TMA4212 - Project 2

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1 Introduction

We will perform a theoretical analysis of a numerical scheme for the PDE,

$$u_t = \mu u_{xx} + f(u), \tag{1}$$

for positive μ. We will then use this to model the spreading of decease in a population.

2 Theory

Consider the scheme

$$U_m^* = U_m^n + \frac{r}{2}(\delta_x^2 U_m^* + \delta_x^2 U_m^n) + kf(U_m^n), \quad r = \mu\frac{k}{h^2} \tag{2a}$$

$$U_m^{n+1} = U_m^* + \frac{k}{2}(f(U_m^*) - f(U_m^n)). \tag{2b}$$

For a linear PDE, i.e. if $f(u) = au$ for some constant a, the scheme becomes

$$U_m^* = U_m^n + \frac{r}{2}(\delta_x^2 U_m^* + \delta_x^2 U_m^n) + kaU_m^n, \quad r = \mu\frac{k}{h^2} \tag{3a}$$

$$U_m^{n+1} = U_m^*(1 + \frac{ka}{2}) - \frac{ka}{2}U_m^n. \tag{3b}$$

We aim to prove the convergence of this numerical method, for the linear reaction function. For this we will need the following theorem.

Theorem 2.1 (Lax' equivalence theorem) *A difference scheme is convergent if and only if it is consistent and stable.*

2.1 Consistency

We wish to study the consistency of our method, this method is split into two parts, firstly the predictor step, U_m^*, and then a correction step. So we start by looking more closely at the prediction step. For this analysis, assume that $U_m^n = u_m^n$. Then we do a recursive expansion of U_m^*,

$$U_m^* = U_m^n + kf(U_m^n) + \frac{r}{2}\left(\delta_x^2 U_m^n + \delta_x^2\left(U_m^n + kf(U_m^n) + \frac{r}{2}(\delta_x^2 U_m^n + ...)\right)\right), \tag{4}$$

by inserting the expression for U_m^* into the implicit part of the equation. We collect terms, and we then get,

$$U_m^* = U_m^n + kf(U_m^n) + r\delta_x^2 U_m^n + \frac{r^2}{2}\delta_x^4 U_m^n + k\frac{r}{2}\delta_x^2 f(U_m^n) + \frac{r^2}{4}\delta_x^4(U_m^* - U_m^n). \tag{5}$$

We will in the following use the central difference approximations for second, forth and sixth derivatives. The last term in the above equation can be written as

$$\frac{r^2}{4}\delta_x^4(U_m^* - U_m^n) = \frac{r^3}{8}\delta_x^6(U_m^* + U_m^n) + k\frac{r^2}{4}aU_m^n = \mathcal{O}(k^3) + k\mathcal{O}(k^2) = \mathcal{O}(k^3). \tag{6}$$

By central difference approximations

$$r\delta_x^2 U_m^n = k\mu\partial_x^2 U_m + \mathcal{O}(kh^2) \tag{7}$$

$$\frac{r^2}{2}\delta_x^4 U_m^n = \frac{k^2}{2}\mu^2\partial_x^4 U_m^n + \mathcal{O}(k^2h^2), \tag{8}$$

$$\frac{k^2\mu}{h^2}\delta_x^2 f(U_m^n) = k^2\mu\partial_x^2 f(U_m^n) + \mathcal{O}(k^2h^2), \tag{9}$$

and Taylor expansion in time, we further rewrite equation (5) and get

$$U_m^* = U_m^n + k\left(f(U_m^n) + \mu\partial_x^2 U_m^n\right) + \frac{k^2}{2}\mu^2\partial_x^4 U_m^n + k^2\mu\partial_x^2 f(U_m^n) + \mathcal{O}(k^3 + kh^2) \tag{10}$$

$$= U_m^n + k\partial_t u_m^n + \frac{k^2}{2}\mu^2\partial_x^4 U_m^n + k^2\mu\partial_x^2 f(U_m^n) + \mathcal{O}(k^3 + kh^2) \tag{11}$$

$$= u_m^{n+1} - \frac{k^2}{2}\partial_t^2 u_m^n + \mathcal{O}(k^3 + kh^2) + \frac{k^2}{2}\mu^2\partial_x^4 U_m^n + k^2\mu\partial_x^2 f(U_m^n) + \mathcal{O}(k^3 + kh^2) \tag{12}$$

$$U_m^* = u_m^{n+1} + \mathcal{O}(k^2 + kh^2). \tag{13}$$

For the next part of the analysis we will be using the second temporal derivatives of the solution,

$$\partial_t^2 u = \partial_t(\mu\partial_x^2 u + f(u)) = \mu\partial_x^2(\partial_t u) + \partial_t f(u) = \mu^2\partial_x^4 u + \mu\partial_x^2 f(u) + \partial_t f(u). \tag{14}$$

We add the correction step of our method (2b), to equation (12), which gives

$$U_m^{n+1} = U_m^n + k\partial_t U_m^n + \frac{k^2}{2}(\mu^2\partial_x^4 U_m^n + \mu\partial_x^2 f(U_m^n)) + \mathcal{O}(kh^2) + \frac{k}{2}(f(U_m^*) - f(U_m^n)) \tag{15}$$

$$= U_m^n + k\partial_t U_m^n + \frac{k^2}{2}\left(\partial_t^2 U_m^n - \partial_t f(U_m^n) + \frac{f(U_m^*) - f(U_m^n)}{k}\right) + \mathcal{O}(kh^2). \tag{16}$$

We now look only at the correction term. We apply that f is linear, and insert the standard first order approximation for the derivative in time,

$$\frac{a(u_m^{n+1} + \mathcal{O}(k^2 + kh^2) - U_m^n)}{k} = \frac{a(u_m^{n+1} - U_m^n)}{k} + \mathcal{O}(k + h^2) = \partial_t f(U_m^n) + \mathcal{O}(k) + \mathcal{O}(k + h^2). \tag{17}$$

Inserting this into the equation we had for U_m^{n+1} we get the following

$$U_m^{n+1} = U_m^n + k\partial_t U_m^n + \frac{k^2}{2}\partial_t^2 U_m^n + \mathcal{O}(k^3 + kh^2) = u_m^{n+1} + \mathcal{O}(k^3 + kh^2). \tag{18}$$

Finally we can now conclude with the following lemma.

Lemma 2.2 *The method described in* (2) *is consistent of order 2 in space and time.*

2.2 Stability

To study the stability of the numerical scheme in equation (3b), we will use von Neumann stability analysis. We assume for the stability analysis that the solution to equation (1) can be Fourier expanded in terms of $u_\beta(x,t) = e^{i\omega(\beta)t}e^{i\beta x}$ on the . In our case, $i\omega(\beta) = a - \beta^2$.

Writing the initial condition as its Fourier series,

$$u(x,0) = \sum_{\beta\in\mathbb{Z}} A_\beta e^{i\beta x}, \quad A_\beta = \frac{1}{2\pi}\int_0^{2\pi} u(x,0)e^{-i\beta x}, \tag{19}$$

and comparing to the PDE using separation of variables we get the solution

$$u(x,t) = \sum_{\beta\in\mathbb{Z}} A_\beta e^{(a-\mu\beta^2)t} e^{i\beta x}. \tag{20}$$

To check for stability of our numerical scheme, we assume that the numerical approximation U_m^n in a single step can be expressed as

$$U_m^n = \sum_{\beta\in\mathbb{Z}} A_\beta \xi^n e^{i\beta x_m}. \tag{21}$$

We consider only one general term, $U_m^n = \xi^n e^{i\beta x_m}$, and then use this to understand the stability of the numerical scheme. Notice that $U_m^{n+1} = \xi U_m^n$. Putting this into equation (3b) and solving for U_m^*, we get

$$\xi U_m^n = U_m^*(1 + \frac{ka}{2}) - \frac{ka}{2}U_m^n \quad \Leftrightarrow \quad U_m^* = cU_m^n, \quad c = \frac{\xi + ka/2}{1 + ka/2}. \tag{22}$$

Putting this expression for U_m^* into the implicit solve step of the scheme (3a) we get

$$cU_m^n = U_m^n + \frac{r}{2}(\delta_x^2 cU_m^n + \delta_x^2 U_m^n) + kaU_m^n \tag{23}$$

The difference operator terms can be calculated

$$\delta_x^2 U_m^n = \xi^n e^{i\beta x_m}(e^{i\beta h} + e^{-i\beta h} - 2) = U_m^n(2\cos\beta h - 2), \quad \delta_x^2 cU_m^n = c\delta_x^2 U_m^n. \tag{24}$$

Assuming $\xi = 0$, we can equate the coefficients of equation (23) and rearrange the second term in equation (22) to arrive at

$$c = 1 + \frac{r}{2}(c+1)(2\cos\beta h - 2) + ka, \tag{25a}$$

$$\xi = c\left(1 + \frac{ka}{2}\right) - \frac{ka}{2}. \tag{25b}$$

Rearranging equation (25a) we get

$$c = \frac{1 + ka - r(1-\cos\beta h)}{1 + r(1-\cos\beta h)} \leq 1 + ka \leq 1 + k|a|, \tag{26}$$

where the inequality follows from both r and $(1-\cos\beta h)$ being non-negative. Notice also that

$$c = \frac{1 + ka - r(1-\cos\beta h)}{1 + r(1-\cos\beta h)} \geq \frac{-k|a|}{1 + r(1-\cos\beta h)} + \frac{-r(1-\cos\beta h)}{1 + r(1-\cos\beta h)} \geq -k|a| - 1. \tag{27}$$

This limits $|c| \leq 1 + k|a|$, and putting this into equation (25b) we get

$$|\xi| \leq |c| \left(1 + \frac{k|a|}{2}\right) + \frac{k|a|}{2} \tag{28}$$

$$\leq 1 + \frac{3}{2}k|a| + \frac{(k|a|)^2}{2} \tag{29}$$

$$\leq 1 + \left(\frac{3}{2}|a| + \tau a^2\right) k \tag{30}$$

$$\leq 1 + \nu k, \ \nu = \left(\frac{3|a|}{2} + \tau a^2\right), \tag{31}$$

where τ is some maximal value of the time step, for instance the whole time period considered. This means the method satisfies the von Neumann stability criterion, $|\xi| \leq 1 + \nu k$, for some constant ν.

Lemma 2.3 *The scheme* (2)*, for a linear function* f*, is stable when used on a problem with periodic or no boundary conditions.*

By theorem 2.1, we therefore get the following result.

Theorem 2.4 *The scheme* (2)*, for a linear function* f*, is convergent when used on a problem with periodic or no boundary conditions.*

3 SI Model

An application of the diffusion reaction equation is in modelling the spread of disease. One model suggested in Murray [1], chapter 13, involves the two parameters S, the susceptible population, as well as I, the infected population. We define the functions

$$S : \mathbb{R}_+ \times [-L, \ L] \times [-L, \ L] \to \mathbb{R}, \tag{32}$$

$$I : \mathbb{R}_+ \times [-L, \ L] \times [-L, \ L] \to \mathbb{R}, \quad L \in \mathbb{R}_+ \tag{33}$$

obeying the partial differential equations

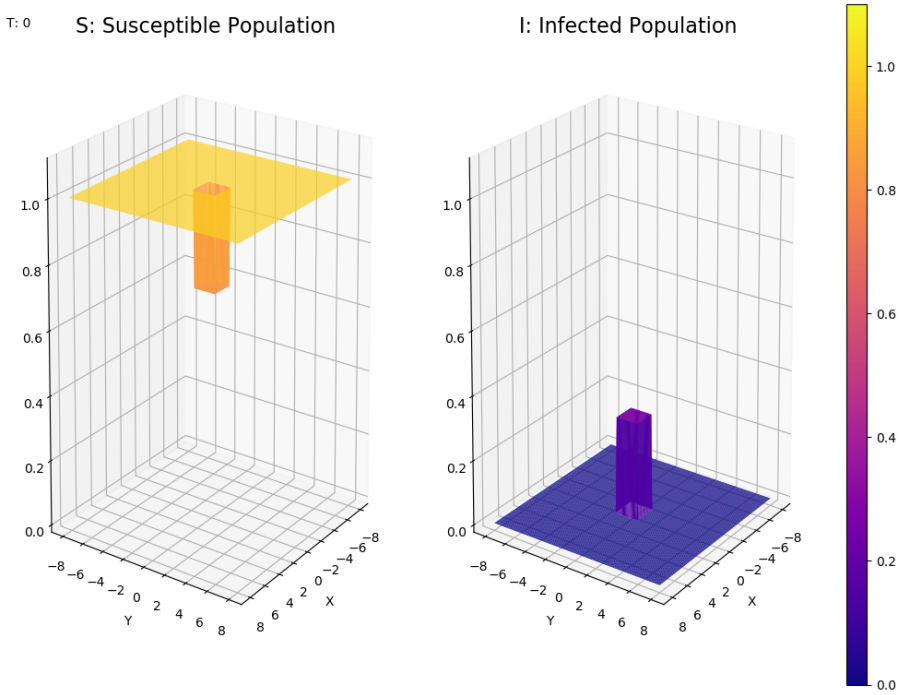
$$\frac{\partial S}{\partial t} = -\beta IS + \mu_S \Delta S, \tag{34}$$

$$\frac{\partial S}{\partial t} = \beta IS - \gamma I + \mu_I \Delta I. \tag{35}$$

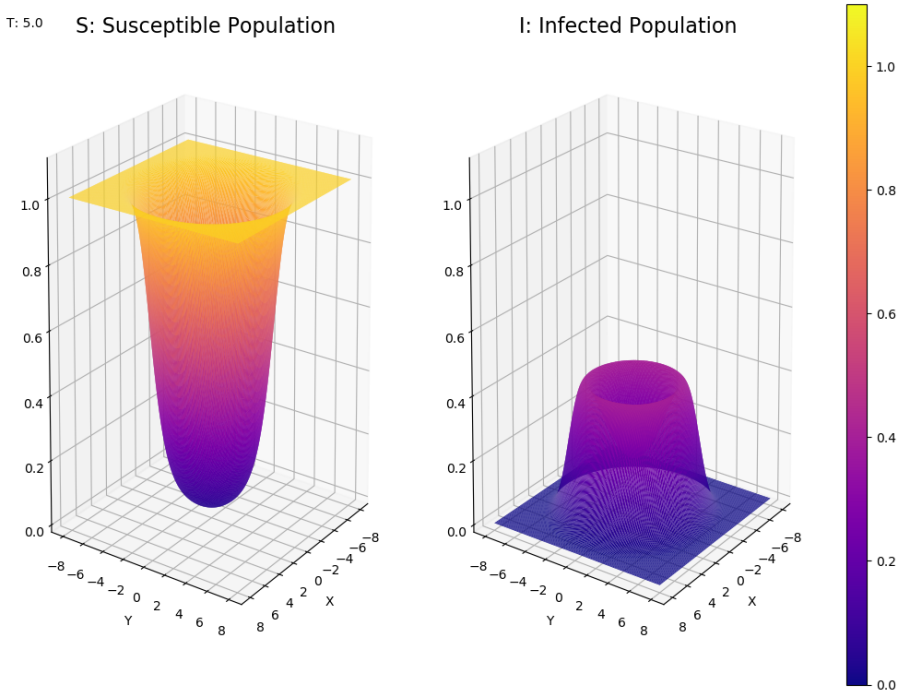
where β and γ are parameters of the model describing the infectiousness of the disease from infected to susceptible people and rate of removal of infected people respectively. Given initial conditions for the susceptible and infected population, this system models an epidemic outbreak of a disease.

For an illustrative case of how the model behaves, we solve forward in time for initial conditions where $S = 1$ on the entire domain, except for a small square in the middle of the domain, where 30% of the population is infected. This is signified by $S = 0.7$ and $I = 0.3$. See figure 1a for an illustration of these initial conditions. The parameters for this simulation are $\beta = 1.5$, $\gamma = 0.5$, $\mu_S = 0.1$ and $\mu_I = 0.2$.

As this example evolves in time, we see a gouge in the susceptible population, and a circularly expanding wave of infected people. A snapshot at time $T = 5$ is shown in figure 1b, and an animation of this specific problem is included in the project hand-in in the file "single_source.gif". From this animation it seems that some of the susceptible population are not infected.



(a) Initial Condition, $T = 0$.



(b) Solution at $T = 5$.

Figure 1: Illustrative time development of an SI-model with the entirety of the population (1) Susceptible at $T = 0$, except for 30% of the population being Infected in a small box the middle of the domain.

In addition, to further test the model, we performed tests with initial non-uniform population distribution. For this we had an initial susceptible population focused around two tops, which can be thought of as cities. We added some infected into one of the cities, and tested how the disease spread. We set the diffusion parameter for susceptibles quite low, while the diffusion rate for infected was set to be quite a lot higher. This was to avoid that the susceptible population would spread out to a uniformly distributed population before the disease could spread. This model gave that the first city quickly became mostly infected. As the disease spread to the second city, the infection came slower, and the infected population did not quite reach the same peak as in the first city. This can be seen in the animation "two_cities.gif".

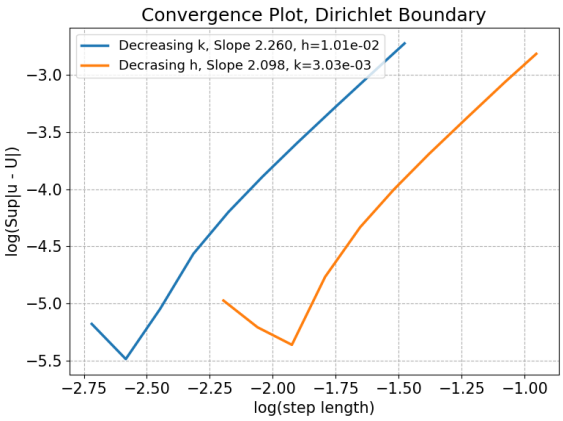


Figure 2: Sup-error at time $T = 0.3$ between a numerical and an exact solution to equation (1) with Dirichlet boundary conditions. Here the exact solution was $u(x,t) = e^{-\pi^2 t}\sin(\pi x) - tx(1-x)$.

4 Numerical Results

In order to empirically verify the consistency orders found theoretically in Lemma 2.2, we use the numerical solver on problems with known exact solutions. This way, we can directly measure the error between the numerical and the exact solution for given step-sizes h and k and compare their relative growth.

This can be seen in figures 2 and 3, where we in order to verify the $\mathcal{O}(k^2 + h^2)$ consistency order in either term hold either h or k constant at a small value for our solutions, and then gradually lower the other step size. We see clearly that the log-log slopes between the Sup-error and the step length have slopes of 2 or higher, indicating second order consistency.

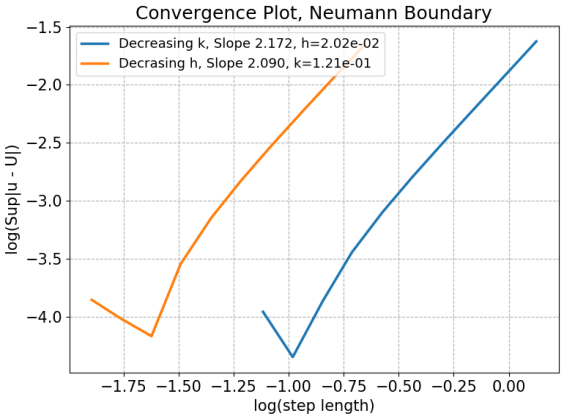


Figure 3: Sup-error at time $T = 12$ between a numerical and an exact solution to equation (1) with Neumann boundary conditions. Here the exact solution was $u(x,t) = \sin(t) + \sin(x)$.

There is however a noticeable upward spike in every convergence line with decreasing step size. This might be due to a lower bound on the error, given by the fixed small value of the step size that is not being reduced. Another contributing factor might be numerical round-off errors, but with sup-error magnitudes between 10^{-4} and $10^{-5.5}$ it is less likely that this is the main contributing factor. Ideally, one would repeat the experiments with lower values for the other step size, and see whether or not the second order convergence continues to lower magnitudes.

5 Conclusion

We have established that the scheme (2) is convergent for problems with periodic or no boundary conditions. Our numerical experiments seem to verify the results from our theoretical analysis.

We further used this, as well as a two dimensional solver. To model the spread of diseases in a population. This yielded results as would be expected. Both from speculations on how the PDE should behave, as well as how real world diseases might spread [1].

References

[1] J. Murray, *Mathematical biology II: spatial models and biomedical applications*. Springer New York, 2001.