BGGN 221 Mathematical Methods
Problem Presentation

Diego Mesa
Brian Luk

1 The Narrative

The year is 2050 and we're engineers working in a lab for Triton Pharmaceuticals. We've just received a new membrane protein that was recently invented and we're to insert it into an empty, newly manufactured lipid bi-layer. Being the phenomenal engineers we are, we decide to calculate some metrics about the proteins' diffusion through the membrane.

Since the membrane is manufactured in long sheets, we will simply cut one down to size and before sending it off to be formed and sealed, we'll inject the membrane proteins in the middle of the sheet and try to model the concentration as a function of length and width of the sheet, and time.

2 The Facts

Modeling the diffusion of particles across the surface of a sphere is hard! We've made some assumptions to try and simplify the problem enough so that we could solve it using the techniques we've learned in class.

The key assumptions we've made:

- We've decide to approximate the sphere as a rectangular sheet that is infinitely thin (diffusion in 2 dimensions).
- The motion of the proteins throughout the membrane will be represented as free moving particles diffusing throughout a liquid. We aren't considering any chemical properties between the proteins and/or the membrane itself.
- We are going to model the initial deposit of membrane proteins into our sheet as a delta function
- The flux at $x = 0$ and $x = L$ are zero, because eventually the membrane would be tied back in on itself, giving us no net flux across that boundary.
- The concentrations at $y = 0$ and $y = W$ are zero because we assume that a constant flow across those edges are going keeping them so.

3 The Setup

- Diffusion in Two Dimensions

$$\frac{\partial}{\partial t} u\left(x,y,t\right) = D * \left(\frac{\partial^2}{\partial x^2} u\left(x,y,t\right) + \frac{\partial^2}{\partial y^2} u\left(x,y,t\right) \right) \tag{1}$$

- Boundary Conditions

$$\frac{\partial}{\partial t}u\,(0,y,t) = \frac{\partial}{\partial t}u\,(L,y,t) = 0 \tag{2}$$
$$u\,(x,0,t) = u\,(x,W,t) = 0 \tag{3}$$

- Initial Conditions

$$u\,(x,y,0) = c * \delta_{xy} \tag{4}$$

4 The Math

4.1 2 Dimensions

Using the separation of variables technique we proceed by trying to find a solution of the form:

$$u\,(x,y,t) = V(x,y)T(t)$$

Preceding in this fashion allows us to now express (1) as the following system:

$$T'(t) - D\lambda_1 T(t) = 0 \tag{5}$$
$$\frac{\partial^2}{\partial x^2}V(x,y) + \frac{\partial^2}{\partial y^2}V(x,y) - (-\lambda_1)V(x,y) = 0 \tag{6}$$

Using the separation of variables technique once more, we can separate

$$V(x,y) = X(x)Y(y) \tag{7}$$

into the following system:

$$X'' - (-\lambda_2)X = 0 \tag{8}$$
$$Y'' + (\lambda_1 - \lambda_2)Y = 0 \tag{9}$$

We can revisit our B.C. in (2) and express it as:

$$X'(0)Y(y)T(t) = X'(L)Y(y)T(t) = 0$$
$$X(x)Y(0)T(t) = X(x)Y(W)T(t) = 0$$

to avoid the trivial cases we are left with

$$X'(0) = X'(L) = 0 \tag{10}$$
$$Y(0) = Y(W) = 0 \tag{11}$$

We can now use these to solve our system described in (8) - (9)

$$X'' + \lambda_2 X = 0 \tag{12}$$

has a characteristic equation of:

$$r^2 + \lambda_2 = 0 \tag{13}$$

When $\lambda_2 < 0$

$$\textit{...trivial solutions} \tag{14}$$

When $\lambda_2 = 0$

$$X(x) = c_o \tag{15}$$

When $\lambda_2 > 0$

$$X(x) = c_1 cos(\sqrt{\lambda_2} x) + c_2 sin(\sqrt{\lambda_2} x) \tag{16}$$

$$X'(x) = -c_1 \sqrt{\lambda_2} sin(\sqrt{\lambda_2} x) + c_2 \sqrt{\lambda_2} cos(\sqrt{\lambda_2} x) \tag{17}$$

Applying our B.C. listed in (10) we find that

$$c_2 = 0$$
$$\lambda_2 = (\frac{m\pi}{L})^2$$
$$X_m(x) = c_m cos(\frac{m\pi}{L} x)$$

We can now examine (9), and in after proceeding in a similar manner as above and applying our B.C. listed in (11) we find that

$$\lambda_3 = (\frac{n\pi}{W})^2 \tag{18}$$

$$\lambda_1 = (\frac{n\pi}{W})^2 + (\frac{m\pi}{L})^2 \tag{19}$$

$$Y_n(y) = d_n sin(\frac{n\pi}{W} y) \tag{20}$$

Now that we have our λ_1 we can use it to solve for (5). As a linear first order ODE we obtain:

$$T_{nm}(t) = b_{mn} e^{-D\lambda_1 t} \tag{21}$$

Now we can substitute our separated functions back into our original equation and combine the constant terms to form:

$$u_{mn}(x, y, t) = a_{mn} e^{-D\lambda_1 t} cos(\frac{m\pi x}{L}) sin(\frac{n\pi y}{W}) \tag{22}$$

Here we can make use of a new technique to solve these types of problems - **double Fourier series**:

$$u(x, y, t) = \sum_{m=0}^{\infty} \sum_{n=1}^{\infty} a_{mn} e^{-D\lambda_1 t} cos(\frac{m\pi x}{L}) sin(\frac{n\pi y}{W}) \tag{23}$$

Now we can finally make use of our I.C to get:

$$u(x,y,0) = c * \delta_{xy} = \sum_{m=0}^{\infty}\sum_{n=1}^{\infty} a_{mn} cos(\frac{m\pi x}{L}) sin(\frac{n\pi y}{W}) \tag{24}$$

We can now take exploit the orthogonality twice to get our coefficients.

$$\int_0^L \int_0^W f(x,y) cos(\frac{p\pi x}{L}) sin(\frac{q\pi y}{W}) = \sum_{m=0}^{\infty}\sum_{n=1}^{\infty} a_{mn} \int_0^L \int_0^W cos(\frac{m\pi x}{L}) sin(\frac{n\pi y}{W}) cos(\frac{p\pi x}{L}) sin(\frac{q\pi y}{W}) \tag{25}$$

We're left with definitions of our constants in terms of p and q, variables that carry over from our orthogonal multiplication.

$$a_{0q} = \frac{2}{LW} \int_0^L \int_0^W f(x,y) sin(\frac{q\pi y}{W}) dydx \tag{26}$$

$$a_{pq} = \frac{4}{LW} \int_0^L \int_0^W f(x,y) cos(\frac{p\pi x}{L}) sin(\frac{q\pi y}{W}) dydx \tag{27}$$

4.2 1 Dimension

We were able to consult several texts for different techniques and applications to analytically solve in two dimensions. However, we were not able to acquire significant insight into the numerical portion of this task. The resources for dealing with a double Fourier series and/or Matlab's PDE Toolbox with something like a delta function for an initial condition, were simply not there. We therefore simplified the problem, approximating the sheet as a one dimensional rod with a delta function right in the middle as our initial condition. The analytical solution for this 1 dimensional case is presented bellow, followed by a numerical approximation of this solution.

Diffusion in one dimension

$$\frac{\partial}{\partial t} u(x,t) = D \frac{\partial^2}{\partial x^2} u(x,t) \tag{28}$$

Our Boundary Condition

$$\frac{\partial}{\partial x} u(-L/2,t) = \frac{\partial}{\partial x} u(L/2,t) = 0 \tag{29}$$

Our Initial Condition

$$u(x,0) = c * \delta_x \tag{30}$$

So we can again assume that we can represent $u(x,t)$ in the following manner:

$$u(x,t) = X(x)T(t) \tag{31}$$

Plugging this into (28) gives us

$$T'(t)X(x) = DT(t)X''(x) \tag{32}$$

We can now split this up into the following system of ODEs:

$$T' + \lambda DT = 0 \tag{33}$$
$$X'' + \lambda X = 0 \tag{34}$$

Solving for (33) as we have done before leaves us with

$$T(t) = Ae^{-\lambda Dt} \tag{35}$$

To solve for (34) we examine the characteristic equation

$$r^2 + \lambda = 0 \tag{36}$$
$$r = 0 \pm i\sqrt{\lambda} \tag{37}$$

As discussed above, when $\lambda < 0$

$$\textit{...trivial case} \tag{38}$$

When $\lambda = 0$

$$X(x) = c_o \tag{39}$$

When $\lambda > 0$

$$X(x) = c_1 cos(\sqrt{\lambda}x) + c_2 sin(\sqrt{\lambda}x) \tag{40}$$

We can now apply our B.C. to obtain

$$X'(x) = -c_1\sqrt{\lambda}sin(\sqrt{\lambda}x) + c_2\sqrt{\lambda}cos(\sqrt{\lambda}x)X'(-L/2) = X'(L/2) = 0 \tag{41}$$

We must solve for

$$2\sqrt{\lambda}c_1 sin(\sqrt{\lambda}\frac{L}{2}) = 2\sqrt{\lambda}c_2 cos(\sqrt{\lambda}\frac{L}{2}) \tag{42}$$

We then arrive at 2 different values of λ

$$\lambda_{sin} = \frac{2\pi n}{L} \tag{43}$$
$$\lambda_{cos} = \frac{2\pi(n+\frac{1}{2})}{L} \tag{44}$$

By principle of superposition we can combine them as:

$$u(x,t) = \sum_{m=0}^{\infty} A_m cos(\frac{2\pi(m+\frac{1}{2})}{L}x)e^{-D(\frac{2\pi(m+\frac{1}{2})}{L})t} + \sum_{n=0}^{\infty} B_n sin(\frac{2\pi n}{L}x)e^{-D(\frac{2\pi n}{L})t} \tag{45}$$

We can now apply our I.C. to pin down the values of A_m and B_n

$$u(x,t) = c * \delta_x = \sum_{m=0}^{\infty} A_m cos(\frac{2\pi(m+\frac{1}{2})}{L}x) + \sum_{n=0}^{\infty} B_n sin(\frac{2\pi n}{L}x) \tag{46}$$

After multiplying both sides by our orthogonal bases, we are left with:

$$A_m \int_{-L/2}^{L/2} cos^2(\frac{2\pi(m+\frac{1}{2})}{L}x)dx = \int_{-L/2}^{L/2} c_o \delta_x cos(\frac{2\pi(m+\frac{1}{2})}{L})dx \tag{47}$$

$$B_n \int_{-L/2}^{L/2} sin^2(\frac{2\pi n}{L}x)dx = \int_{-L/2}^{L/2} c_o \delta_x sin(\frac{2\pi n}{L})dx \tag{48}$$

This reduces to a more familiar form:

$$A_m = \frac{2}{L}\int_{-L/2}^{L/2} c_o \delta_x cos(\frac{2\pi(m+\frac{1}{2})}{L})dx \tag{49}$$

$$B_n = \frac{2}{L}\int_{-L/2}^{L/2} c_o \delta_x sin(\frac{2\pi n}{L})dx \tag{50}$$

We can then recall that, on any $[a,b]$ that contains 0, we can say that:

$$\int_a^b \delta(x) = 1 \tag{51}$$

$$\int_a^b \delta(x)g(x) = g(0) \tag{52}$$

This allows us to simplify (49) and (50) to the following:

$$A_m = \frac{2c_o}{L} \tag{53}$$

$$B_n = 0 \tag{54}$$

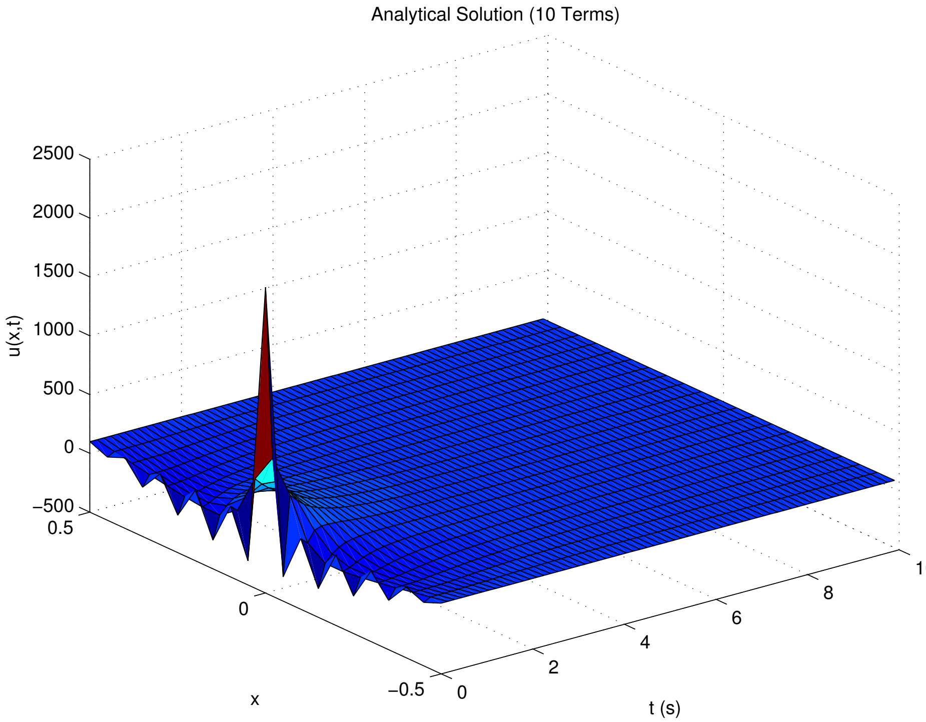

Figure 1: Analytical Solution using 10 terms

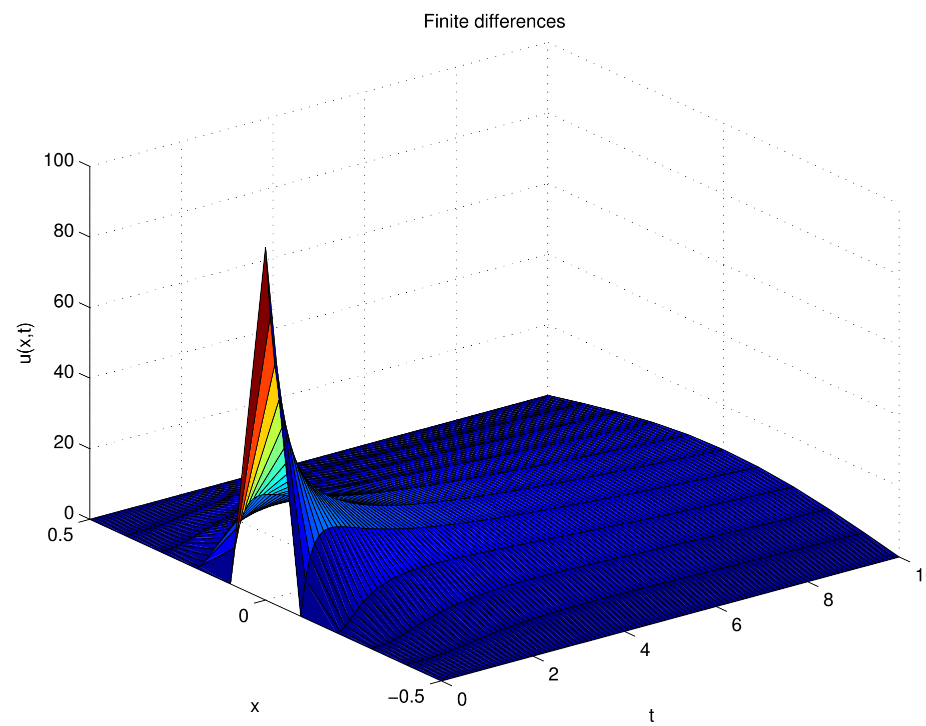

Figure 2: Finite Difference Approximation

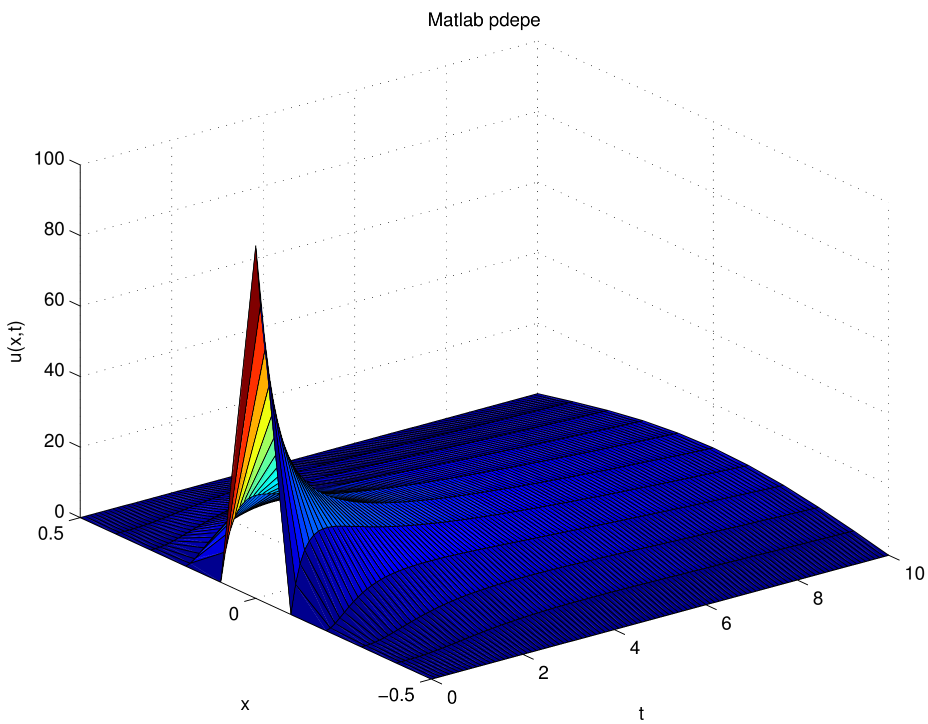

Figure 3: MATLABs pdepe

```
function project_1D_case

%constants
L = 1; % length = 1um
D = 0.01; % diffusion coefficient = .01um^2/s
c_0 = 100; % initial concentration = 1umol/m^2

% analytical solution
tRange = 10;        %s
xSkip = 5;
tSkip = 15;

%defining points on the grid
[X, T] = meshgrid(-L/2:0.01:L/2, 0:0.01:tRange);
A0 = c_0/L;

lastTerm = 0*X;
for i = 1:10
    An = 2*c_0/L;
    sqrtLambda = ((2*(i+(1/2)))*pi)/L;
    currentTerm = An * cos(X * sqrtLambda) .* exp(T * (-D * (sqrtLambda)^2));
    lastTerm = lastTerm + currentTerm;
end

U = A0 + lastTerm;

%surf analytical
figure(1);
surf(T(1:tSkip:end, 1:xSkip:end), ...
     X(1:tSkip:end, 1:xSkip:end), ...
     U(1:tSkip:end, 1:xSkip:end));
title('Analytical Solution (10 Terms)')
xlabel('t (s)')
ylabel('x')
zlabel('u(x,t)')

%finite differences method
dx = 0.1;
dt = 0.1;
xmesh = -L/2:dx:L/2;
tmesh = 0:dt:10;
nx = length(xmesh); % number of points in x dimension
nt = length(tmesh); % number of points in t dimension
stepsize = D * dt / dx^2; % stepsize for numerical integration
conc_fd = zeros(nt, nx);
conc_fd(1, :) = (xmesh == 0)*c_0; % initial conditions; delta impulse at center
conc_fd(:, 1) = 0; % left boundary conditions; zero value
con_fd(:, nx) = 0; % left boundary conditions; zero value
for t = 1:nt-1
    for x = 2:nx-1
        conc_fd(t+1, x) = conc_fd(t, x) + stepsize * ...
            (conc_fd(t, x-1) - 2 * conc_fd(t, x) + conc_fd(t, x+1));
    end
```

```
end

figure(2)
surf(tmesh,xmesh,conc_fd')
title('Finite differences')
xlabel('t')
ylabel('x')
zlabel('u(x,t)')

% pdepe method
sol_pdepe = pdepe(0,@pdefun,@ic,@bc,xmesh,tmesh);

figure(3)
surf(tmesh,xmesh,sol_pdepe')
title('Matlab pdepe')
xlabel('t')
ylabel('x')
zlabel('u(x,t)')


% function definitions for pdepe:
% --------------------------------------------------------------

function [c, f, s] = pdefun(x, t, u, DuDx)
% PDE coefficients functions

c = 1;
f = D * DuDx; % diffusion
s = 0; % homogeneous, no driving term

end
% --------------------------------------------------------------

function u0 = ic(x)
% Initial conditions function

u0 = (x==0)*c_0; % delta impulse at center

end
% --------------------------------------------------------------

function [pl, ql, pr, qr] = bc(xl, ul, xr, ur, t)
% Boundary conditions function

pl = ul; % zero value left boundary condition
ql = 0;  % no flux left boundary condition
pr = ur; % zero value right boundary condition
qr = 0;  % no flux right boundary condition

end

end % end project
```