Physical Modelling of Complex Systems: Assignment 8

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Contents

1 Fisher-Kolmogorov equation

In the lecture, we discussed the Fisher-Kolmogorov equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(1-u)\,, \tag{1.1}$$

and considered travelling wave solutions of this equation, i.e. solutions of the type $u(x,t) = f(x-ct) \equiv f(z)$, with boundary conditions $\lim_{z\to-\infty} f(z) = 1$ and $\lim_{z\to+\infty} f(z) = 0$.

1.1 Minimal speed and the phase portrait method

We will show, using the phase portrait method, that wavelike solutions to the Fisher-Kolmogorov equation must have a minimal speed c_{min}. Therefore, we are interested in the following differential equation in the variable z (with primes denoting derivatives with respect to z)

$$u'' + cu' + u(1-u) = 0\,, \tag{1.2}$$

which is now an ordinary second-order differential equation instead of a partial differential equation. To proceed, we apply a well-known trick to transform this into a set of two first-order ODE's by defining $v = u'$, such that the above equation is equivalent to the system

$$\begin{cases} u' &= v \\ v' &= -cv - u(1-u) \end{cases} . \tag{1.3}$$

This is now a two-component system, for which we can apply the usual techniques. The fixed points of the above system are $(0,0)$ and $(1,0)$. The Jacobian matrix of the above system is

$$J(u,v) = \begin{pmatrix} 0 & 1 \\ -1+2u & -c \end{pmatrix} . \tag{1.4}$$

Evaluating the Jacobian at $(1,0)$ gives

$$J(1,0) = \begin{pmatrix} 0 & 1 \\ 1 & -c \end{pmatrix} . \tag{1.5}$$

Since $\det J(1,0) = -1 < 0$, this fixed point is guaranteed to be a saddle node, for all values of c. Evaluating the Jacobian at the origin, we find

$$J(0,0) = \begin{pmatrix} 0 & 1 \\ -1 & -c \end{pmatrix} . \tag{1.6}$$

The characteristic equation of this matrix is

$$\lambda^2 + c\lambda + 1 = 0\,, \tag{1.7}$$

which gives the eigenvalues

$$\lambda_\pm = \frac{-c \pm \sqrt{c^2-4}}{2} . \tag{1.8}$$

The nature of the origin as fixed point depends on the value of c. Indeed, if $c < 2$, the square root above is an imaginary number and $\lambda_\pm$ is a pair of complex conjugated eigenvalues. In this case, the fixed point will be a stable spiral. However, if $c > 2$, both $\lambda_\pm$ will be real and negative eigenvalues, such that the fixed point is a stable node. Recall that we are looking for wavelike solutions that connect the two fixed points. If $c < 2$, the origin is a stable spiral, and if we start from the fixed point[1] $(1, 0)$ and approach the origin, the solution will start to spiral around the origin. This causes the solution to go in the half-plane $u < 0$. However, this is not physical or biological, since we would like u to represent populations or concentrations for instance, in which we impose that $u \geq 0$ at all times. Therefore, we need to exclude these spiraling trajectories from our solutions, which gives the condition $c > 2$, such that the minimal speed is $c_{\min} = 2$.

1.2 Numerical integration

Consider now the interval $[-20, 20]$ for x and an initial condition

$$u_{\text{in}}(x, 0) = \frac{e^{-x^2}}{2} \,. \tag{1.9}$$

By discretizing space and time, we numerically integrate the Fisher-Kolmogorov equation with the above initial condition. The discretization is done as follows. An interval $[a, b]$ is divided into N parts (always chosen to be equidistant in our code). Let $u_n(t)$ be the value at the n-th point in this partition of the interval. Then we can numerically integrate the equations

$$\frac{\mathrm{d}u_1}{\mathrm{d}t} = \frac{1}{\Delta x^2}(u_2(t) - u_1(t)) + f(u_1(t)) \tag{1.10}$$

$$\frac{\mathrm{d}u_n}{\mathrm{d}t} = \frac{1}{\Delta x^2}(u_{n+1}(t) - 2u_n(t) + u_{n-1}(t)) + f(u_n(t)) \quad n = 2, 3, \ldots, N-1 \tag{1.11}$$

$$\frac{\mathrm{d}u_n}{\mathrm{d}t} = \frac{1}{\Delta x^2}(u_{N-1}(t) - u_N(t)) + f(u_N(t)) \tag{1.12}$$

in time (similar to how we integrated ODE's in previous assignments). Here, $f(u)$ denotes the reaction function, which is the logistic function $f(u) = u(1-u)$ for the Fisher-Kolmogorov equation.

To see if the numerical integration scheme works, we can apply it in a test case, where we 'turn off' the reaction part of the Fisher-Kolmogorov equation and only keep the diffusion part. Therefore, the exercise is to solve a diffusion equation, for which we easily find an analytic expression which can then be compared with a numerical integration.

As seen in the lecture on the diffusion equation by professor Carlon, if we have an initial condition $g(x)$ (which is given by equation (1.9) for this exercise), then the solution at time t of the diffusion equation is given by (note that we set $D = 1$)

$$u(x, t) = \int g(x_0) \frac{1}{\sqrt{4\pi t}} e^{-(x-x_0)^2/4t} \, \mathrm{d}x_0 \,. \tag{1.13}$$

[1]What we really mean is "if we start from an initial condition that is arbitrarily close to the fixed point $(1, 0)$". In the following sections, where we again look for orbits between fixed points, we will keep on abusing this terminology.

Substituting our initial condition, we find

$$u(x,t) = \frac{1}{2\sqrt{4\pi t}} e^{-x^2/4t} \int \exp\left[-\frac{4t+1}{4t} x_0^2 + \frac{x}{2t} x_0\right] \mathrm{d}x_0 \,. \tag{1.14}$$

The remaining integral is a generalization of the Gaussian integral, for which we can use the result

$$\int \exp\left(-ax^2 + bx + c\right) \mathrm{d}x = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a} + c\right) , \tag{1.15}$$

such that the solution, after some straightforward algebraic manipulations, is

$$u(x,t) = \frac{1}{2\sqrt{4t+1}} \exp\left(-\frac{x^2}{4t+1}\right) . \tag{1.16}$$

In Figure 1.1 below, we plot this exact solution at time $t = 20$, along with the numerically obtained solution for a particular discretization of space and time. Both agree very well, although small deviations are visible at the endpoints of the interval. For lower values of t, the two graphs match even better, while for higher t, the deviations become large and we have to be cautious and need to improve the discretization. However, it turns out that in the following exercises we will not need solutions with $t > 20$, such that we can conclude our numerical scheme to be adequate to obtain solutions for this assignment.

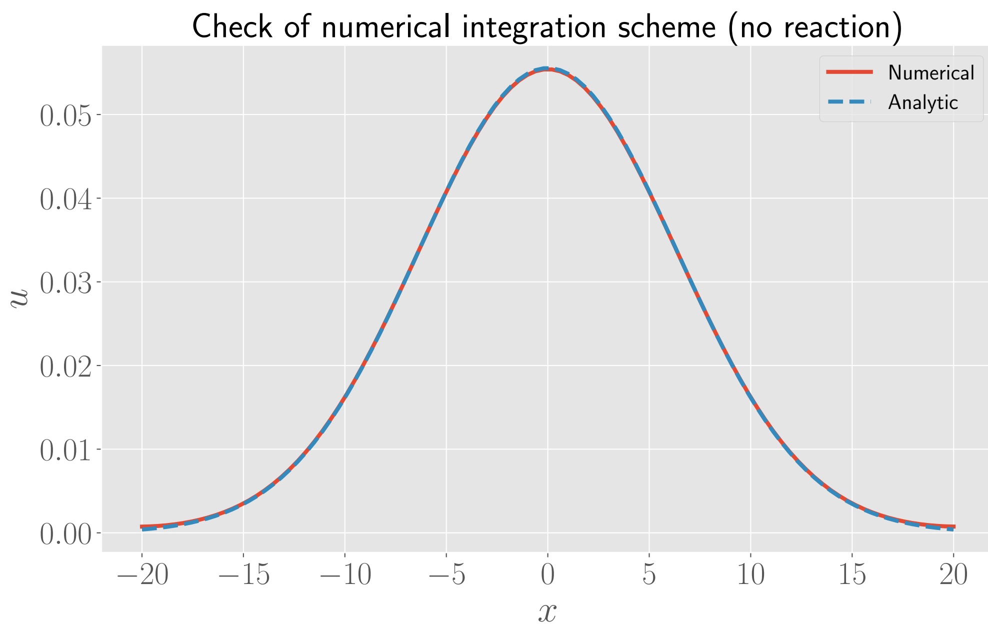

Figure 1.1: Test of the numerical scheme, without including the reaction part, by comparing the numerical result with the analytic calculation for the diffusion equation. Both solutions are evaluated at $t = 20$ (more details in the Python notebook).

Now that we are fairly confident that our numerical scheme works, we use it to obtain the solution to the Fisher-Kolmogorov equation with the initial condition given in equation

(1.9). The result for different values of t is shown in Figure 1.2 below. The perturbation at the origin grows in size, and the solution has two travelling waves: one going in the positive x direction, while the other goes in the negative x direction. The solution tends to grow towards 1. However, due to the logistic growth in the Fisher-Kolmogorov equation, as soon as $u(x,t) \approx 1$ at a certain position x, the solution stops growing. This is in agreement with our earlier observation that $u = 1$ is a stable steady state. Hence we conclude that the solution is indeed a travelling wave, going from the unstable steady state $u = 0$ towards the stable steady state $u = 1$. Note that at early times, the curve is not very smooth around the origin, possibly because at early times, the solution is still strongly varying. We could improve the discretization of space by either increasing N, or choosing for a partition which does not give equidistant values for x, but takes more samples where the initial condition varies strongly. However, since we are mainly interested in later times (because the wave has to converge to the minimal speed) and want to reduce the computation time, we will not delve deeper into this minor issue.

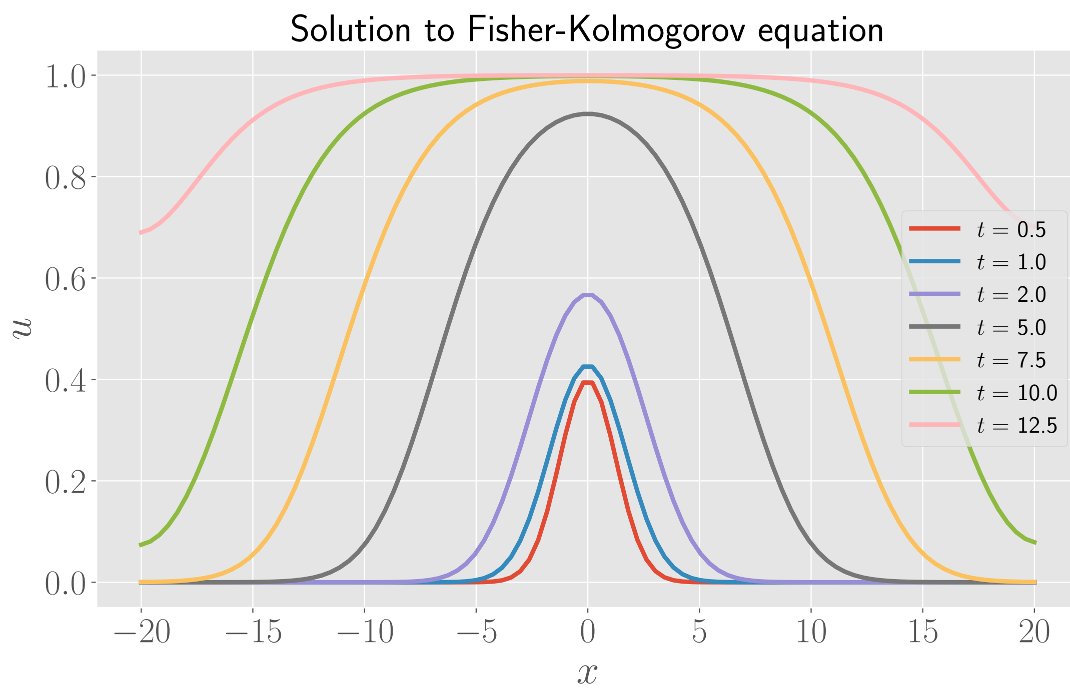

Figure 1.2: Solution to the Fisher-Kolmogorov equation for various values of t (shown in the legend). The solution is a travelling wave with one wave propagating in the positive x direction, and another in the negative x direction.

To estimate the speed of the wave, we let us inspire by the lecture. There, the idea to determine the speed of a travelling wave was to plot a straight line at $u = A$, with A some arbitrary number. We then determine at various times t the location $x_A(t)$ such that $u(x_A(t), t) = A$. This method is applied and shown in Figure 1.3 below, taking t

values between 1.5 and 6.5, with a separation of $\Delta t = 1$ between each plot. Since $\Delta t = 1$ between successive plots, we estimate the speed by estimating the difference $\Delta x_A(t) = x_A(t_{n+1}) - x_A(t_n)$, which gives a speed $c^* \approx 1.8$ of the wave.

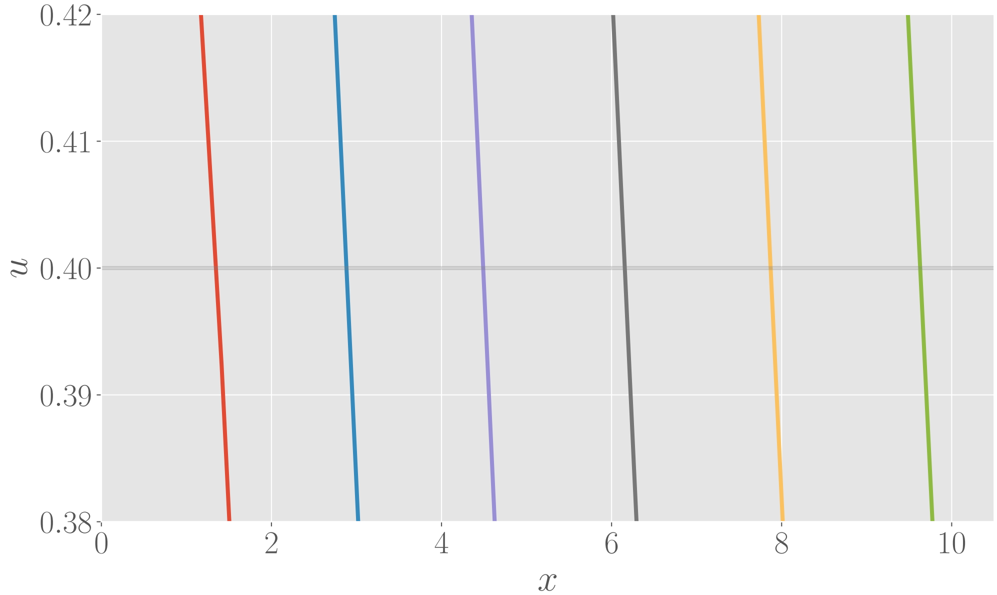

Figure 1.3: Close-up around $u = A = 0.4$ of solutions for various values of t with separation $\Delta t = 1$ between successive plots to estimate the speed of the wave.

This method to determine the speed is also implemented in a Python function. To get a reliable estimate numerically, we should have a finer partition of the interval and therefore increase the value of N. We find that $c^* \approx 1.8247$. However, for higher values of N, the discretization of time must be improved as well, so one should be careful when applying this function and check the numerical scheme once the discretization is changed.

We conclude that the speed of the wave is equal to the minimal speed $c_{\min} = 2$: the convergence to the minimal velocity is known to be very slow, as mentioned in the assignment, such that the value we determine is around 10% lower.

1.3 Approximate solution

We now find an approximate solution of the Fisher-Kolmogorov equation, which can be found by considering the change of variables $\xi = z/c$. Defining $g(\xi) = u(z)$, the Fisher-Kolmogorov equation can be rewritten if we use equation (1.2), along with the fact that

$$\frac{\mathrm{d}u}{\mathrm{d}z} = \frac{\mathrm{d}\xi}{\mathrm{d}z}\frac{\mathrm{d}g}{\mathrm{d}\xi} = \frac{1}{c}g' \,, \tag{1.17}$$

such that we find the equivalent equation

$$\frac{1}{c^2} g''(\xi) + g'(\xi) + g(\xi)(1 - g(\xi)) = 0\,. \tag{1.18}$$

Since the minimal velocity is 2, we assume we can neglect the first term, and therefore find

$$\frac{\mathrm{d}g}{\mathrm{d}\xi} = -g(1-g)\,. \tag{1.19}$$

We can solve the above equation by separation of variables, such that

$$\int \frac{\mathrm{d}g}{g(1-g)} = -\int \mathrm{d}\xi\,. \tag{1.20}$$

The integral on the left hand side is computed by using partial fractions, noting that

$$\frac{1}{g(1-g)} = \frac{1}{g} + \frac{1}{1-g}\,, \tag{1.21}$$

and hence we find

$$\ln \frac{g}{1-g} = -\xi\,, \tag{1.22}$$

from which we then find the solution

$$g = \frac{e^{-\xi}}{1+e^{-\xi}} = \frac{1}{1+e^{\xi}}\,. \tag{1.23}$$

Written down in the original variables, this becomes

$$u(z) = \frac{1}{1+e^{z/c}}\,. \tag{1.24}$$

This solution satisfies the boundary conditions specified in the first exercise, namely, that $u \to 1$ for $x \to -\infty$, and $u \to 0$ for $x \to +\infty$.

In Figure 1.4 below, we compare the approximate solution (with $c = c_{\min} = 2$) with the solution obtained from the numerical integration found earlier. At early times, the approximate solution is significantly larger than the numerical integration for $x \leq 10$. This is because the initial conditions of both solutions are quite different, as seen from Figure 1.5. The initial condition for the numerical integration goes to zero much faster in this range than the approximate solution. Therefore, the approximate solution has a 'head start' relative to the numerically integrated solution. For later times, both solutions have a similar shape (see for example the curves at $t = 10$). It appears that the wave of the approximate solution is faster than the numerical integration, but this is explained by the slow convergence to the minimal velocity, as mentioned earlier.

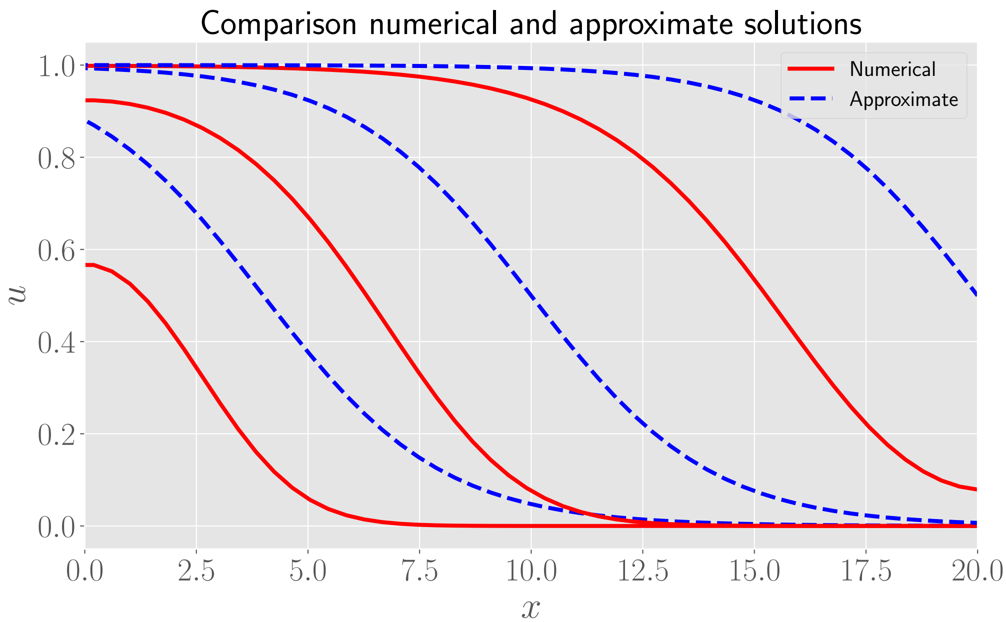

Figure 1.4: Comparison between the approximate solution and the numerical integration of the Fisher-Kolmogorov equation. Times shown are (from left to right) $t = 2, 5$ and 10.

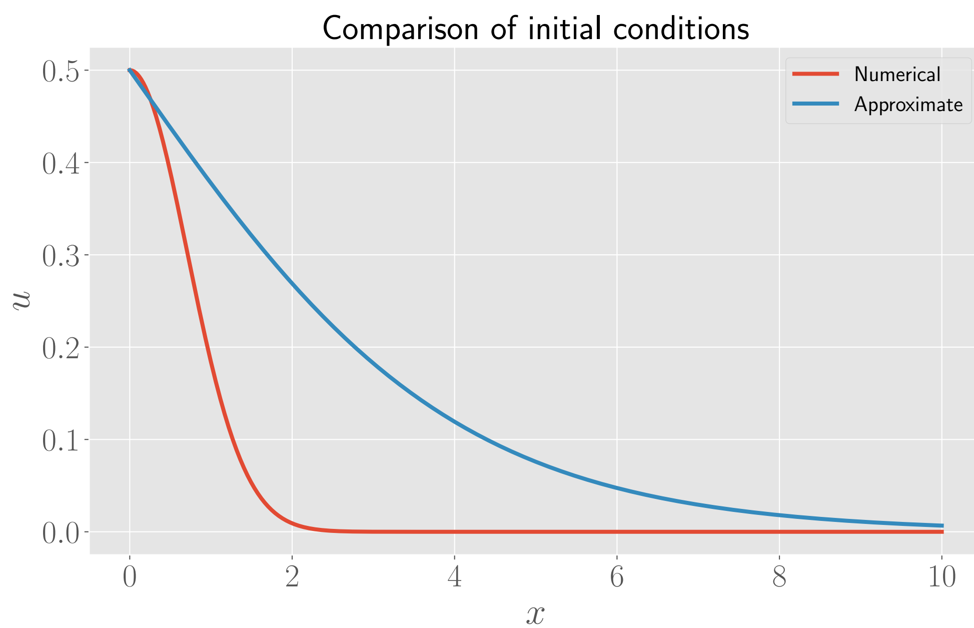

Figure 1.5: Comparison of initial conditions of the approximate solution and the numerical integration.

2 Travelling waves in bistable systems

In the Fisher-Kolmogorov model from the previous section, the homogeneous steady state solutions were unstable ($u = 0$) or stable ($u = 1$). In this section, we consider the alternative model

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(u-a)(1-u)\,, \tag{2.1}$$

with $0 < a < 1$. In this case, there are two homogeneous stable steady state solutions, namely $u = 0$ and $u = 1$, and an unstable one, $u = a$. We again look for solutions of the form $u(x,t) = f(x - ct) = f(z)$, with boundary conditions $\lim_{z\to-\infty} f(z) = 1$ and $\lim_{z\to+\infty} f(z) = 0$. Below, we fix $a = 1/4$.

2.1 Spatial dynamical system and fixed points

First, note that we can rewrite the above differential equation as

$$u'' + cu' + u(u-a)(1-u) = 0\,, \tag{2.2}$$

where primes denote derivatives with respect to z. Proceeding as in the previous section, we define $v = u'$, such that the above equation becomes a two-component dynamical system

$$\begin{cases} u' &= v \\ v' &= -cv - u(u-a)(1-u) \end{cases}\,. \tag{2.3}$$

This system has three fixed points: $(0,0), (1,0)$ and $(a,0)$. We want to show that there exists a unique velocity c^* for a wavelike solution. To determine the value of c^* numerically, we look for a trajectory in the (u,v) plane connecting the two saddle nodes $(1,0)$ and $(0,0)$ (i.e., a *heteroclinic orbit*), starting from $(1,0)$. The Jacobian associated to the above system of differential equations is

$$J(u,v) = \begin{pmatrix} 0 & 1 \\ 3u^2 - 2(1+a)u + a & -c \end{pmatrix}\,. \tag{2.4}$$

At the origin, the $J_{12}(0,0)$ component is a, so $\det J(0,0) = -a < 0$ and the origin is a saddle node. At the fixed point $(a,0)$, the $J_{12}(a,0)$ component is $a(a-1)$ such that $\det J(a,0) = -a(a-1) > 0$. Since $\operatorname{tr} J(a,0) = -c < 0$, this implies that the fixed point $(a,0)$ is a stable node or stable spiral. Finally, evaluating the Jacobian at the fixed point $(1,0)$, we have

$$J(1,0) = \begin{pmatrix} 0 & 1 \\ 1-a & -c \end{pmatrix}\,, \tag{2.5}$$

and therefore $\det J(1,0) = a - 1 < 0$, so this is a saddle node as well. The characteristic equation for this matrix is

$$\lambda^2 + c\lambda + a - 1 = 0\,, \tag{2.6}$$

which has solutions

$$\lambda_\pm = \frac{-c \pm \sqrt{c^2 - 4(a-1)}}{2}\,, \tag{2.7}$$

with corresponding eigenvectors

$$\mathbf{v}_+ = \begin{pmatrix} 1 \\ \lambda_+ \end{pmatrix}\,, \quad \mathbf{v}_- = \begin{pmatrix} 1 \\ \lambda_- \end{pmatrix}\,. \tag{2.8}$$

2.2 Heteroclinic orbit and wavelike solution

To find a trajectory in the (u, v)-plane connecting the saddle nodes $(1, 0)$ and $(0, 0)$, starting from $(1, 0)$, we use an initial point (u_0, v_0) close to $(1, 0)$ and which lies along the direction of the repulsive eigenvector $\mathbf{v}_+$, for some parameter value of c. If we let this point flow along the phase portrait of the dynamical system (2.3), the solution will (i) cross the u-axis before the origin is reached, (ii) flow to infinity or (iii) reach the origin (i.e. the trajectory is a heteroclinic orbit), depending on the value of c. After some trial and error runs, it turns out that for c between 0.35 and 0.355, a heteroclinic orbit is reached. To determine the optimal value of c, we solve the differential equation for various values of c in this range. The code checks if the solutions are closer than a distance ϵ (taken to be 10^{-3} in the notebook) away from the origin, and saves the corresponding values of c. We then take c^* as the mean of these values, resulting in $c^* = 0.35365$. In Figure 2.1, we show the heteroclinic orbit for this value of c^*.

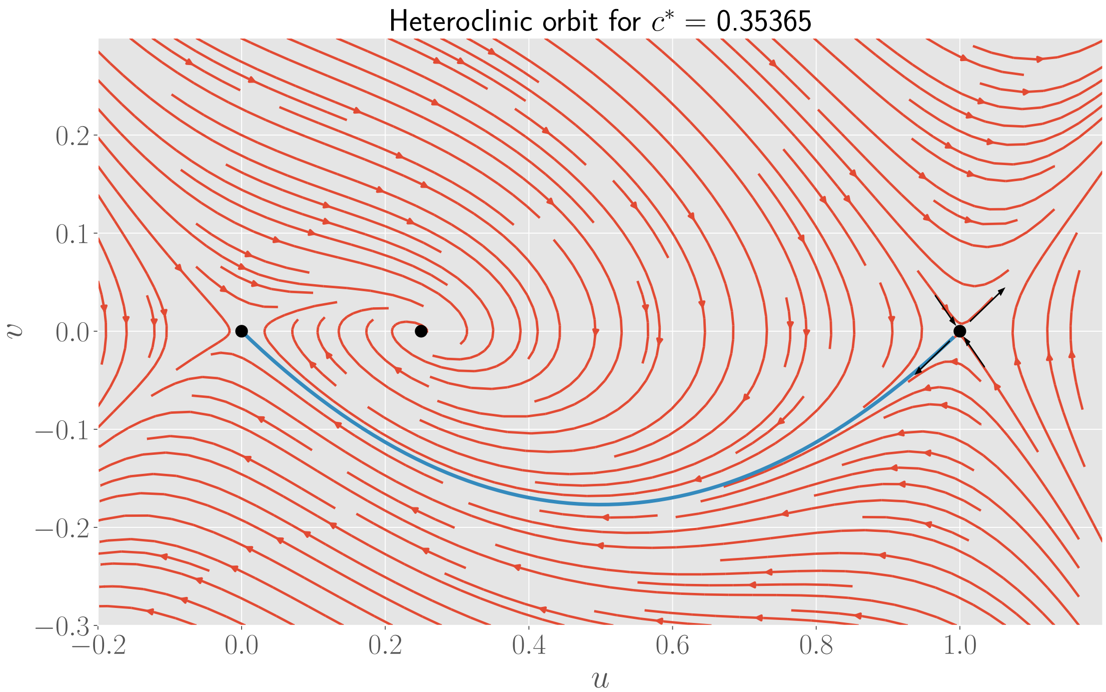

Figure 2.1: A heteroclinic orbit (blue curve) is generated from (u_0, v_0) if $c^* = 0.35365$. The fixed points are shown as black dots. The arrows denote the direction of repulsion or attraction of the saddle node $(1, 0)$.

Using as initial condition

$$u_{\text{in}}(x, 0) = \frac{1}{1 + e^x}\,, \tag{2.9}$$

we find that the solution $u(x, t)$ of the above differential equation is a wave with speed c^*. To verify this, we proceed as in the first section. Choosing an arbitrary A, we plot the numerically obtained solution for a few values of t and determine the position $x_A(t)$ such that $u(x_A(t), t) = A$. We take as separation in time $\Delta t = 1/c^* \approx 2.83$, such that the location of $x_A(t)$ should increase by 1 in successive plots. In Figure 2.2, the solutions are plotted, and we can verify that this is indeed the case by considering the close-up in Figure 2.3. So we conclude that the above initial condition leads to a wavelike solution with speed c^*.

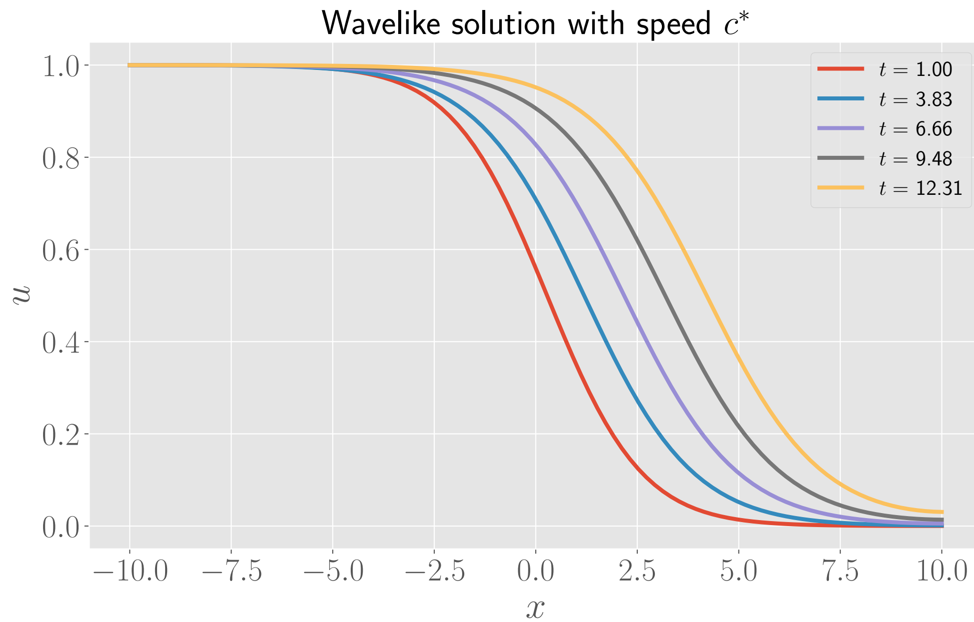

Figure 2.2: Plot of the solution for various values of t, shown in the legend, with separation $\Delta t = 1/c^* \approx 2.83$.

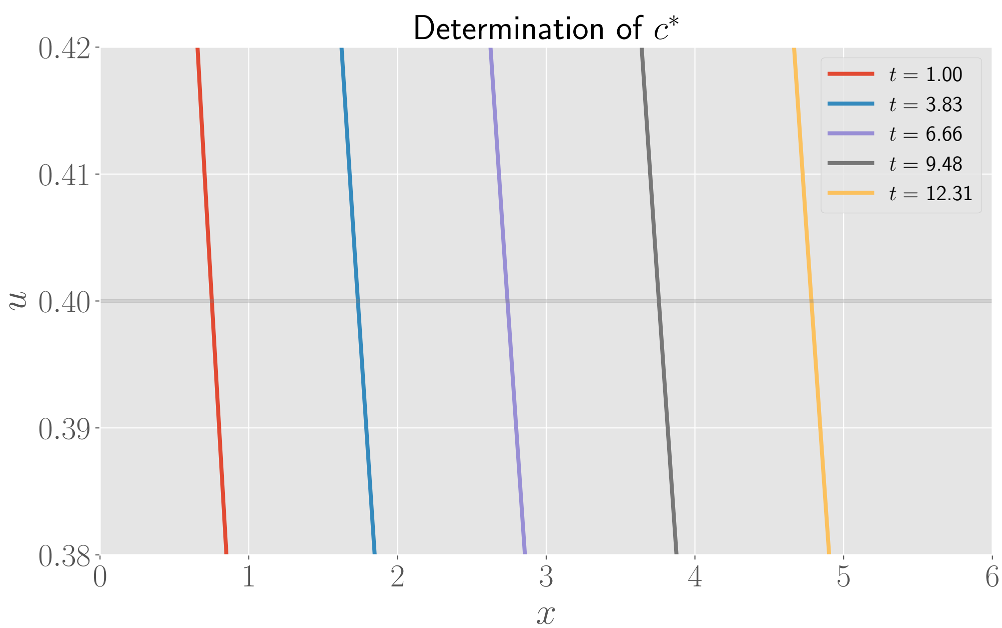

Figure 2.3: Close-up of the solutions shown in Figure 2.2 around $u = A = 0.4$ to determine the speed of the wave.

3 Special solution of the Fisher-Kolmogorov equation

Recall that the Fisher-Kolmogorov equation is

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(1-u)\,. \tag{3.1}$$

We now show that

$$u(z) = \frac{1}{(1+Ae^{z/\sqrt{6}})^2} \tag{3.2}$$

where A is an arbitrary constant and $z = x - ct$, is a travelling wave solution of the Fisher-Kolmogorov equation with wave velocity equal to $c = 5/\sqrt{6}$. We will refer to this solution as the 'special solution'.

We first compute each term in the Fisher-Kolmogorov equation. For the left hand side, we find

$$\text{LHS} = \frac{\partial u}{\partial t} = \frac{2c}{\sqrt{6}} \frac{Ae^{z/\sqrt{6}}}{(1+Ae^{(x-ct)/\sqrt{6}})^3}\,. \tag{3.3}$$

For the right hand side, the spatial derivative term is

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x}\left(-\frac{2A}{\sqrt{6}} \frac{e^{(x-ct)/\sqrt{6}}}{(1+Ae^{(x-ct)/\sqrt{6}})^3}\right) \\ &= -\frac{2A}{\sqrt{6}}\frac{1}{\sqrt{6}} e^{(x-ct)/\sqrt{6}} \left(\frac{1+Ae^{(x-ct)/\sqrt{6}} - 3Ae^{(x-ct)/\sqrt{6}}}{(1+Ae^{(x-ct)/\sqrt{6}})^4}\right) \\ &= \frac{Ae^{(x-ct)/\sqrt{6}}}{(1+Ae^{(x-ct)/\sqrt{6}})^4}\left(-\frac{1}{3}+\frac{2}{3}Ae^{(x-ct)/\sqrt{6}}\right)\,. \end{aligned} \tag{3.4}$$

The second term in the right hand side can be written as

$$u(1-u) = \frac{Ae^{(x-ct)/\sqrt{6}}}{(1+Ae^{(x-ct)/\sqrt{6}})^4}\left(2 + Ae^{(x-ct)/\sqrt{6}}\right)\,. \tag{3.5}$$

Summing both together, the full right hand side is given by

$$\text{RHS} = \frac{5}{3}\frac{Ae^{(x-ct)/\sqrt{6}}}{(1+e^{(x-ct)/\sqrt{6}})^4}\left(1+Ae^{(x-ct)/\sqrt{6}}\right) = \frac{5}{3}\frac{Ae^{(x-ct)/\sqrt{6}}}{(1+Ae^{(x-ct)/\sqrt{6}})^3}\,. \tag{3.6}$$

Comparing with the left hand side in equation (3.3), we conclude that $u(z)$ is indeed a solution if we require

$$\frac{2c}{\sqrt{6}} = \frac{5}{3}\,, \tag{3.7}$$

which indeed gives a speed $c = 5/\sqrt{6}$ for this wavelike solution.

Figure 3.1 below shows a plot of the special solution in the (u, v)-plane, with $v = u'$, along with the phase portrait of the dynamical system from equation (1.3) for $c = 5/\sqrt{6}$. The special solution is a heteroclinic orbit, connecting the two saddle nodes $(1, 0)$ and $(0, 0)$.

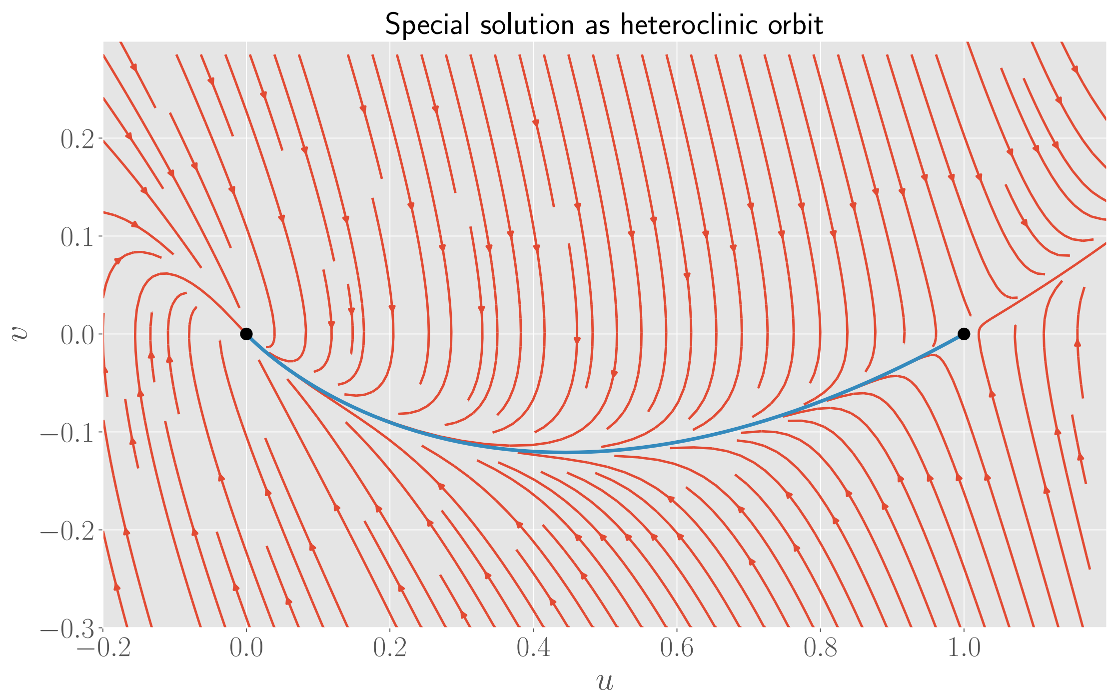

Figure 3.1: Plot of the special solution, shown in blue, in phase space along with the phase portrait. The solution is a heteroclinic orbit, connecting the fixed points $(1, 0)$ and $(0, 0)$ (black dots).

We compare this wave with the solution we obtained numerically in the first section in Figure 3.2 below. As expected, the special solution is slightly faster than the numerically integrated solution. In fact, the shape of the wave of this special solution resembles the shape of the approximate solution from the first exercise, and hence our discussion from that exercise can be repeated here. Indeed, Figure 3.3 compares these two solutions, and we see the approximate solution is a good approximation to the special solution. The approximate solution consistently has larger values for u, but has the same shape as the special solution.

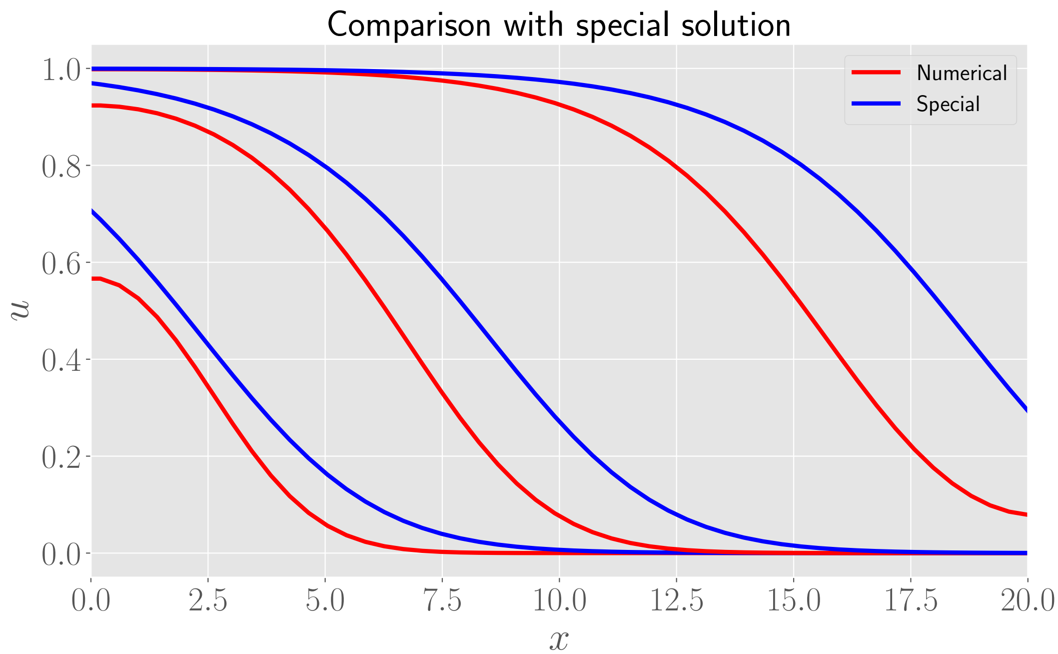

Figure 3.2: Comparison between special solution and numerical integration. Times shown are (from left to right) $t = 2, 5$ and 10.

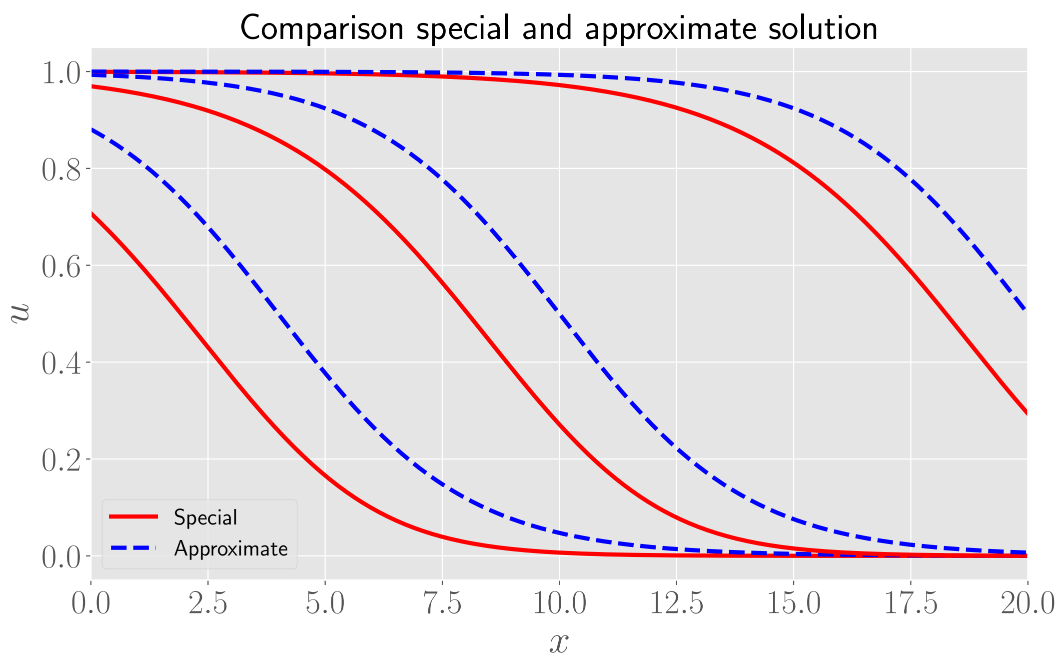

Figure 3.3: Comparison between special solution and approximate solution. Times shown are (from left to right) $t = 2, 5$ and 10.