Diffusion Phenonema Seminar

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0.1. Introduction

These lectures are largely based on Chapter 7 of Bank's text [**?**]. Another very useful reference is Logan's text [**?**], which is used in Math 842-43 (the applied mathematics sequence.)

We're going to need a whole bunch of terminology, some of which I'll stick here. First some notation and facts from calculus:

(1) $\mathbf{n}$: an outward pointing unit normal vector defined at each point on the boundary$\partial\Omega$ of a 2- or 3-dimensional solid Ω which is usually assumed to be an open connected set with an orientable boundary.
(2) $\bigtriangledown f$: the gradient of the scalar function f of the spatial variables. E.g., in the case of three space dimensions, we obtain the vector valued function $\bigtriangledown f = \left\langle \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right\rangle = \langle f_x, f_y, f_z \rangle$
(3) $\bigtriangledown \cdot \mathbf{F}$: the divergence of a vector function $\mathbf{F}$ where each coordinate depends on the spatial variables. E.g., if $\mathbf{F} = \langle F, G \rangle$, then $\bigtriangledown \cdot \mathbf{F} = \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = F_x + G_y$.
(4) A function is *smooth* in a domain if is has continuous partial derivatives in all its variables in the domain under consideration.
(5) Gauss Divergence Theorem: Under suitable smoothness conditions

$$\int_\Omega \bigtriangledown \cdot \mathbf{F} dx = \int_{\partial\Omega} \mathbf{F} \cdot \mathbf{n} dx.$$

Here I'm using the convention that "dx" represents the appropriate differential element. For example, if $\mathbf{F}$ is 3-dimensional, dx represents differential volume and in calculus notation we would have used three integral signs.

Incidentally, GDT is rather more ordinary than you might think. Consider what it means in one dimension.

0.2. Conservation and Balance Laws

Imagine that a physical quantity is distributed over a spatial region R. This region could be 1-3 dimensional, and a generic point is referenced by the letter $\mathbf{x}$. Thus, $\mathbf{x}$ could reference a location x on the real line, a point (x, y) in a two-dimensional region or (x, y, z) in a three-dimensional region.

Next, suppose that the variable N is to represent a physical quantity like population, mass, energy, etc., that is distributed over space and may vary with time. Then it is necessary to measure the *concentration* (or *density*) of this substance. For example, in that case of a single space dimension (the simplest case) we would have that $N = N(x, t)$ and if the units of the physical quantity are Q, then the units of N are given by

$$[N] = \frac{Q}{L},$$

where L is length. BTW, Q and L would be called *fundamental units.* Some other fundamental units are mass M and time T. We will assume that the physical quantity N is neither created or destroyed unless we are given an explicit mechanism for doing so, like a source or decay function.

Now suppose that Ω is a subregion of R with boundary $\partial\Omega$. In words, a conservation law takes the form:

Time rate of change of total Q inside Ω equals

- Amount of Q flowing out of Ω across $\partial\Omega$ per unit time +

Amount of Q being sourced or sinked (created or destroyed is one interpretation) in Ω (of course, sourced is positive and sinked is negative.)

Actually, the name is a slight misnomer. Traditionally, the law I have just described is a *balance law,* while a *conservation law* is a balance law in which there is no source term.

We need one more term, namely a "flux" term Φ that represents the amount of $\mathbf{\Phi}$ that flows across a unit spatial element of $\partial\Omega$ per unit time. Such a function can be very complicated and depend not only on spatial coordinates and time, but even N and its derivatives. Notice that $\mathbf{\Phi}$ is a vector quantity, because flows have a direction as well as a magnitude. Finally, we want to allow for the possibility that the material is being sourced or sinked according to a "source" (rate) function f whose units are $[N]/T$. This function could depend on time, position and even N. We'll suppress its argument list. Now we're going to express it in symbols. We're ready for the integral formulation, which starts as

$$\frac{d}{dt}\int_{\Omega} N(\mathbf{x}, t) dx = -\int_{\partial\Omega} \mathbf{\Phi} \cdot \mathbf{n} dx + \int_{\Omega} f dx$$

and is transformed by GDT to the so-called integral formulation of conservation/balance

$$\frac{d}{dt}\int_{\Omega} N(\mathbf{x}, t) dx = \int_{\Omega} \left(- \bigtriangledown \cdot \mathbf{\Phi} + f\right) dx.$$

Now we make a crucial assumption about N, namely that it is smooth in all if its variables and we assume that Ω is a bounded region. Then we may take the derivative sign inside and obtain

$$\int_{\Omega} \left\{ \frac{\partial N(\mathbf{x}, t)}{\partial t} - \left(- \bigtriangledown \cdot \mathbf{\Phi} + f\right) \right\} dx.$$

But this is true for all subregions Ω of R. Assuming the integrand is continuous, the only way for this to be true is that

$$N_t(\mathbf{x}, t) + \bigtriangledown \cdot \mathbf{\Phi} = f,$$

which is the so-called *differential form* of a conservation/balance law.

The next question to be answered is the form of the flux term. Perhaps the most famous of these is Ficke's law, that asserts that the quantity tends to flow from higher concentration to lower at a rate proportional to the concentration gradient. In symbols

$$\mathbf{\Phi} = -D \bigtriangledown N.$$

In the most general case D is a tensor quantity, that is, in our setting, a matrix. Moreover, in all cases, D is assumed to be a symmetric positive definite matrix, so that by some orthogonal change of coordinates we can view D as a diagonal matrix with positive diagonal entries. If they are all equal, we can take D to be a positive scalar, which could be a function of position and other variables, even N itself.

In this case the differential form of conservation becomes

$$N_t(\mathbf{x}, t) = \bigtriangledown \cdot (D \bigtriangledown N) + f.$$

This is the most general form of the diffusion equation. Let's specialize to the case where D is a constant, a very common and useful case. The diffusion equation now takes the form

$$N_t(\mathbf{x}, t) = D \bigtriangleup N + f,$$

where $\bigtriangleup$ is the Laplacian operator. Sometimes other coordinate systems are preferable to cartesian. In cylindrical and spherical coordinates, for example, we have the formulas

$$\begin{aligned} \bigtriangleup N &= \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial N}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 N}{\partial \theta^2} \\ \bigtriangleup N &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial N}{\partial r}\right) + \frac{1}{r^2 \sin\phi}\frac{\partial}{\partial \phi}\left(\sin\phi\frac{\partial N}{\partial \phi}\right) + \frac{1}{r^2 \sin^2\phi}\frac{\partial^2 N}{\partial \theta^2} \end{aligned}$$

In the case of spherical coordinates with functions that are independent of angle, the Laplacian simplifies to

$$\bigtriangleup N = \frac{\partial^2 N}{\partial r^2} + \frac{2}{r}\frac{\partial N}{\partial r}$$

and in cylindrical coordinates to

$$\bigtriangleup N = \frac{\partial^2 N}{\partial r^2} + \frac{1}{r}\frac{\partial N}{\partial r}.$$

0.3. Simple Cases: Instantaneous Sources

A Pure IVP. We start with this pure IVP

$$\begin{aligned} \frac{\partial N}{\partial t} &= D\frac{\partial^2 N}{\partial x^2}, \ -\infty < x < \infty, \ t > 0 \\ N(x, 0) &= f(x), \ -\infty < x < \infty. \end{aligned}$$

Here $f(x)$ is assumed to be well behaved and decaying rapidly, so that Fourier transforms can be applied. Do so and obtain

$$\frac{\partial \widehat{N}}{\partial t} = -D\xi^2 \widehat{N},$$

so that one obtains

$$\widehat{N} = \widehat{f} e^{-D\xi^2 t} = \widehat{f} \left\{ \widehat{\frac{e^{-x^2/(4Dt)}}{\sqrt{4\pi Dt}}} \right\}$$

and thus the convolution theorem yields that

$$N(x,t) = f(x) \star \frac{e^{-x^2/(4Dt)}}{\sqrt{4\pi Dt}} = \int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi Dt}} e^{-(x-y)^2/(4Dt)} f(y)dy.$$

Point Sources. Consider a point source with intensity M, that is, an initial distribution

$$f(x) = M\delta(x)$$

which gives solution

$$N(x,t) = \frac{M}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}.$$

Transport Terms

Introduce a transport term into the problem, so that the flux term is now

$$\mathbf{\Phi} = -D \bigtriangledown N + v_0,$$

where $v_0$is a constant speed at which the material is being transported spatially. (In higher dimensions this speed would be a velocity vector.) The conservation system now becomes

$$\begin{aligned} \frac{\partial N}{\partial t} &= D\frac{\partial^2 N}{\partial x^2} - v_0 N, \ -\infty < x < \infty, \ t > 0 \\ N(x,0) &= f(x), \ -\infty < x < \infty. \end{aligned}$$

A change of variables $z = x - v_0 t$ leads to the equation $N_t = DN_{zz}$ and hence by what we have already done, a solution

$$N(x,t) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi Dt}} e^{-(x-v_0t-y)^2/(4Dt)} f(y)dy.$$

Of course, this gives us a nice formula in the case that $f(x) = M\delta(x)$, namely,

$$N(x,t) = \frac{M}{\sqrt{4\pi Dt}} e^{-\frac{(x-v_0t)^2}{4Dt}}.$$

Radial Diffusion with Exponential Growth. In this case the PDE becomes

$$\frac{\partial N}{\partial t} = D\left(\frac{\partial^2 N}{\partial r^2} + \frac{2}{r}\frac{\partial N}{\partial r}\right) + aN,$$

where a is a growth rate (or a decay rate.) To get a feel for the growth term, imagine that there is no dispersion, but simply exponential growth at a fixed point. What we then have is an ODE $dN/dt = aN$. This is useful in population models of animal growth that try to account for reproduction and dispersion in a single model. It can be shown (see [?]) that a solution to this problem with an instantanious point source at $r = 0$ and $t = 0$ $M\delta(r)$ is given by

$$N(x,t) = \frac{M}{4\pi Dt} \exp\left(at - \frac{r^2}{4Dt}\right).$$

0.4. Simple Cases: Continuous Sources

These sources make their appearances in boundary conditions or continuous interior sources. We'll stick to the former.

Rectilinear Diffusion with a Constant Boundary Condition. Here a simple model problem in one space dimension is

$$\begin{aligned} \frac{\partial N}{\partial t} &= D\frac{\partial^2 N}{\partial x^2},\ 0 < x < \infty,\ t > 0 \\ N(x,0) &= f(x),\ 0 < x < \infty \\ N(0,t) &= N_*. \end{aligned}$$

The solution to this problem is obtained by Laplace transforms and is

$$N = N_* \operatorname{erfc} \frac{x}{\sqrt{4Dt}}$$

where

$$\operatorname{erfc} z = 1 - \operatorname{erf} z = 1 - \frac{2}{\sqrt{\pi}} \int_0^z e^{-\xi^2} d\xi$$

0.5. Model Problems for Study

We will focus on radial diffusion. We're not going to consider a "point source" and we may want to only consider a finite domain. Furthermore, we want to allow for some complex reaction terms. So here is the general statement:

Model Radial Problem:

$$\begin{aligned} \frac{\partial N}{\partial t} &= D\left(\frac{\partial^2 N}{\partial r^2} + \frac{1}{r}\frac{\partial N}{\partial r}\right) + f(r,t,N),\ 0 < r_0 < r < R \le \infty,\ t > 0 \\ N(r,0) &= f(r), \end{aligned}$$

together with suitable boundary conditions at $r = r_0$ and $r = R$. However, problems with $r_0 = 0$ or $R = \infty$ present special problems if we intend to construct numerical approximations to these solutions. Note that Banks focuses on problems where there are explicit analytical solutions, even if, for all practical purposes, these solutions are themselves very difficult to calculate. So we have to finess the special boundary conditions, and there are many ways that we can do this.

EXAMPLE 0.5.1. We can impose Dirichlet boundary conditions, which means that we specify the value of N at each boundary. These values can be constant or even vary with t. If these are ordinary functions, these problems are handled fairly easily by the Octave script `fcnradrR.m` For example, suppose we had just written the code and wanted to test it. Let's pull the standard programmer's trick and try it out on a problem with a known solution. So start with the solution.

Say $N(r,t) = e^{r^2/2-t}$, $1 \le r \le 2$ and $t \ge 0$. Assume diffusion coefficient $D = 1$. Now compute the derivatives and get with a little work that

$$N_t - \frac{1}{r}(rN_r)_r = -\left(3 + r^2\right) N,$$

so the test problem is

$$\begin{aligned} N_t &= -\frac{1}{r}(rN_r)_r - \left(3 + r^2\right) N,\ 1 < r < 2,\ t > 0, \\ N(1,t) = e^{1/2-t}, &\qquad N(2,t) = e^{2-t},\ t > 0, \\ N(r,0) &= e^{r^2/2}. \end{aligned}$$

Now massage the file `fcnradrR.m` so that it satisfies these conditions. (Check the latest version in my Public directory.) Then type interactively in an octave session (which BTW I recorded using the diary feature):

```
octave:2> % script:  radialDirichlet.m

octave:2> % the solution to this problem is N(r,t)=exp(r^2/2-t)
octave:2> % get the initializations out of the way
octave:2> n = 20;rnodes = linspace(1,2,n+1)';rnodes = rnodes(2:n);

octave:3> % next the initial condition
octave:3> y0 = exp(rnodes.*rnodes/2);
octave:4> % calculate the solution
octave:4> sln = lsode('fcnradrR',y0,[0,2]);
octave:5> % plot solution and exact solution at t=2
octave:5> clearplot;hold on;grid
octave:6> plot(rnodes,sln(2,:)')
octave:7> plot(rnodes,exp(rnodes.*rnodes/2-2))
octave:8> % looks nice...let's see the max error
octave:8> e1 = norm(sln(2,:)'-exp(rnodes.*rnodes/2-2),inf)
e1 = 0.00030499
octave:9> % not bad...let's test the quality of our solution
octave:9> % since spatial error is O(dr^2), halving the stepsize
octave:9> % should cut the error down by about 4.  let's see..
octave:9> n = 40;rnodes = linspace(1,2,n+1)';rnodes = rnodes(2:n);

octave:10> y0 = exp(rnodes.*rnodes/2);
octave:11> sln = lsode('fcnradrR',y0,[0,2]);
octave:12> % we won't bother with plots..
octave:12> e2 = norm(sln(2,:)'-exp(rnodes.*rnodes/2-2),inf)
e2 = 7.6389e-05
octave:13> e1/e2
ans = 3.9927
octave:14> % well, it gives a reduction factor of about 4.  good
enough.
octave:14> quit
```

You might note that in the face of an unknown solution, halving step size or other modifications have another application: if you have doubts about the validity of the solution, due to some instability in the numerical scheme, half step sizes and see if you get similar results. If not, you need to rethink your numerical parameters or the scheme itself.

EXAMPLE 0.5.2. Next, let's try to solve a problem with a left flux condition (a.k.a. "Neumann condition"). Suppose that what is happening in two dimensional space is that we now are injecting an amount q (per unit time) of the material N along the boundary of a circle $r = r_0$. Remember that the flux function in two dimensions represents material flowing across the boundary. If the total amount flowing across the circle is $q(t)$, then that the correct identity at the boundary is

$$\text{flux} = -DN_r = \frac{q(t)}{2\pi r_0},$$

so that $N_r = q(t)/(2\pi r_0 D)$. Now massage the file `fcnradfluxR.m` so that it satisfies these conditions for our test problem $N(r,t) = e^{r^2/2-t}$. Since we know that $N_r(1,t) = e^{1/2-t}$, we see that the correct choice for $q(t)$ is $q(t) = -2\pi e^{1/2-t}$. Plug this into the file and now test our results with an interactive Octave session:

```
octave:2> % script:  radialNeumann.m

octave:2> % the solution to this problem is N(r,t)=exp(r^2/2-t)
octave:2> % get the initialization out of the way
octave:2> n = 20;rnodes=linspace(1,2,n+1)';rnodes=rnodes(1:n);
octave:3> % next the initial condition
octave:3> y0 = exp(rnodes.*rnodes/2);
octave:4> % calculate the solution
octave:4> sln = lsode('fcnradfluxR',y0,[0,2]);
octave:5> % plot solution and exact solution at t=2
octave:5> clearplot;hold on;grid
octave:6> plot(rnodes,sln(2,:)')
octave:7> plot(rnodes,exp(rnodes.*rnodes/2-2))
octave:8> % not as good as the Dirichlet problem, but this is typical
octave:8> % check the maximum error
octave:8> e1 = norm(sln(2,:)'-exp(rnodes.*rnodes/2-2),inf)
e1 = 0.00054433
octave:9> % ok, let's halve the stepsize
octave:9> n = 40;rnodes=linspace(1,2,n+1)';rnodes=rnodes(1:n);
octave:10> y0 = exp(rnodes.*rnodes/2);
octave:11> sln = lsode('fcnradfluxR',y0,[0,2]);
octave:12> plot(rnodes,sln(2,:)')
octave:13> e2 = norm(sln(2,:)'-exp(rnodes.*rnodes/2-2),inf)
e2 = 0.00013627
octave:14> e1/e2
ans = 3.9945
octave:15> % once again, about 4.
octave:15> quit
```

EXAMPLE 0.5.3. Now suppose that we want to model a population that obeys the governing equations

$$\begin{aligned} \frac{\partial N}{\partial t} &= D\left(\frac{\partial^2 N}{\partial r^2} + \frac{1}{r}\frac{\partial N}{\partial r}\right) + f(r,t,N),\ 0 < r < \infty,\ t > 0 \\ N(r,0) &= M\delta(r),\ 0 < r < \infty. \end{aligned}$$

(There is another implicit condition: the solution should remain bounded.) The muskrat population example of Banks [**?**, p. 336] serves as an example of a diffusion phenomenon with exponential growth ($f = aN$), where a is a positive growth rate.

Delta conditions are really difficult to code up numerically because they are a pretty severe form of discontinuity. We can finess this into a more numerically amenable problem as follows: ask ourselves what happens a small time after time $t = 0$. We expect the instantaneous pulse to evolve into a smooth Gaussian-like distribution. A good clue is the explicit form to the exponential growth rate problem ([**?**, p. 335])

$$N(r,t) = \frac{M}{4\pi Dt} e^{at - r^2/(4Dt)}.$$

So we can treat this instantaneous source problem as a problem with a flux condition at the left boundary, but rather than have an instantaneous source at $t = 0$, we can spread out the pulse over a short time in a smooth fashion by defining

$$q(t) = \frac{2M}{\sigma\sqrt{2\pi}} e^{-t^2/\left(2\sigma^2\right)}$$

where σ is a small variance. Note that

$$\int_0^\infty q(t)dt = M.$$

So we will replace the instantaneous source by a continuous source that emits about the same amount, M, over a relatively short time span by using the above formula for $q(t)$ with a suitable choice of σ.

Exercise 0.6. Take a critical look at the example of Banks [**?**, p. 336]. Solve this problem numerically using the function file fcnradfluxR.m. You might use $M = 1$ as in the previous example and an interval from 1 to something like 150, along with $\sigma = 1$ to mimick an instantaneous source. As Banks mentions, you could use $a = 2.65/\text{yr}$ and $D = 12.2$. Look at the graphs and see if the radius of the front roughly corresponds to the data given. What are the approximate populations in the years $2, 4, 6, 8$ and 10 where we count 1905 as year zero? Do you believe this model?

Exercise 0.7. Suppose that we model (criminal) drug sales as radiating from a single steady source whose location we know and obeying a radial diffusion law. Now $N(r,t)$ represents the density of drug incidents. Here are issues to think about and we will discuss them in seminar:

1. How can we set up the function files to handle a continuous constant source of radial diffusion, given a constant diffusion coefficient and the size of the source. What are the appropriate boundary conditions? (Do this for a continuous model as in Example 0.5.3 so that it is ready to go for the rest of this problem.)

2. Now suppose that we are given drug crime data on a grid (map of the city, really). How can we translate this into information about $N(r,t)$?

3. Given this information about $N(r,t)$, how can we use it to estimate the diffusion coefficient of the model?

4. (Harder!) What if we don't know the center, but believe there is one?

Bibliography