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Kunnskap for en bedre verden

TMA4212 - Numerical solution of differential equations by difference methods

Finite difference methods for diffusion-reaction equations

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1 Introduction

Reaction-diffusion systems are mathematical models that are given by equations of the form

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

These equations describe many phenomena in physics, chemistry, and biology, including heat conduction, chemical reactions, and the spread of infectious diseases. Due to the nature of differential equations, and their complexity, analytical solutions are often not possible to find, which means that the use of numerical methods is necessary to find approximations to the solutions.

In this paper, we study numerical schemes for solving reaction-diffusion equations, with a focus on error analysis, before moving on to an epidemiological situation by incorporating reaction-diffusion dynamics into an SIR model to study the spread of a infectious disease under various circumstances.

2 Stability and consistency

2.1 Intro

As we are well aware, time-dependent PDE's with diffusion terms should be solved by implicit methods. However, as in the case of reaction-diffusion equations, using implicit methods to solve the entire system requires solutions of nonlinear equations for every step, which can quickly become very computationally expensive. In order to avoid this, one option is to use an implicit method for the diffusion term and an explicit method for the reaction term. One example of such would be a scheme based on forward and backward Euler in time and a central difference scheme in space. In order for this scheme to be convergent and accurately solve the problem at hand, it needs to be both stable and consistent.

We want to solve the aforementioned reaction-diffusion equation, by using a modified version of the well-known Crank-Nicholson scheme:

$$U_m^* = U_m^n + \frac{r}{2}(\delta_x^2 U_m^* + \delta_x^2 U_m^n) + kf(U_m^n)$$
$$U_m^{n+1} = U_m^* + \frac{k}{2}(f(U_m^*) - f(U_m^n)), \quad r = \mu\frac{k}{h^2}$$

For pure diffusion, i.e. $f = 0$ this is the usual Crank-Nicholson, while for pure reaction $\mu = 0$ this equates to a second order Runge-Kutta method. In our error analysis we will assume f to be linear of the form $f(u) = au$.

2.2 Stability

A numerical scheme is said to be stable if small perturbations, such as initial condition errors or numerical round-off errors, do not grow exponentially as the computations proceed. In order to analyze the stability, we introduce the notion of the growth factor ξ such that $u_m^{n+1} = \xi u_j^n$, and perform a von Neumann analysis.

Second order central difference approximation is:

$\delta_x^2 U_m^n = \frac{U_{m+1}^n - 2U_m^n + U_{m-1}^n}{h^2}$

We now assume a solution on the form: $U_m^n = \hat{U}^n e^{im\theta}$

Where $\theta = l * h, \quad l \in \mathbb{R}, \quad$ and $\hat{U}^{n+1} = \xi\hat{U^n}$

By combining these, we get the following.

$\delta_x^2 U_m^n = \frac{e^{i(m+1)\theta} - 2e^{im\theta} + e^{-i(m-1)\theta}}{h^2} \hat{U}^n$

Plug this into the first step of the scheme:

$U_m^* = U_m^n + \frac{r}{2}(\frac{e^{i(m+1)\theta} - 2e^{im\theta} + e^{i(m-1)\theta}}{h^2} \hat{U}^* + \frac{e^{i(m+1)\theta} - 2e^{im\theta} + e^{i(m-1)\theta}}{h^2} \hat{U}^n) + kaU_m^n$

$\Rightarrow \hat{U}^* e^{im\theta} = \hat{U}^n e^{im\theta} + \frac{r}{2} e^{im\theta}(\frac{e^{i\theta} - 2 + e^{-i\theta}}{h^2} \hat{U}^* + \frac{e^{i\theta} - 2 + e^{-i\theta}}{h^2} \hat{U}^n) + ka\hat{U}^n e^{im\theta}$

Divide by $e^{im\theta}$:

$\Rightarrow \hat{U}^* = \hat{U}^n + \frac{r}{2}(\frac{e^{i\theta} - 2 + e^{-i\theta}}{h^2} \hat{U}^* + \frac{e^{i\theta} - 2 + e^{-i\theta}}{h^2} \hat{U}^n) + ka\hat{U}^n$

$\Rightarrow (1 - \frac{r(e^{i\theta} - 2 + e^{-i\theta})}{2h^2})\hat{U}^* = \hat{U}^n + \frac{r}{2} \frac{e^{i\theta} - 2 + e^{-i\theta}}{h^2} \hat{U}^n + ka\hat{U}^n = (1 + \frac{r(e^{i\theta} - 2 + e^{-i\theta})}{2h^2} + ka)\hat{U}^n$

$\hat{U}^* = \frac{(1 + \frac{r(e^{i\theta} - 2 + e^{-i\theta})}{2h^2} + ka)}{(1 - \frac{r(e^{i\theta} - 2 + e^{-i\theta})}{2h^2})} \hat{U}^n$

Which after simplifying and using the trigonometric identity: $e^{i\theta} + e^{-i\theta} = 2cos(\theta)$ becomes:

$\hat{U}^* = \frac{1 + \frac{r}{h^2}(cos(\theta) - 1) + ak}{1 - \frac{r}{h^2}(cos(\theta) - 1)} \hat{U}^n$

Now we plug this into the second step:

$U_m^{n+1} = \hat{U}^* e^{im\theta} + \frac{ka}{2} e^{im\theta}(\hat{U}^* - \hat{U}^n)$

$\Rightarrow \hat{U}^{n+1} = \hat{U}^* + \frac{ka}{2}(\hat{U}^* - \hat{U}^n) = (1 + \frac{ka}{2})\hat{U}^* - \frac{ka}{2}\hat{U}^n$

$\Rightarrow \hat{U}^{n+1} = ((1 + \frac{ka}{2}) \frac{1 + \frac{r}{h^2}(cos(\theta) - 1) + ak}{1 - \frac{r}{h^2}(cos(\theta) - 1)} - \frac{ka}{2})\hat{U}^n$

This means that, as described in Strikwerda 2004, the amplification factor and the Neumann criterion for stability is as follows:

$|\xi| = |((1 + \frac{ka}{2}) \frac{1 + \frac{r}{h^2}(cos(\theta) - 1) + ak}{1 - \frac{r}{h^2}(cos(\theta) - 1)} - \frac{ka}{2})| \leq 1$

$\Rightarrow |\frac{1 + \frac{r}{h^2}(cos(\theta) - 1) + ak}{1 - \frac{r}{h^2}(cos(\theta) - 1)}| \leq 1$

By squaring both sides, substituting in r and solving with respect to h, we find that the step length in the spatial dimension must satisfy:

$h \leq (\frac{2\mu(1 - cos(\theta))}{a})^{\frac{1}{4}}$

Now we substitute $\theta = lh$, $1 - cos(lh) = 2sin^2(\frac{lh}{2}) \approx (\frac{lh}{2})^2$ and $k = \frac{\mu k}{h^2}$ and get:

$k \leq \frac{ah^2}{l^2}$

Where a and l both are real numbers, and we therefore a quadratic relationship between the spatial and temporal step sizes:

$\underline{k \leq Ch^2}$ $\square$

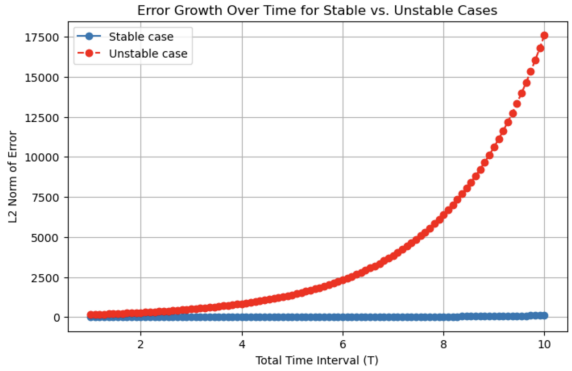

Figure 1: The stable case satisfies $k \leq Ch^2$, while the unstable one does not

From figure 1 we see that when the von Neumann condition is satisfied, the error is bounded, and does not increase when the total time the scheme is run for increases. When the condition is broken however, an increase in the size of the time domain inevitably leads to an exponential increase in the error of the numerical approximation. This is just what is expected, and confirms the theoretical results.

2.3 Consistency

For a numerical method to be of any real use, it is also important that it satisfies the consistency principle. A numerical scheme is consistent if the local truncation error τ_m^n satisfies the following:

$\tau_m^n \to 0 \quad \forall m, n \quad \text{when} \quad h, k \to 0$

In the case of the modified Crank-Nicholson scheme, we have for the first step:

$u^* = u^n + \frac{r}{2}(\delta_x^2 u^* + \delta_x^2 u^n) + kau^n + \tau^*$

Where $\tau^* = \tau_{ck} + \tau_e$

The local truncation error achieved by discretisizing the diffusion term by the Crank-Nicholson method is known to be $\tau_{ck} = \mathcal{O}(k^2) + \mathcal{O}(h^2)$, and we are thus left with analyzing τ_e. This is equivalent to analyzing the truncation error from estimating $u_t = au$ by the scheme $U^{n+1} = U^n + kaU^n$. Thus we want to look at $u^{n+1} = u^n + kau^n + \tau_e$. Taylor's formula from Owren 2017, chapter 2 gives $u^{n+1} = u^n + ku_t^n + \mathcal{O}(k^2)$. Substituting $u_t = au$ into Taylor's formula to get $u^{n+1} = u^n + kau^n + \mathcal{O}(k^2)$. Solving for u^n and substituting into $\tau_e = u^{n+1} - u^n - kau^n$ gives $\tau_e = \mathcal{O}(k^2)$.

As it's clear the second step of our scheme, which is explicit, adjusts the approximation of our reaction term by removing $\frac{k}{2}au_m^n$ and then adding an improved approximation $\frac{k}{2}u_m^*$ from the implicit-explicit step. We see that our final truncation error will be $\tau = \tau_{ck} + RK2(\tau_e)$, where we from our second step get $u_m^{n+1} = u_m^* + \frac{k}{2}(au_m^* - au_m^*) + RK2(\tau_e)$. Remembering that the first step gives $u_m^* = u_m^n + kau_m^n$ and substitution into our second step we get

$$u_m^{n+1} = u_m^n + kau_m^n + \frac{k}{2}(au_m^n + ka^2u_m^n - au_m^n) + RK2(\tau_e),$$

and simplifying gives

$$u_m^{n+1} = u_m^n + kau_m^n + \frac{k^2a^2}{2}u_m^n + RK2(\tau_e).$$

Again expanding using Taylor's formula with $u_t = au$ and $(au)_t = a^2u$ we get

$$u_m^{n+1} = u_m^n + kau_m^n + \frac{k^2a^2}{2}u_m^n + \mathcal{O}(k^3).$$

Comparing the two expressions we see that $RK2(\tau_e) = \mathcal{O}(k^3)$. So for the local truncation error τ of our complete scheme, the $RK2(\tau_e)$ term is smaller than τ_{ck}, so we conclude that $\tau = \mathcal{O}(k^2) + \mathcal{O}(h^2)$.

It's however good to see that the second step improves on the truncation error of the naively treated reaction term, which might be usefull for when $f(u)$ isn't linear and as well-behaved as in our case.

2.4 Convergence

We have now proven that the method is not only stable, but also consistent. From this follows a rather fortunate outcome, namely that it is also convergent. This is a consequence of the Lax equivalence theorem as described in Owren 2017, which states that "A consistent difference scheme is convergent if and only if it is stable."

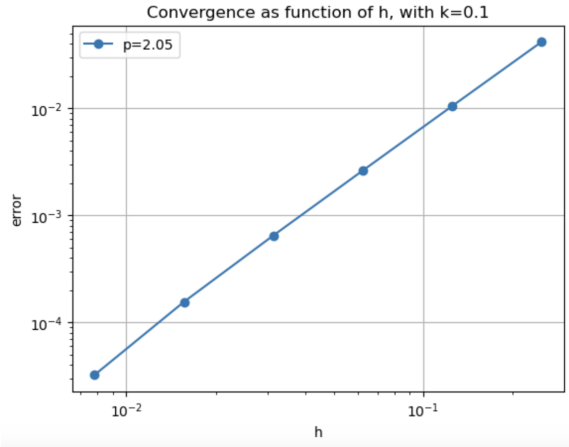

Figure 2: Decreasing step size in space leads to smaller error term

This convergence can be observed in figure 2, which clearly shows convergence of order $p = 2$ in the spatial direction. This is exactly what was calculated during the consistency analysis and also holds for the convergence in time.

3 Modelling infectious diseases

We will look at models for how an infectious disease might spread. At a given time t, a population N can be divided into three groups of people. S denotes people susceptible to the disease, I denotes people who carry and can transfer the disease and R denotes the part of the population who no longer can get the disease due to immunity or death. It's assumed that at $t = 0$ no one is immune to the disease.

3.1 Simple SIR

Our goal is to study how the disease will develop over space and time, but in order to get some intuition for how the model behaves we look at the SIR model described in Britton 2003, chapter 3, which describes the spread of the disease over time:

$$\frac{dS}{dt} = -\beta SI,$$
$$\frac{dI}{dt} = \beta SI - \gamma I,$$
$$\frac{dR}{dt} = \gamma I.$$

We are assuming a scaled model where $S(t) + I(t) + R(t) = 1$. From this model we see that the parameter β governs the rate at which infected people transmits the disease to susceptible people, while γ determines the rate at which people stop being infectious.

3.2 Development in space and time

In order to extend the model to include a space dimension, we consider the following model from Murray 2003, chapter 13:

$$S_t = -\beta SI + \mu_S \Delta S,$$
$$I_t = \beta SI - \gamma I + \mu_I \Delta I.$$

We no longer keep track of group R and the newly introduced parameter μ_* describe how fast people move around. These are reaction-diffusion equations of the form $u_t = \mu u_{xx} + f(u)$ with reaction terms $f_s(S, I) = -\beta SI$ and $f_i(S, I) = \beta SI - \gamma I$ respectively.

3.3 Simulation of model using finite difference method

We denote the numerical approximation of S and I at point $(t = kn, x = hm)$ by $U^n_{s,m}$ and $U^n_{i,m}$.

As discussed earlier these reaction-diffusion equations should be solved using an implicit method. The numerical scheme discussed in section 2 lends it self as a convenient scheme due to the explicit method for the reaction term, which in our model correlates to the cross terms, i.e. the terms where the equations depend on each other. Thus the method analogously extends to solving our system of two PDE's by first performing the implicit-explicit intermediate step for both equations, followed by performing the purely explicit steps as such:

$$U^*_{s,m} = U^n_{s,m} + \frac{r}{2}(\delta^2_x U^*_{s,m} + \delta^2_x U^n_{s,m}) + k f_s(U^n_{s,m}, U^n_{i,m}),$$
$$U^*_{i,m} = U^n_{i,m} + \frac{r}{2}(\delta^2_x U^*_{i,m} + \delta^2_x U^n_{i,m}) + k f_i(U^n_{s,m}, U^n_{i,m}),$$
$$U^{n+1}_{s,m} = U^*_{s,m} + \frac{k}{2}(f_s(U^*_{s,m}, U^*_{i,m}) - f_s(U^n_{s,m}, U^n_{i,m})),$$
$$U^{n+1}_{i,m} = U^*_{i,m} + \frac{k}{2}(f_i(U^*_{s,m}, U^*_{i,m}) - f_i(U^n_{s,m}, U^n_{i,m})), \quad r = \mu\frac{k}{h^2}.$$

We let our space domain be $[0, 1]$ as it works nicely with the notion of our total scaled population $N(t, x) = 1$ and thus integrating N for any fixed t over our spacial domain results in the total population coming out to be equal to 1.

For the initial condition of our model we assume a part of the population close to the center of our spacial domain is infected. Due to this the values of S at the boundaries is 1 and the values of I at the boundaries is 0. Further we would like to impose on the values at the boundaries to be constant, that is $g(t)_{s,0} = g(t)_{s,1} = 1$ and $g(t)_{i,0} = g(t)_{i,1} = 0$.

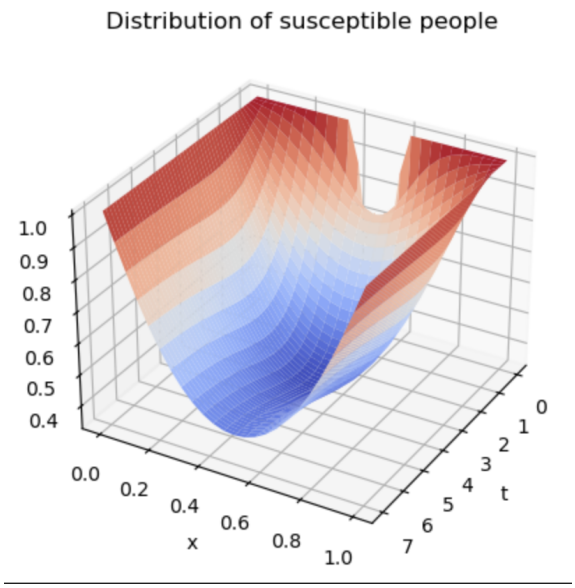

Figure 3: Plotted here is the distribution of the susceptible population, that being not infected, not dead and not immune, over time.

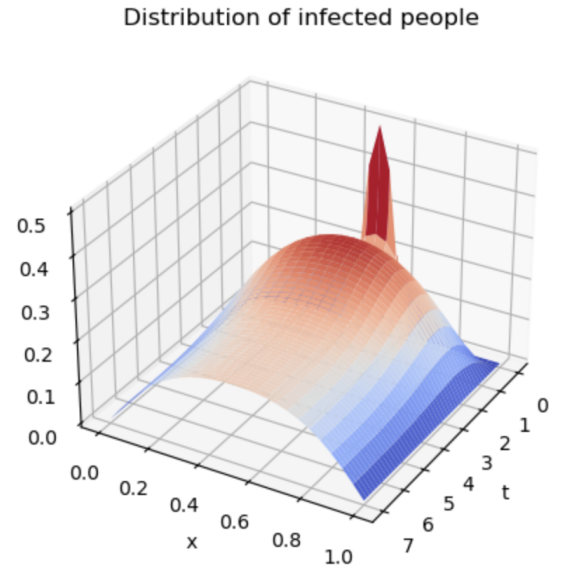

Figure 4: Plotted here is the distribution of the infected population over time.

Figures 3 and 4 shows how the disease spreads over time, given a set of conditions and parameters. The population is normalized to size 1, all of whom are susceptible at time $t = 0$ except for a at the very center, which is the location of the epicenter of the disease. The infection rate is $\beta = 3$ and the recovery rate is $\gamma = 1$. The dynamics appear diffusive, with the susceptible population redistributing across the domain and gradually reducing. Especially in the center, where the infection started, just about half of the initial population are either deceased, infected, immune or have spread to other parts of the spatial domain. As both the population and the contagion disperses, the number of infected people flattens out, before it gradually starts decreasing, likely due to the infection rate being $\frac{1}{3}$ of the recovery rate.

The model captures the expected dynamics of an epidemic outbreak, with initial growth, peak infections, and eventual decline due to recovery. Sharp peaks in infections indicate a period of rapid spread, which is typical in real-world outbreaks. These results align with classical epidemiological

models, demonstrating how reaction-diffusion equations capture these propagation effects very well. The numerical implementation via the scheme from section 1 ensures stability, allowing accurate tracking of the disease over time.

4 Conclusion

In this paper, we analyzed numerical methods for solving reaction-diffusion equations, focusing on error analysis, and their application to modelling the spread of an infectious disease. Reaction-diffusion equations, which describe many naturally occuring processes, require numerical methods due to the complexity of their analytical solutions.

We first performed a theoretical consistency and stability analysis of a proposed numerical scheme for solving a linear reaction-diffusion equation. With proofs and associated numerical experiments, we confirmed the theoretical features of the method, checking its accuracy and stability under different conditions.

In the second part of the paper, we applied numerical techniques to the SIR model extended to space. By simulating the spread of an infectious disease over space and time, we explored how different parameters, such as diffusion rates and transmission coefficients, influences the development of an epidemic. The results demonstrated how numerical methods can provide insights into real world scenarios such as in this case.

Overall, this project confirmed the importance of numerical stability and accuracy in solving time-dependent PDE's. The findings highlight the need for careful method selection when modeling dynamical systems.

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