Rutgers 642:613 - Fall 2003

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Conservation Laws and Diffusion

http://www.math.rutgers.edu/~sontag/613.html

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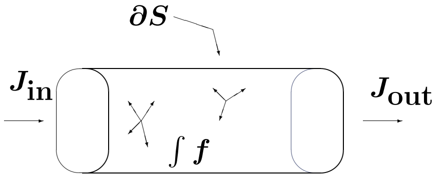
total change in S = total created + net inflow



$$\int_S [c(x,t+h)-c(x,t)]dx = \int_t^{t+h}\int_S f(x,t)dx - \int_t^{t+h}\int_{\partial S} J\cdot n\,dA$$

so dividing by h and taking limits as $h \to 0$ we get:

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

but (divergence, or Gauss') theorem says that

$$\int_S \nabla J\,dx \;=\; \int_{\partial S} J\cdot n\,dA$$

where *divergence* of $J = (J_1, J_2, J_3)$, $x = (x_1, x_2, x_3)$:

$$\text{div}\, J \;=\; \text{“}\nabla\cdot J\text{”} \;=\; \frac{\partial J_1}{\partial x_1} + \frac{\partial J_2}{\partial x_2} + \frac{\partial J_3}{\partial x_3}$$

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

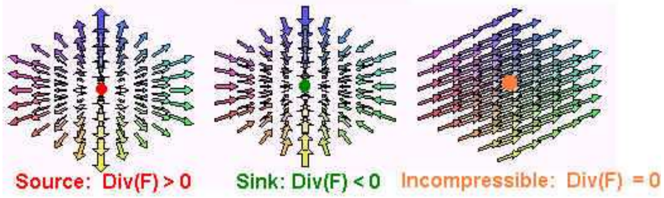
then, on the interval of time $[t, t+h]$, the net amount of chemical *exiting* through the boundary of S is

$$\int_t^{t+h}\int_{\partial S} J\cdot n\,dA$$

where n is the outward unit normal to the boundary

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:

$$\int_S \frac{\partial c}{\partial t}\,dx \;=\; \int_S f(x,t)\,dx - \int_S \nabla J\,dx$$

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

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

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 ⇝ "flux $J(x,t) \propto -\nabla c(x,t)$"

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 = *diffusion coefficient*)
and, in general, $\frac{\partial c}{\partial t} = f - \operatorname{div} J$ (div = "$\nabla\cdot$")
⇝

$$\boxed{\frac{\partial c}{\partial t} \;=\; D\nabla^2 c \,+\, f}$$

where ∇^2 is the "Laplacian" (often "Δ") 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:

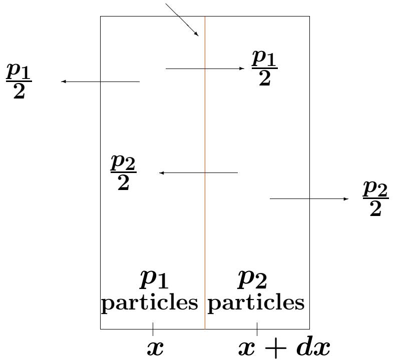
$$\frac{\partial c}{\partial t} \;=\; D\,\frac{\partial^2 c}{\partial x^2} \,+\, f$$

(note: $\frac{1}{D} \propto \sqrt[3]{\text{volume}}$, or equivalently to $\sqrt[3]{\text{mass}}$)

with no f nor additional constraints, eventually → 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



probabilistic intuition
(in one space dimension)

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 $\frac{p_1}{2} - \frac{p_2}{2}$, which is proportional to $c(x,t) - c(x+dx,t)$, which is proportional to $-\frac{\partial c}{\partial x}$ (analogously in $\mathbb{R}^3$: $-\nabla c(x,t)$)

Remark: Speed of Diffusion (dim 1)

(ignore 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

$$\lim_{x\to\pm\infty} x^2 \frac{\partial c}{\partial x}(x,t) = 0\,, \quad \lim_{x\to\pm\infty} x\,c(x,t) = 0\,.$$

(c is small at infinity) $\forall\, t$. Define, for each t:

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

which measures how the density "spreads out"
Then:

$$\sigma^2(t) \;=\; 2D\,t \,+\, \sigma^2(0) \quad \forall\, t > 0$$

in particular, if the initial ($t = 0$) population is concentrated near $x = 0$ ("δ function"), then $\boxed{\sigma^2(t) \approx 2D\,t}$

Proof

use PDE and integrate by parts:

$$\frac{C}{D}\frac{d\sigma^2}{dt} = \frac{1}{D}\frac{\partial}{\partial t}\int_{-\infty}^{+\infty} x^2 c\,dx = \frac{1}{D}\int_{-\infty}^{+\infty} x^2\frac{\partial c}{\partial t}\,dx$$

$$= \int_{-\infty}^{+\infty} x^2\frac{\partial^2 c}{\partial x^2}\,dx = \left[x^2\frac{\partial c}{\partial x}\right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} 2x\frac{\partial c}{\partial x}\,dx$$

$$= -\,[2xc]_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} 2c\,dx = 2\int_{-\infty}^{+\infty} c(x,t)\,dx \;=\; 2\,C$$

Cancelling C, we obtain

$$\frac{d\sigma^2}{dt}(t) \;=\; 2D$$

and hence, integrating over t we have, as wanted:

$$\sigma^2(t) \;=\; 2Dt + \sigma^2(0)\,.$$

if $c(x,0) = 0$ for all $|x| > \varepsilon$ then (with $c = c(x,0)$):

$$\int_{-\infty}^{+\infty} x^2 c\,dx = \int_{-\varepsilon}^{+\varepsilon} x^2 c\,dx \le \varepsilon^2\int_{-\varepsilon}^{+\varepsilon} c\,dx = \varepsilon^2 C(0)$$

so $\sigma^2(0) \le \varepsilon \approx 0$

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

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^{-3} seconds
(typical order of magnitude in cell),
then how much time needed to travel 1 meter?

since $x^2 = 2Dt$, solve $(10^{-6})^2 = 2D10^{-3} \rightsquigarrow D = 10^{-9}/2$
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

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 "δ"
think as "spread from a point source"
moreover, for arbitrary continuous g

$$c(x,t) \;=\; \int_{-\infty}^{+\infty}\frac{C}{\sqrt{4\pi Dt}}e^{-\frac{(x-\xi)^2}{4Dt}}g(\xi)\,d\xi$$

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 ($r^2 = x_1^2 + \dots x_d^2$), 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 ≈ 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:

ending	possible sequences	count	
-4	−1−1−1−1	1	x
-2	−1−1−1+1,−1−1+1−1,...	4	xxxx
0	−1−1+1+1,−1+1+1−1,...	6	xxxxxx
2	1+1+1−1,1+1−1+1,...	4	xxxx
4	1+1+1+1	1	x

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

$$\sigma^2(t) = E(X_1+\ldots+X_t)^2 = \sum_{i=1}^{t}\sum_{i=1}^{t} EX_iX_j = \sum_{i=1}^{t} EX_i^2 = \sigma^2 t$$

since independent (so $EX_iX_j = 0$ 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, $E(\sqrt{x_1^2+\ldots+x_d^2})$