Reaction-Diffusion Equations

Let $c(x, t)$ be the density of a chemical around a point $x = (x_1, x_2, x_3)$ in space, at time $t$.

Consider a region $S$ and let $C_S(t)$ be the total amount of chemical inside $S$ at time $t$, i.e.: $C_S(t) = \int_S c(x, t) \, dx$.

Let $J(x, t)$ be the flux of $c$, a (possibly time-dependent) vector field which indicates the direction of flow, and the average amount of the chemical crossing, per unit time, a unit area perpendicular to $J$.

Then, on the interval of time $[t, t + h]$, the net amount of chemical exiting through the boundary of $S$ is $\int_S \int_{\partial S} J \cdot n \, dA$.

Let $f(x, t)$ be the amount of the chemical being created (or destroyed, if $< 0$) at a point $x$ in space, at time $t$.

$(\forall$ smooth vector field $J$, net flow through the boundary of a region [bounded open subset of $\mathbb{R}^n$ with smooth or piecewise smooth boundary] = total divergence in the region).

So we conclude:

$$\int_S \frac{\partial c}{\partial t} \, dx = \int_S f(x, t) \, dx - \int_{\partial S} J \cdot n \, dA$$

and since this happens for all $S$, no matter how small ("function with zero integral on all regions must be zero")

$$\frac{\partial c}{\partial t} = f - \nabla J$$

This applies in general; next: flux due to diffusion.
**What is Diffusion?**

one of the fundamental processes by which “particles” (atoms, molecules, even bigger objects) move

**Fick’s Law, 1855, based upon experimental observation:** movement [higher → lower] concentration regions
\[ \text{“flux } J(x, t) \propto -\nabla c(x, t) \text{”} \]

applies to movement of particles in a solution; proportionality constant depends on sizes of molecules (solvent, solute) and temperature and, when across membranes, permeability & thickness

main physical explanation is probabilistic, based on thermal motion of individual particles due to environment (e.g. molecules of solvent) constantly “kicking” the particles (Brown 1828: pollen grains suspended in water move in a rapid but very irregular fashion; relation to Fick’s Law explained mathematically in Einstein’s Ph.D. thesis, 1905)

**Diffusion Equation**

so \( J(x, t) = -D \nabla c(x, t) \) \((D = \text{diffusion coefficient})\) and, in general, \( \frac{\partial c}{\partial t} = f - \text{div } J \) (div = “\( \nabla \)”)

\[ \frac{\partial c}{\partial t} = D \nabla^2 c + f \]

where \( \nabla^2 \) is the “Laplacian” (often “\( \Delta \)”) operator:

\[ \nabla^2 c = D \left( \frac{\partial^2 c}{\partial x_1^2} + \frac{\partial^2 c}{\partial x_2^2} + \frac{\partial^2 c}{\partial x_3^2} \right) \]

and in particular in dimension one:

\[ \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} + f \]

(note: \( \frac{1}{D} \propto \sqrt{\text{volume}}, \text{or equivalently to } \sqrt{\text{mass}} \))

with no \( f \) nor additional constraints, eventually \( \rightarrow \text{homogeneous concentration over space}; \) but usually there are additional boundary conditions, creation and absorption rates, etc, superimposed on pure diffusion, so there’s a “trade-off” between the “smoothing out” effects of diffusion and other influences

**why \( J(x, t) \propto -\nabla c(x, t) \)?**

“virtual wall” of unit area

suppose particles move right or left with equal probability, so half of the \( p_1 \) particles in the first box move right, and the other half move left; similarly for second box flux (rightward) through virtual wall proportional to \( \frac{p_1 - p_2}{2} \), which is proportional to \( -\frac{\partial c}{\partial x} \) (analogously in \( \mathbb{R}^3: -\nabla c(x, t) \))

**Remark: Speed of Diffusion (dim 1)**

(ignoring reaction term “\( f \)” for now; will add back later)

*Suppose \( c \) satisfies diffusion equation \( \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \).*

Assume also that the following hold:

\[ c = \int_{-\infty}^{+\infty} c(x, t) \, dx \]

is independent of \( t \) (constant population), and

\[ \lim_{x \to \pm\infty} x^2 \frac{\partial c}{\partial x}(x, t) = 0 \quad \text{and} \quad \lim_{x \to \pm\infty} xc(x, t) = 0. \]

\((c \text{ small at infinity}) \forall t\). Define, for each \( t \):

\[ \sigma^2(t) = \frac{1}{C} \int_{-\infty}^{+\infty} x^2 c(x, t) \, dx \quad \text{(second moment finite)} \]

which measures how the density “spreads out”

Then:

\[ \sigma^2(t) = 2Dt + \sigma^2(0) \quad \forall t > 0 \]

in particular, if the initial \((t = 0)\) population is concentrated near \( x = 0 \) (“\( \delta \) function”), then \( \sigma^2(t) \approx 2Dt \)
Proof
use PDE and integrate by parts:
\[
\frac{C d\sigma^2}{D dt} = \int_{-\infty}^{+\infty} x^2 c \, dx = \int_{-\infty}^{+\infty} x^2 \frac{\partial c}{\partial t} \, dx
\]
\[
= \left[ x^2 \frac{\partial c}{\partial x} \right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} 2x \frac{\partial c}{\partial x} \, dx
\]
\[
= -2c(x) x^2 \left. \right|_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} 2c \, dx = 2 \int_{-\infty}^{+\infty} c(x,t) \, dx = 2 C
\]
Cancelling $C$, we obtain
\[
\frac{d\sigma^2}{dt}(t) = 2D
\]
and hence, integrating over $t$ we have, as wanted:
\[
\sigma^2(t) = 2D t + \sigma^2(0)
\]
if $c(x,0) = 0$ for all $|x| > \varepsilon$ then (with $c = c(x,0)$):
\[
\int_{-\infty}^{+\infty} x^2 c \, dx = \int_{-\varepsilon}^{+\varepsilon} x^2 c \, dx \leq \varepsilon^2 \int_{-\varepsilon}^{+\varepsilon} c \, dx = \varepsilon^2 C(0)
\]
so $\sigma^2(0) \leq \varepsilon \approx 0$
so, in a rough sense, diffusion has “speed” $\propto \sqrt{t}$
(a different, probabilistic, interpretation is given later)

**travelling distance $L$ requires time $L^2$**
diffusion is simple and energetically “cheap”:
no need for building machinery for locomotion; no loss due to conversion to mechanical energy (e.g. cellular motors)
at the right scales, very efficient: fast method for nutrients and signals that must be carried along for short distances,.
. . . but not for long distances. . . example:
if can travel $10^{-6} m (= 1 \mu m)$ in $10^{-9}$ seconds (typical order of magnitude in cell),
then how much time needed to travel 1 meter?
since $x^2 = 2Dt$, solve $(10^{-6})^2 = 2D (10^{-9}) \Rightarrow D = 10^{-9}/2$
so, $1 = 10^{-9} t \Rightarrow t = 10^{9}$ seconds, i.e. about 27 years (!)
not a feasible way to move things along a large organism,.
. . . or even a big cell (e.g., long neuron)
⇒ circulatory systems, cell motors, microtubules, etc.

Suggested Problem
Show that, under analogous conditions to those in the theorem shown for dim 1,
in dimension $d$ (e.g.: $d = 2, 3$) one has the formula:
\[
\sigma^2(t) = 2dDt + \sigma^2(0)
\]
(for $d = 1$, this is the same as previously)
the proof will be completely analogous, except that the first step in integration by parts (uv = (uv)' - u'v, the Leibnitz rule for derivatives) must be generalized to vectors ($\nabla \cdot$ acts like a derivative) and the second step (the Fundamental Theo of Calc) should be replaced by an application of Gauss’ divergence theorem

the “fundamental solution”
for $n = 1$, this is one solution of the diffusion equation:
\[
c_0(x,t) = \frac{C}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}
\]
(where $C$ is any constant – verify by plugging-in)
for $t = 0$ solution is not well-defined; it tends to “$\delta$” think as “spread from a point source”
moreover, for arbitrary continuous $g$
\[
c(x, t) = \int_{-\infty}^{+\infty} \frac{C}{\sqrt{4\pi Dt}} e^{-\frac{(x-u)^2}{4Dt}} g(u) \, du
\]
solves diff eq and has initial condition $c(x,0) = g(x)$ (continuous function, satisfies PDE for $t > 0$)
convolution $c_0 * g$ with “Green’s function” for PDE
more generally ($r^2 = x_1^2 + \ldots x_d^2$), this is a solution:
\[
c_0(x,t) = \frac{C}{(4\pi Dt)^{d/2}} e^{-\frac{r^2}{4Dt}}
\]
with radial ($d = 2$) or spherical ($d = 3$) symmetry
probabilistic interpretation: random walks
above looks \(\approx\) Gaussian (normal) distribution... coincidence?
intuition (dimension 1, but similar for arbitrary \(d\)):

each individual particle is undergoing Brownian motion
if particles move independently (small, no collisions) then, concentration in a region \(R\) is proportional to the probability of any given particle being in \(R\)

so, soln of diffusion equation \(c(x, t)\) should be proportional to the probability density of the random variable that gives the position of a random-walk at time \(t\)

if starting at \(x = 0\), one obtains Gaussian distribution \(c_0\)
intuition from discrete steps:
suppose we can move left or right with a unit displacement and equal probability (each step independent of the rest) what is the position after \(t\) steps?
do a histogram, let us say for 4 steps:

<table>
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<th>Ending</th>
<th>Possible Sequences</th>
<th>Count</th>
</tr>
</thead>
<tbody>
<tr>
<td>-4</td>
<td>-1-1-1-1</td>
<td>1 x</td>
</tr>
<tr>
<td>-2</td>
<td>-1-1-1+1,-1-1+1-1,</td>
<td>4 xxxx</td>
</tr>
<tr>
<td>0</td>
<td>-1+1+1+1,-1+1+1-1,</td>
<td>6 xxxxxx</td>
</tr>
<tr>
<td>2</td>
<td>1+1+1-1,1+1-1-1,</td>
<td>4 xxxx</td>
</tr>
<tr>
<td>4</td>
<td>1+1+1+1</td>
<td>1 x</td>
</tr>
</tbody>
</table>

tends to normal (Central Limit Theorem), and has variance:

\[
\sigma^2(t) = E(X_1^2 + \ldots + X_t)^2 = \sum_{i=1}^{t} \sum_{j=1}^{t} E X_i X_j = \sum_{i=1}^{t} E X_i^2 = \sigma^2 t
\]

since independent (so \(E X_i X_j = 0\) for \(i \neq j\)) again this leads to the formula “\(\sigma(t)\) proportional to \(\sqrt{t}\)” exercise: prove that the average displacement of a Gaussian r.v. is proportional to \(\sqrt{t}\) (hint: substitute \(u = x/\sigma\)):

\[
E(|X|) = \frac{2}{\sigma \sqrt{2\pi}} \int_{0}^{\infty} x e^{-x^2/(2\sigma^2)} dx = \frac{\sigma}{\sqrt{\pi}}
\]
similarly, \(E(\sqrt{x_1^2 + \ldots + x_t^2})\)