Math 19. Solving the Diffusion-Reaction Equation

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1 Modeling the Density of Protein

It is known that the concentration of certain proteins at any cell in an embryo determines whether or not a particular gene is expressed in that cell. We will consider a cell model of an embryo where

$$u(t, x, y)$$

is the density of protein at time t and position (x, y). We will consider our embryo to be square, $[0, L] \times [0, L]$, where Protein is produced along the left-hand edge according to

$$u(t, 0, y) = \sin\left(\frac{\pi y}{L}\right).$$

Observe that this function is zero at $(0, 0)$ and $(0, L)$. Assume also that

$$\begin{aligned} u(t, x, 0) &= 0 \\ u(t, x, L) &= 0 \\ u(t, L, y) &= 0. \end{aligned}$$

The protein will diffuse according to the equation

$$\frac{\partial u}{\partial t} = \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - ru.$$

Eventually, we will reach a steady-state

$$\mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - ru = 0. \tag{1}$$

2 Separation of Variables

If we assume that our solution has the form

$$u(x, y) = A(x)B(y),$$

then

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &= A''(x)B(y) \\ \frac{\partial^2 u}{\partial y^2} &= A(x)B''(y), \end{aligned}$$

and equation (1) becomes

$$\mu \left[A''(x)B(y) + A(x)B''(y)\right] - A(x)B(y) = 0 \tag{2}$$

or equivalently

$$\mu \left(\frac{A''(x)}{A(x)} + \frac{B''(y)}{B(y)} \right) = r. \tag{3}$$

if we divide both sides of equation (2) by $A(x)B(y)$. The first term of the expression inside the parentheses of the last equation is a function of x and the second term is a function of y. Since x and y are independent variables and the equation is equal to a constant r, both of these terms must be constant. Thus, rewriting equation (3) as

$$\frac{B''(y)}{B(y)} = \frac{r}{\mu} - \frac{A''(x)}{A(x)} = \lambda,$$

where λ is a constant, we can assume that

$$\frac{1}{A}A'' = \frac{r}{\mu} - \lambda \tag{4}$$

$$\frac{1}{B}B'' = \lambda. \tag{5}$$

Our boundary conditions now become

$$\begin{aligned} A(0)B(y) &= \sin\left(\frac{\pi y}{L}\right), \\ A(L)B(y) &= 0, \\ A(x)B(0) &= 0, \\ A(x)B(L) &= 0. \end{aligned}$$

3 Solving $B'' = \lambda B$

To solve $B'' = \lambda B$, we must consider consider three cases: λ is positive, negative, or zero.

- If $\lambda > 0$, then our solution is

$$B = \alpha e^{\sqrt{\lambda}\,y} + \beta e^{-\sqrt{\lambda}\,y}.$$

- If $\lambda = 0$, then

$$B = \alpha + \beta y.$$

- If $\lambda < 0$, then

$$B = \alpha \cos \sqrt{-\lambda}\, y + \beta \sin \sqrt{-\lambda}\, y. \tag{6}$$

Considering the boundary condition $A(0)B(y) = \sin \pi/L$, the only consistent case occurs when $\lambda < 0$. If we let $\alpha = 0$ and $\beta = 1$ in equation (6), then we can let

$$B(y) = \sin\left(\frac{\pi y}{L}\right) = \sin \sqrt{-\lambda}\, y,$$

and $\lambda = -\pi^2/L^2$. Notice that the boundary conditions

$$\begin{aligned} A(x)B(0) &= 0, \\ A(x)B(L) &= 0. \end{aligned}$$

are satisfied

4 Solving $A'' = (r/\mu - \lambda)A$

The Equation

$$\frac{1}{A}A'' = \frac{r}{\mu} - \lambda$$

now becomes

$$A'' = \left(\frac{r}{\mu} + \frac{\pi^2}{L^2}\right) A.$$

To simplify matters, we will let

$$c = \frac{r}{\mu} + \frac{\pi^2}{L^2}.$$

Thus, we need to solve the equation

$$A'' = cA.$$

In this case, we already know that $c > 0$; consequently our solutions must be of the form

$$A(x) = \alpha e^{\sqrt{c}\,x} + \beta e^{-\sqrt{c}\,x}.$$

Since

$$A(0)B(y) = (\alpha + \beta)\sin\left(\frac{\pi y}{L}\right) = \sin\left(\frac{\pi y}{L}\right),$$

we know that $\alpha + \beta = 1$. Since $A(L)B(y) = 0$ for all y with $0 \leq y \leq L$, it must be the case that

$$\alpha e^{\sqrt{c}\,L} + \beta e^{-\sqrt{c}\,L} = 0$$

or

$$\alpha e^{\sqrt{c}\,L} + (1-\alpha)e^{-\sqrt{c}\,L} = 0$$

Solving this last equation for α, we obtain

$$\begin{aligned} \alpha &= -\frac{1}{e^{2\sqrt{c}\,L} - 1} \\ \beta &= \frac{e^{2\sqrt{c}\,L}}{e^{2\sqrt{c}\,L} - 1} \end{aligned}$$

5 Putting Everything Together

We finally have the solution that we have been seeking,

$$\begin{aligned} u(x, y) &= A(x)B(y) \\ &= \left[\alpha e^{\sqrt{c}\,x} + \beta e^{-\sqrt{c}\,x}\right]\sin\left(\frac{\pi y}{L}\right) \\ &= \left[\left(-\frac{1}{e^{2\sqrt{c}\,L} - 1}\right)e^{\sqrt{c}\,x} + \left(\frac{e^{2\sqrt{c}\,L}}{e^{2\sqrt{c}\,L} - 1}\right)e^{-\sqrt{c}\,x}\right]\sin\left(\frac{\pi y}{L}\right) \\ &= \frac{-e^{\sqrt{c}\,x} + e^{2\sqrt{c}\,L}e^{-\sqrt{c}\,x}}{e^{2\sqrt{c}\,L} - 1}\sin\left(\frac{\pi y}{L}\right), \end{aligned}$$

where

$$c = \frac{r}{\mu} + \frac{\pi^2}{L^2}.$$

Well, we never claimed that this solution would be pretty, but if we look at the graph of the protein distribution in our square cell, it is actually quite nice.