Math 5120 Spring 2009 – Some notes on numerical solution of diffusion equations and reaction-diffusion equations

Consider the problem

$$PDE: \quad c_t = Dc_xx + ac(1-c) \qquad \text{for } 0 < \text{x} < \text{L and t} > 0,$$

with boundary conditions

$$BC: \quad c_x(0,t) = 0 \ \text{ and } \ \mathrm{c_x(L,t) = 0},$$

and initial conditions

$$IC: \quad c(x,0) = f(x) \qquad \text{for } 0 < \text{x} < \text{L}.$$

Here, $D > 0$, $a > 0$, $L > 0$ are given constants, and $f(x)$ is the specified initial data. Note that we have imposed no-flux boundary conditions at both ends of our interval. We will touch on other boundary conditions later.

Note that the partial derivative of c with respect to t can be approximated by a difference quotient:

$$c_t(x,t) \approx \{c(x,t+\Delta t) - c(x,t)\}/\Delta t$$

provided $0 < \Delta t << 1$. Similarly, the spatial derivatives of c can be approximated by difference quotients.

$$\begin{aligned} c_x(x,t) \approx& \{c(x+\Delta x,t) - c(x,t)\}/\Delta x && (1)\\ \approx& \{c(x,t) - c(x-\Delta x,t)\}/\Delta x && (2)\\ \approx& \{c(x+\Delta x,t) - c(x-\Delta x,t)\}/(2\Delta x). && (3) \end{aligned}$$

provided $0 < \Delta x << 1$. Further,

$$c_{xx}(x,t) \approx \frac{c(x-\Delta x,t) - 2c(x,t) + c(x+\Delta x,t)}{(\Delta x)^2}$$

again provided $0 < \Delta x << 1$. Only the approximation to c_{xx} might be surprising. One way to motivate it is to write the RHS of this expression as

$$\frac{\frac{c(x+\Delta x,t)-c(x,t)}{\Delta x} - \frac{c(x,t)-c(x-\Delta x,t)}{\Delta x}}{\Delta x},$$

that is, as a difference quotient of difference quotient approximations of c_x. Alternatively, we can write Taylor Series expansions of $c(x-\Delta x,t)$ and $c(x+\Delta x,t)$ about (x,t) to obtain:

$$\begin{aligned} c(x-\Delta x,t) &= c(x,t) - c_x(x,t)\Delta x + \tfrac{1}{2}c_{xx}(x,t)(\Delta x)^2 - \frac{1}{6}c_{xxx}(x,t)(\Delta x)^3 + \frac{1}{24}c_{xxxx}(x,t)(\Delta x)^4 + ...\\ c(x+\Delta x,t) &= c(x,t) + c_x(x,t)\Delta x + \tfrac{1}{2}c_{xx}(x,t)(\Delta x)^2 + \frac{1}{6}c_{xxx}(x,t)(\Delta x)^3 + \frac{1}{24}c_{xxxx}(x,t)(\Delta x)^4 + ... \end{aligned}$$

It follows from these that

$$
\begin{aligned}
c(x-\Delta x,t)-2c(x,t)+c(x+\Delta x,t) &= \{c(x,t)-2c(x,t)+c(x,t)\}+\{-c_x(x,t)+c_x(x,t)\}\Delta x \\
&+ \{\tfrac{1}{2}c_{xx}(x,t)+\tfrac{1}{2}c_{xx}(x,t)\}(\Delta x)^2 \\
&+ \left\{-\frac{1}{6}c_{xxx}(x,t)+\frac{1}{6}c_{xxx}(x,t)\right\}(\Delta x)^3 \\
&+ \left\{\frac{1}{24}c_{xxxx}(x,t)+\frac{1}{24}c_{xxxx}(x,t)\right\}(\Delta x)^4+... \\
&= c_{xx}(x,t)(\Delta x)^2+\frac{1}{12}c_{xxxx}(x,t)(\Delta x)^4+...
\end{aligned}
$$

Dividing by $(\Delta x)^2$, we see that

$$
\begin{aligned}
\frac{c(x-\Delta x,t)-2c(x,t)+c(x+\Delta x,t)}{(\Delta x)^2} &= c_{xx}(x,t)+\frac{1}{12}c_{xxxx}(x,t)(\Delta x)^2+... \\
&\approx c_{xx}(x,t).
\end{aligned}
$$

We will approximate the PDE as follows. We divide the interval $[0,L]$ into subintervals of length Δx where $(N+1)\Delta x = L$ and we divide time into steps of length Δt starting at $t=0$. We use the difference quotient approximations for c_t and c_{xx} just discussed to write down a 'finite-difference' approximation to the PDE at the spatial points $x_j = j\Delta x$ for $j=0,1,...,N+1$, and at times $t_n = n\Delta t$ for $n=0,1,2,....$ Let $C_j^n \approx c(j\Delta x, n\Delta t)$ satisfy the equations

$$
\frac{C_j^{n+1}-C_j^n}{\Delta t} = D\frac{C_{j-1}^n-2C_j^n+C_{j+1}^n}{(\Delta x)^2}+aC_j^n(1-C_j^n). \tag{4}
$$

for $j=0,1,...,N+1$ and $n=0,1,2,....$

Next, we approximate the boundary conditions as follows:

$$
\frac{C_1^n-C_{-1}^n}{(2\Delta x)} = 0, \tag{5}
$$

and

$$
\frac{C_{N+2}^n-C_N^n}{(2\Delta x)} = 0. \tag{6}
$$

From (5), we see that $C_{-1}^n = C_1^n$ and from (6) that $C_{N+2}^n = C_N^n$. Equation (4) for $j=0$ involves C_0^{n+1}, C_0^n, C_{-1}^n, and C_1^n, and in this equation we set $C_{-1}^n = C_1^n$ as per (5). Equation (4) for $j=N+1$ involves C_{N+1}^{n+1}, C_{N+1}^n, C_N^n, and C_{N+2}^{n+1}, and in this equation we set $C_{N+2}^n = C_N^n$ as per (6). Writing (4) as an equation for C_j^{n+1} and using these substitutions for $j=0$ and $j=N+1$, our system of equations is

$$
\begin{aligned}
C_0^{n+1} &= C_0^n+\frac{D\Delta t}{(\Delta x)^2}(-2C_0^n+2C_1^n)+a\Delta t C_0^n(1-C_0^n), \qquad (7) \\
C_j^{n+1} &= C_j^n+\frac{D\Delta t}{(\Delta x)^2}(C_{j-1}^n-2C_j^n+C_{j+1}^n)+a\Delta t C_j^n(1-C_j^n) \quad \text{for j = 1,...,N}, \\
C_{N+1}^{n+1} &= C_{N+1}^n+\frac{D\Delta t}{(\Delta x)^2}(2C_N^n-2C_{N+1}^n)+a\Delta t C_{N+1}^n(1-C_{N+1}^n).
\end{aligned}
$$

If we know C_j^n for $j = 0, ..., N+1$, these formulas allow us to calculate C_j^{n+1} for $j = 0, ..., N+1$. Since we have initial data $c(x, 0) = f(x)$, we start with $C_j^0 = f_j = f(j\Delta x)$ for $j = 0, ..., N+1$. Then we use (7) to calculate C_0^1, C_1^1, ..., C_{N+1}^1. After this we use (7) again to calculate C_0^2, C_1^2, ..., C_{N+1}^2. In this way, we march forward in time, computing an approximation solution at each time $t_{n+1} = (n+1)\Delta t$. The method we just described is called the Forward Euler method applied to Fisher's Equation. It works reasonably well for Δt and Δx sufficiently small, provided these numerical parameters also satisfy the condition $\frac{D\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$. This combination of terms comes up often so we give it a name, $\lambda = \frac{D\Delta t}{(\Delta x)^2}$. So the condition for the Forward Euler method behaving reasonably is that $0 < \lambda < \frac{1}{2}$. This is illustrated in Fig.1. On the left, the timestep Δt and spacestep Δx are chosen such that $\lambda = 0.4$, while on the right, they are chosen so that $\lambda = 1.0$. The solution on the right grows to magnitude 10^{23} by $t = 1$.

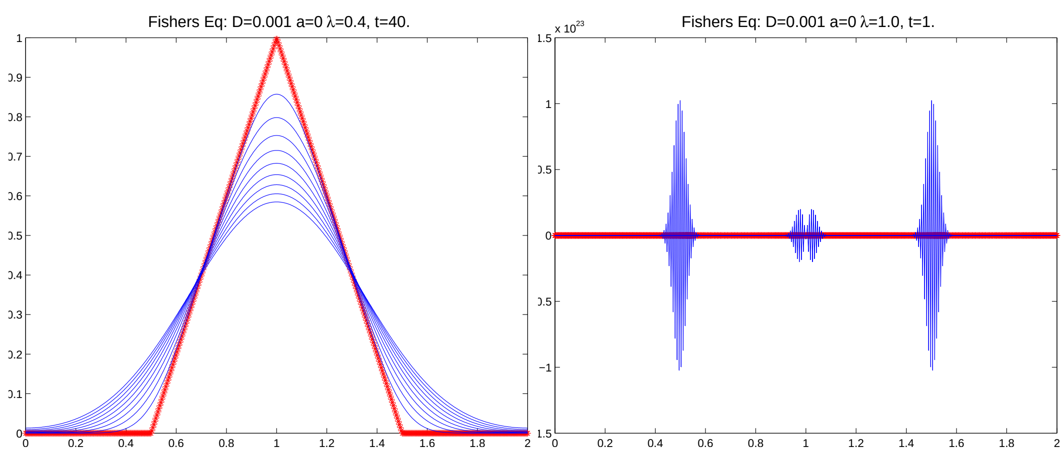

Figure 1: Left: Diffusion Equation solved with Forward Euler method with $\lambda = D\Delta t/(\Delta x)^2 = 0.4$. Right: Diffusion Equation solved with Forward Euler method with $\lambda = D\Delta t/(\Delta x)^2 = 1.0$.

Fig.2 shows the results of a calculation with $a = 1.0$ and $\lambda = 0.4$. The solution $c(x, t)$ grows to 1 in two waves moving outward from the initial region of nonzero c.

We can do some analysis which explains why we have the restriction $\lambda \leq \frac{1}{2}$ for the Forward Euler method. To do this it is very useful to write equations (7) in matrix-vector form. Let $\mathbf{C}^n \in \mathbb{R}^{N+2}$ denote the vector whose entries are the values $C_0^n, C_1^n, C_2^n, ..., C_{N+1}^n$ in that order, and let $\mathbf{C}^{n+1}$ be

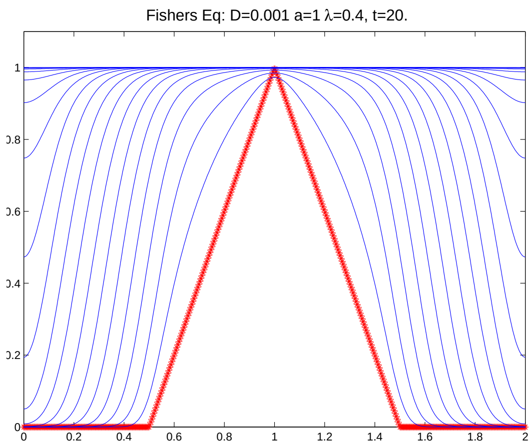

Figure 2: Fisher's Equation solved with Forward Euler method with $\lambda = D\Delta t/(\Delta x)^2 = 0.4$ for $a = 1$.

defined similarly. Let A be the $(N+2)\times(N+2)$ matrix defined by

$$A = \begin{bmatrix} -2 & 2 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ & & \ddots & \ddots & \ddots & & \\ 0 & \dots & \dots & 1 & -2 & 1 & 0 \\ 0 & \dots & \dots & & 1 & -2 & 1 \\ 0 & \dots & \dots & & 0 & 2 & -2 \end{bmatrix}. \tag{8}$$

and let $M = I + \lambda A$, where I is the $(N+2)\times(N+2)$ identity matrix. Then equations (7) can be written

$$\mathbf{C}^{n+1} = M\mathbf{C}^n. \tag{9}$$

The solution after n timesteps can therefore be written in terms of the initial values as

$$\mathbf{C}^n = M^n\mathbf{C}^0. \tag{10}$$

where M^n means the nth power of the matrix M. Suppose the matrix A has eigenvalue α and corresponding eigenvector $\mathbf{X}$. Then the matrix M has eigenvalue $1+\lambda\alpha$ and the corresponding eigenvector is $\mathbf{X}$. The matrix A has $N+2$ eigenvalues which we denote by $\alpha^{(p)}$ and corresponding eigenvectors $\mathbf{X}^{(p)}$ for $p = 0, 1, ..., N+1$. Suppose for a moment that $\mathbf{C}^0 = \mathbf{X}^{(p)}$ for some p. Then, from (10) it follows that $\mathbf{C}^n = (1+\lambda\alpha^{(p)})^n\mathbf{X}^{(p)}$. If $|1+\lambda\alpha^{(p)}| > 1$, then the initial vector gets amplified by a factor that grows without bound as n gets larger. This could be the origin of the unstable behavior of the numerical method. To decide if this is the case, it would be useful to know the eigenvalues and eigenvectors of A and therefore M.

The matrix A has eigenvectors $\mathbf{X}^{(p)}$ with components $X_j^{(p)} = \cos\left(\frac{\pi p j \Delta x}{L}\right) = \cos\left(\frac{\pi p j}{N+1}\right)$. (Why does it make sense that the eigenvectors are given by cosines? Think about the separation of variables solution for the diffusion equation with boundary conditions $c_x(0,t) = 0$ and $c_x(L,t) = 0$.) The corresponding eigenvalues of A are $\alpha^{(p)} = -4\sin^2\left(\frac{\pi p}{2(N+1)}\right)$. The eigenvalues of M are therefore $\mu^{(p)} = 1 - 4\lambda\sin^2\left(\frac{\pi p}{2(N+1)}\right)$. The eigenvalues of M are between -1 and 1 if $0 < \lambda \leq \frac{1}{2}$. For $\lambda \leq \frac{1}{2}$ the Forward Euler method is stable; for $\lambda > \frac{1}{2}$ it is unstable and the solution grows unboundedly.

So far, we have considered the boundary conditions $c_x(0,t) = 0$ and $c_x(L,t) = 0$. If we want to change the boundary condition at $x = 0$ to $c(0,t) = g_0$ for some constant g_0, we have only to modify the equations (7) a little. The only change is to replace the first equation (the $j = 0$ one) in (7) with the equation

$$C_0^{n+1} = g_0. \tag{11}$$

This is useful for setting up a problem for which a travelling wave would develop as shown in Fig.3.

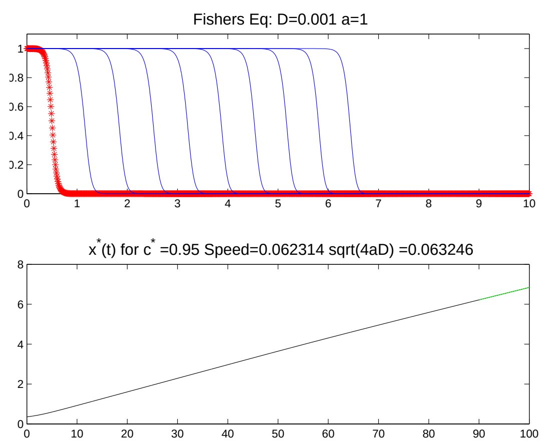

Figure 3: Fisher's Equation solved with Forward Euler method with $\lambda = D\Delta t/(\Delta x)^2 = 0.4$ for $a = 1$.

The Forward Euler scheme works fine as long as $\lambda \leq \frac{1}{2}$. To get a more accurate solution, we choose smaller values of Δx and Δt. Suppose we have computed with some values $\Delta x = \Delta x_0$ and $\Delta t = \Delta t_0$ for which $\lambda \leq \frac{1}{2}$. Suppose we decide to halve Δx, so $\Delta x^{\text{new}} = \frac{1}{2}\Delta x_0$. To keep λ the same value, we would have to set $\Delta t^{\text{new}} = \frac{1}{4}\Delta t_0$ and would therefore have to do four times as many timesteps to get to the same time t as with the original Δt_0. This rapid increase in the number of timesteps can get to be costly as we reduce Δx. It would be nice to have a method for which we could choose Δt without having to worry about stability.

We can get an idea of how to achieve this by considering a much simpler problem

$$\frac{dy}{dt} = -\beta y \qquad \text{where} \quad \beta > 0. \tag{12}$$

Since, $\frac{dy}{dt} \approx \frac{y(t+\Delta t)-y(t)}{\Delta t}$, we can define a finite-difference method for this ODE by

$$\frac{Y^{n+1} - Y^n}{\Delta t} = -\beta Y^n. \tag{13}$$

This is the Forward Euler method for this simple ODE. We can rewrite equation (13) as

$$Y^{n+1} = (1 - \beta \Delta t)\, Y^n. \tag{14}$$

The solution to this equation at time $t_n = n\Delta t$ is

$$Y^n = (1 - \beta \Delta t)^n\, Y^0. \tag{15}$$

Note that this scheme is therefore stable if $|1 - \beta\Delta t| \leq 1$, and unstable otherwise. If $\beta >> 1$, a very small value of Δt is needed to satisfy the stability condition. Consider the alternative method

$$\frac{Y^{n+1} - Y^n}{\Delta t} = -\beta \tfrac{1}{2}(Y^n + Y^{n+1}). \tag{16}$$

which we rewrite as

$$Y^{n+1} = \frac{1 - \frac{1}{2}\beta\Delta t}{1 + \frac{1}{2}\beta\Delta t} Y^n, \tag{17}$$

which has solution

$$Y^n = \left(\frac{1 - \frac{1}{2}\beta\Delta t}{1 + \frac{1}{2}\beta\Delta t}\right)^n Y_0. \tag{18}$$

Since the factor $\left(\frac{1 - \frac{1}{2}\beta\Delta t}{1 + \frac{1}{2}\beta\Delta t}\right)$ is no greater than 1 in magnitude for any $\Delta t > 0$ since $\beta > 0$, we see that this method is stable for any $\Delta t > 0$. The key to acheiving this was to include enough of the unknown future value Y^{n+1} on the right hand side of the approximate ODE.

We can do a very similar thing in the context of the diffusion equation or Fisher's equation. Again, let A by the matrix defined in (8). The Forward Euler method we considered earlier can be written

$$\mathbf{C}^{n+1} - \mathbf{C}^n = \lambda A \mathbf{C}^n.$$

Consider instead the method

$$\mathbf{C}^{n+1} - \mathbf{C}^n = \lambda A \tfrac{1}{2} \left(\mathbf{C}^n + \mathbf{C}^{n+1}\right). \tag{19}$$

This can be rewritten as

$$(I - \tfrac{1}{2}\lambda A)\mathbf{C}^{n+1} = (I + \tfrac{1}{2}\lambda A)\mathbf{C}^{n}. \tag{20}$$

This is the analog of (17) for the ODE. It can be shown that (20) is stable no matter what the choice of $\Delta t > 0$ and therefore for any choice of $\lambda > 0$. This method is known as the Crank-Nicolson method. Not only is it more stable than the Forward Euler method; it is also more accurate in that Forward Euler makes an error that is $O(\Delta t) + O((\Delta x)^2)$, while Crank-Nicolson makes an error that is $O((\Delta t)^2) + O((\Delta x)^2)$. The Crank-Nicolson method can be made a component of the method for solving Fisher's equation. It is still a good idea to evaluate the reaction term $aC(1-C)$ using known values of C because otherwise we would have a nonlinear system of equations to solve to determine the new values $\mathbf{C}^{n+1}$. I combined the Crank-Nicolson method for the diffusion terms with a method known as the 4th order Runge-Kutta method for the reaction terms. It gives the results shown in Fig.4.

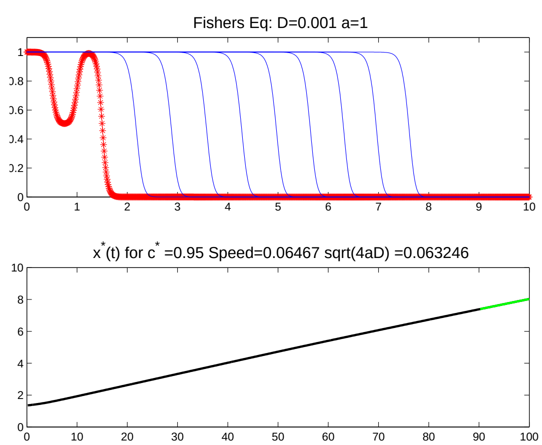

Figure 4: Fisher's Equation solved with Crank-Nicolson method combined with the 4th order Runge-Kutta method, and run with $\lambda = D\Delta t/(\Delta x)^2 = 2.0$ for $a = 1$.