Chemokine Project

Montana Ferita

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Below is a short write-up detailing the mathematics behind the chemokine concentration equation.

Deriving the 1D diffusion equation

Suppose a chemokine is diffusing across a 1D space and we are interested in how the chemokine concentration c changes over space and time. That is, we interested in the function $c(x, t)$.

First, let's discretize our 1D space into evenly spaced squares where i denotes the location of the square.

c_{i-2}	c_{i-1}	c_i	c_{i+1}	c_{i+2}

Let's focus on the c_i square. We want to determine how c_i changes over time, so we want to find dc_i/dt. Suppose the chemokine enters the c_i square from the left (c_{i-1}) and right (c_{i+1}) at rate D with units of length^2/time. Furthermore, suppose the chemokine leaves the c_i square at rate D and goes to either the left (c_{i-1}) or right (c_{i+1}) square. The change in the chemokine concentration at c_i is the following:

$$\frac{dc_i}{dt} = \underbrace{Dc_{i+1}}_{\text{entering from the right}} + \underbrace{Dc_{i-1}}_{\text{entering from the left}} - \underbrace{2Dc_i}_{\text{leaving to the left and right}}$$

We can rewrite this as

$$\frac{dc_i}{dt} = D(c_{i+1} - c_i) + D(c_{i-1} - c_i)$$

Recall one way to write the derivative of a function $f(x)$, is

$$\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

so $f'(x) \approx f(x + \Delta x) - f(x)$.

Looking at the first part of dc/dt we can have $f(x+\Delta x) = c_{i+1}$ and $f(x) = c_i$. So we have,

$$\frac{dc_i}{dt} = D\frac{c_i}{dx}\bigg|_{x=i} + D(c_{i-1} - c_i)$$

We can rewrite $D(c_{i-1} - c_i)$ as $-D(c_i - c_{i-1})$ to mirror our structure. Now $f(x + \Delta x) = c_i$ and $f(x) = c_{i-1}$.

$$\frac{dc_i}{dt} = D\frac{c_i}{dx}\bigg|_{x=i} - D\frac{c_i}{dx}\bigg|_{x=i-1}$$

The second order central difference approximation of $f''(x)$ is

$$f''(x) = \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2}$$

which we can rewrite as

$$f''(x) = \frac{\dfrac{f(x + \Delta x) - f(x)}{\Delta x} - \dfrac{f(x) - f(x - \Delta x)}{\Delta x}}{\Delta x}$$

Thus, by taking the derivative again, we have

$$\frac{dc_i}{dt} = D\frac{d}{dx}\left(\frac{dc_i}{dx}\right)$$

Consequently, we arrive at the 1D diffusion equation:

$$\frac{dc}{dt} = D\frac{d^2c}{dx^2}$$

Finding the general solution

For our problem, let's consider an infinite domain and suppose we have one cancer cell at $x = 0$ that is continuous emitting a chemokine. Furthermore, suppose the chemokine is being degraded at a constant rate δ. Our equation now becomes

$$\frac{dc}{dt} = D\frac{d^2c}{dx^2} - \delta c$$

As our chemokine is being constantly emitted and degraded, the chemokine concentration is constant, so $dc/dt = 0$. This simplification makes it a lot easier to solve our equation. Our equation now becomes

$$\frac{d^2c}{dx^2} = \frac{\delta}{D}c$$

For a second, let's ignore the δ/D, so we have

$$\frac{d^2c}{dx^2} = c$$

We need to find a function whose second derivative is itself. The exponential function satisfies this condition,

$$c(x) = Ae^{x} + Be^{-x}$$

where A and B are coefficients. Our original equation was slightly different and has δ/D term in front of c. To account for this difference, we can adjust our previous equation to be

$$c(x) = Ae^{\lambda x} + Be^{-\lambda x}$$

where $\lambda = \sqrt{\delta/D}$.

Solving for the coefficients

Now we would like to solve for the coefficients A and B. Two conditions we would like to satisfy are

1. As $x \to \pm\infty$, then $c \to 0$
2. c is continuous at $x = 0$

For the first condition, we need to restrict the domain for each term in $c(x)$, so $c \to 0$ as $x \to \pm\infty$. We have

$$\begin{aligned} c(x) =& Ae^{\lambda x}, \ \ -\infty < x < 0 \\ c(x) =& Be^{-\lambda x}, \ \ 0 < x < \infty \end{aligned}$$

For the second condition, we want c to be continuous at $x = 0$. By letting $x = 0$, we find that c is continuous when $A = B$. Now we will only need to find one coefficient.

Suppose M (mass/length^{2}time) is the flux of the chemokine released by the cancer cell. Recall Fick's first law ($J = -Ddc/dx$) where the flow of the chemokine goes from a high to low concentration. For symmetry, suppose the cancer cell at $x = 0$ releases half of M to each side. Consequently, we have

$$\begin{aligned} -D\frac{d}{dx}(Be^{-\lambda x}) =& \frac{M}{2} \quad \text{at } x = 0 \\ D\lambda B =& \frac{M}{2} \\ B\sqrt{D\delta} =& \frac{M}{2} \\ B =& \frac{M}{2\sqrt{D\delta}} \end{aligned}$$

Therefore, we have

$$
\begin{aligned}
c(x) &= \frac{M}{2\sqrt{D\delta}} e^{\sqrt{\delta/D}x}, \quad -\infty < x < 0 \\
c(x) &= \frac{M}{2\sqrt{D\delta}} e^{-\sqrt{\delta/D}x}, \quad 0 < x < \infty
\end{aligned}
$$

We can extend this result to consider multiple cancer cells emitting a chemokine. To find the chemokine concentration at a given position, we can use the superposition principle to sum the chemokine concentration from each individual cancer cell.