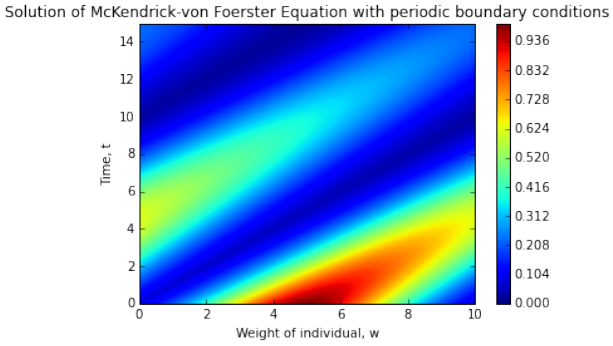
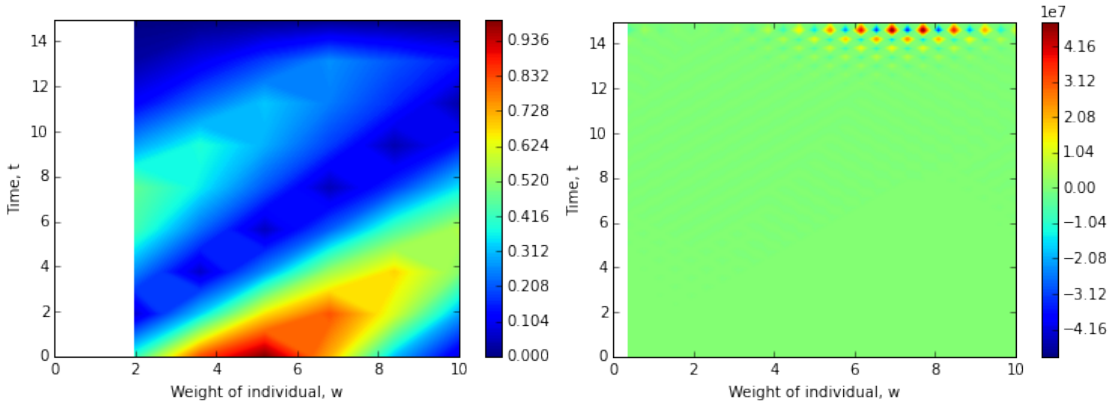


Figure 5.3: The numerical solution of the McKendrick-von Foerster Equation with periodic boundary conditions.

5.2 Diffusion Term & Implicit Methods

Issues begin to arise when we consider the diffusion term within the upwind/downwind approximations, however Figure 5.4 illustrates what happens when we decrease $k < 1$ (by increasing the number of grid points with in the mesh-grid).



(a) Solution $k = 2$ (b) Solution $k = 0.4$

Figure 5.4: Comparison of the upwind/downwind scheme.

Even though the diffusion term should increase the analytic stability of the solution, we find that it also increase the instability of the numerical approximations. To solve this we take a new approach, by using implicit approximations instead of the explicit approximations.

Instead of finding an equation for u_j^{n+1} in terms of $u_i^n, i = ..., j-1, j, j+1, ...$ we aim to find an equation in the form $C \cdot \mathbf{u}^{n+1} = c \cdot \mathbf{u}^n$. If we begin to consider the McKendrick-von Foerster Equation with non-constant coefficients so that

$$L(u) = u_t + (g(w) \cdot u)_w + \mu(w) \cdot u \tag{5.10}$$

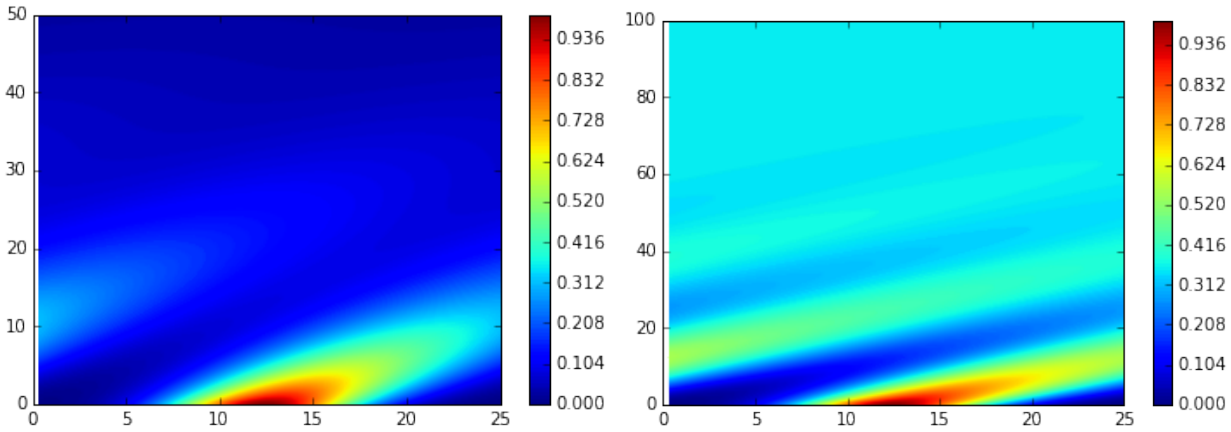
then using the approximation from Hartvig et al. (2011), which relies upon the semi-implicit derivative for products in Press (1992), we can construct a first order implicit approximation

$$D_j^n(u) = \frac{u_j^n - u_j^{n-1}}{h} + \frac{g_j^{n-1}u_j^n - g_{j-1}^{n-1}u_{j-1}^n}{k} + \mu_j^{n-1}u_j^n. \tag{5.11}$$

This method is stable under the assumption that g, μ are non-linear, however we note that the approximation for the derivative in weight is only first order. To look for a higher order method we consider the average of the forwards and backwards derivatives, and add in the diffusion term to yield a finite difference equation

$$D_j^n(u) = \frac{u_j^n - u_j^{n-1}}{h} + \frac{g_{j+1}^{n-1}u_{j+1}^n - g_{j-1}^{n-1}u_{j-1}^n}{2k} + \mu_j^{n-1}u_j^n - \frac{D_{j+1}^{n-1}u_{j+1}^n - 2D_j^{n-1}u_j^n + D_{j-1}^{n-1}u_{j-1}^n}{k^2}. \quad (5.12)$$

A simulation of this scheme shows the solution, while it diffuses to a stationary distribution of $u_{\text{stab}}(t, x) = 0$, is calculated without numerical error and thus the scheme is stable. However we note that the inclusion of the $\mu \cdot u$ term will kill the population over time, much like the solution of the McKendrick-von Foerster Equation without diffusion. Comparing this to the solution of the equation with $\mu = 0$ we see that the solution tends to a constant over time. Closer to the solution that we aim to see earlier in Chapter 3.



(a) $\mu = 0.05$ (b) $\mu = 0$

Figure 5.5: The numerical solution of the McKendrick-von Foerster Equation with periodic boundary conditions and diffusion.

5.2.1 Integral Coefficients

Finally, we consider modelling the integral coefficients using the approximation in Equation 5.12 derived from the work of Hartvig et al. (2011). However, we find that this scheme converges to the $u(t, x) = 0$ solution extremely quickly for any values of K, β, σ, α. Evidence of this is seen in Figure 5.6 where the solution is clearly decreasing in magnitude over time.

5.3 Discussion

While problems in partial differential equation theory do have numerical methods the study of the non-linear equations is still in it's infancy and methods are not thoroughly developed. Much of the research and time spent around constructing our attempt at solving the McKendrick-von

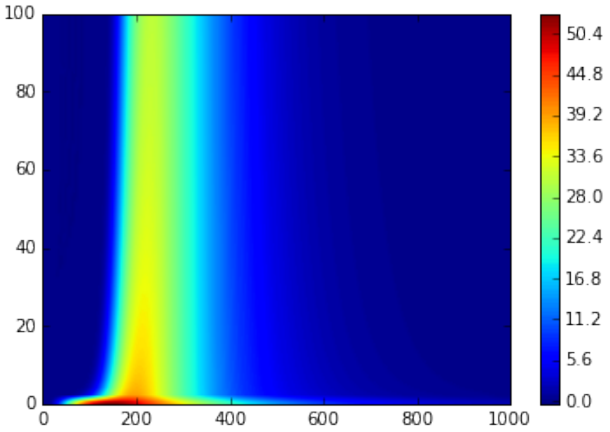


Figure 5.6: The numerical solution of the McKendrick-von Foerster Equation with periodic boundary conditions.

Foerster Equation with diffusion and non-linear coefficients has come from studying the problem with constants instead of functions and experimentation with approximations which are stable for those methods.

Clearly from our study in Figure 5.4 and Figure 5.5 we see that while the diffusion term can greatly improve the stability of the solution to the equations we will need to study the death term $\mu(w) \cdot u(t, w)$ if we are to avoid this dominating the derivative and making the finite difference equation converge to a $u(t, x) = 0$ steady state solution.

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