PDE Models
until now only functions of time (concentrations, populations) from now on, consider functions that also depend on *space*

e.g. morphogen concentration as function of space and time

*Drosophila* embryo stained for protein products of *giant* (blue), *eve* (red), and *Kruppel*
(other colors indicate areas where two or all genes are expressed)
Another example

or study space-dependence of a particular protein in a single cell gradients of G-proteins in response to chemoattractant binding to receptors in surface of *Dictyostelium discoideum* amoebas
space variables $x=(x_1, x_2, x_3)$ \((x, y)\) or \((x, y, z)\) in dim 2/3

densities “$c(x, t)$” understood intuitively in the following sense:

$C(R, t) =$ amount of a type of particle (or \# individuals, mass of proteins of certain type, etc.) in region $R$ of space, at time $t$

the density around point $x$, at time $t$, $c(x, t)$, is:

$$c(x, t) = \frac{C(\Delta R, t)}{\text{vol}(\Delta R)}$$

for “small” cubes $\Delta R$ around $x$, i.e. a “local average”

so $C(R, T) = \int \int \int_R c(x, t) \, dx$ for all regions $R$

(more theoretical: start with $C$, defined as measure on subsets of $\mathbb{R}^3$; density $c$ is derivative)

scalar quantities $c(x, t)$ or vectors ($\neq$ chemicals, etc)
Reaction term: creation or degradation rate

\[ \sigma(x, t) = \text{reactions among chemicals “near” each other} \]
(or individuals, bacteria, ...)

\( \sigma \) is rate per unit volume per unit of time:

\[ \sum(R, [a, b]) = \]
\[ \# \text{ particles created (eliminated) in region } R \text{ during time } [a, b] \]

\[ \sigma(x, t) = \frac{\sum(\Delta R, [t, t + \Delta t])}{\text{vol}(\Delta R) \times \Delta t}, \]
(for “small” cubes \( \Delta R \) around \( x \), “small” time increments \( \Delta t \))

\[ \sum(R, [a, b]) = \int_a^b \int \int \int_R \sigma(x, t) \, dx \, dt \]
for all regions \( R \) and time intervals \([a, b]\)
Conservation or balance principle

*increase (decrease) of quantity in a region = net creation + net influx*

$R =$ volume w/uniform cross-section in the $y, z$ axes

density $c(x, y, z, t) = c(x, t)$

reaction rate $\sigma(x, y, z, t) = \sigma(x, t)$

assume nothing can "escape" through the $y, z$ directions

cross sectional area $= A$
$J(x, t) = \text{flux at } (x, t)$

$= \# \text{ particles that cross a unit area}$

perpendicular to $x$,

in the positive direction,

*per unit of time*

net flow through a cross-sectional area during a time interval $[a, b]$:

$$\int_{a}^{b} J(x, t) A \, dt$$

one gets from $\int_{y} \int_{z} = A$:

$$C(R, t) = \iiint_{R} c(\vec{x}, t) \, d\vec{x} = \int_{x_1}^{x_2} c(x, t) A \, dx$$

$$\Sigma(R, [a, b]) = \iiint_{R} \sigma(\vec{x}, t) \, d\vec{x} \, dt = \int_{a}^{b} \int_{x_1}^{x_2} \sigma(x, t) A \, dx \, dt$$
Balancing in a segment

Consider a segment $x \leq \xi \leq x + \Delta x$ and a time interval $[t, t + \Delta t]$.

\[ \Delta C \]

\[ J_{\text{in}} \rightarrow J_{\text{out}} \]

\[ \Sigma = \int \sigma \]

\[ x \quad \text{to} \quad x + \Delta x \]
Some basic equalities

- net flow through cross-area at \( x \):
  \[ J_{\text{in}} = \int_{t}^{t+\Delta t} J(x, \tau) A d\tau \]

- and at \( x + \Delta x \):
  \[ J_{\text{out}} = \int_{t}^{t+\Delta t} J(x + \Delta x, \tau) A d\tau \]

- net creation (elimination):
  \[ \Sigma = \int_{t}^{t+\Delta t} \int_{x}^{x+\Delta x} \sigma(\xi, \tau) A d\xi d\tau \]

- starting amount in segment:
  \[ C_t = \int_{x}^{x+\Delta x} c(\xi, t) A d\xi \]

- ending amount in segment:
  \[ C_{t+\Delta t} = \int_{x}^{x+\Delta x} c(\xi, t + \Delta t) A d\xi \]

total change balances:

\[ C_{t+\Delta t} - C_t = \Delta C = J_{\text{in}} - J_{\text{out}} + \Sigma \]
putting it all together:

\[
\int_{x}^{x+\Delta x} \left( c(\xi, t + \Delta t) - c(\xi, t) \right) A \, d\xi = \\
\int_{t}^{t+\Delta t} \left( J(x, \tau) - J(x + \Delta x, \tau) \right) A \, d\tau + \int_{t}^{t+\Delta t} \int_{x}^{x+\Delta x} \sigma(\xi, \tau) A \, d\xi \, d\tau
\]

divide by “A\Delta t”; let \( \Delta t \to 0 \), and apply FTC:

\[
\int_{x}^{x+\Delta x} \frac{\partial c}{\partial t} (\xi, t) \, d\xi = J(x, t) - J(x + \Delta x, t) + \int_{x}^{x+\Delta x} \sigma(\xi, t) d\xi
\]

next divide by \( \Delta x \), let \( \Delta x \to 0 \), and again FTC:

\[
\frac{\partial c}{\partial t} = - \frac{\partial J}{\partial x} + \sigma
\]

basic equation that we will use from now on
flux \( J(x, t) \) now vector, indicates maximal-flow direction at \((x, t)\)
magnitude = # particles crossing unit area \( \perp \) \( J \) per unit time

Gauss’ theorem \( \Rightarrow \)

\[
\frac{\partial c}{\partial t} = - \text{div} \ J + \sigma
\]

where divergence of \( J = (J_1, J_2, J_3) \) at \( x = (x_1, x_2, x_3) \) is:

\[
\text{div} \ J = " \nabla \cdot \ J" = \frac{\partial J_1}{\partial x_1} + \frac{\partial J_2}{\partial x_2} + \frac{\partial J_3}{\partial x_3}.
\]

in scalar case, \( \text{div} \ J \) is just \( \frac{\partial J}{\partial x} \)

until now, everything was quite abstract
next we specialize to very different types of fluxes
flux is due to transport: e.g. luggage transporting tape, wind carrying particles, water carrying dissolved substance, etc.

main observation:

\[
\text{flux} = \text{concentration} \times \text{velocity}
\]

(depending on local conditions: \(x\) and \(t\))

flow direction; say constant speed

larger flux smaller flux
approximate by locally-constant density:

unit volumes, $c = 5$

imagine counter “clicks” when particle passes right endpoint

flow at $v = 3$ units/sec

total flux in one second is 15 units = $cv$
\[
J(x, t) = c(x, t) \nu(x, t)
\]

since \( \frac{\partial c}{\partial t} = -\text{div } J + \sigma \), we obtain the transport equation:

\[
\frac{\partial c}{\partial t} = -\frac{\partial (cv)}{\partial x} + \sigma
\]
or, equivalently:

\[
\frac{\partial c}{\partial t} + \frac{\partial (cv)}{\partial x} = \sigma
\]

or more generally, in any dimension:

\[
\frac{\partial c}{\partial t} = -\text{div } (cv) + \sigma
\]
or, equivalently:

\[
\frac{\partial c}{\partial t} + \text{div } (cv) = \sigma
\]

special case: constant velocity \( \nu(x, t) \equiv \nu \):

\[
\frac{\partial c}{\partial t} = -\nu \frac{\partial c}{\partial x} + \sigma
\]
or, equivalently:

\[
\frac{\partial c}{\partial t} + \nu \frac{\partial c}{\partial x} = \sigma
\]

in dimension one, or more generally, in any dimension:

\[
\frac{\partial c}{\partial t} = -\nu \text{div } c + \sigma
\]
or, equivalently:

\[
\frac{\partial c}{\partial t} + \text{div } c = \sigma
\]
\[ \frac{\partial c}{\partial t} + \text{div} (cf) = 0 \]

(continuity equation of fluid mechanics)
where are now writing "f" instead of "v" for the velocity

another interpretation:
suppose each particle moves according to ODE \( \frac{dx}{dt} = f(x, t) \)
i.e. if particle in location \( x \) at time \( t \), its velocity should be \( f(x, t) \)
equation shows how ODE for particles translates to PDE for densities

"Liouville equation"

if \( \text{div} (f) = 0 \), as in Hamiltonian mechanics, and with constant \( v \):
\[ \frac{\partial c}{\partial t} + \sum_i \frac{\partial c}{\partial x_i} f_i, \text{ where } f_i \text{ is the } i\text{th coordinate of } f \]
Probabilistic interpretation

single particles; init conds distributed according to density $c(x, 0)$

ask what is the probability density at time $t$

density is solution of $\frac{\partial c}{\partial t} + \text{div}(cf) = 0$:

think of ensemble of particles, all evolving simultaneously

(assume small enough that they never collide)
special case in which the reaction is linear: $\sigma = \lambda c$
decay or growth proportional to population (at given time & place)

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = \lambda c$$

($\lambda > 0$ growth, $\lambda < 0$ decay)

**Theorem:** Every solution (in dim 1) of form:

$$c(x, t) = e^{\lambda t} f(x - vt)$$

for some (unspecified) differentiable single-variable function $f$.

Conversely, $e^{\lambda t} f(x - vt)$ is a solution, for any $\lambda$ and $f$.

note: when $t = 0$, $c(x, 0) = f(x)$, “initial condition” in time
last part very easy to prove; only need to verify the PDE:

\[
\left[ \lambda e^{\lambda t} f(x - vt) - ve^{\lambda t} f'(x - vt) \right] + ve^{\lambda t} f'(x - vt) = \lambda e^{\lambda t} f(x - vt)
\]

proving only solutions are these is a little more work:
must prove that every solution of \( \frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = \lambda c \), where \( v \) and \( \lambda \) are given real constants), must have the form
\( c(x, t) = e^{\lambda t} f(x - vt) \), for some appropriate “f”
start with very special case \( v = 0 \)
then for each fixed \( x \), we have an ODE: \( \frac{\partial c}{\partial t} = \lambda c \)
and for each \( x \), ODE has unique solution \( c(x, t) = e^{\lambda t} c(x, 0) \)
so can take \( f(x) \) as the function \( c(x, 0) \)
key step: reduce the general case to this case,
by “traveling” along the solution
formally: given solution \( c(x, t) \), introduce a new variable
\( z = x - vt \), so that \( x = z + vt \), and
consider the auxiliary function \( \alpha(z, t) := c(z + vt, t) \)
note \( \frac{\partial \alpha}{\partial z}(z, t) = \frac{\partial c}{\partial x}(z + vt, t) \), but, more interestingly:

\[
\frac{\partial \alpha}{\partial t}(z, t) = v \frac{\partial c}{\partial x}(z + vt, t) + \frac{\partial c}{\partial t}(z + vt, t).
\]

now use the PDE \( v \frac{\partial c}{\partial x} = \lambda c - \frac{\partial c}{\partial t} \) to get:

\[
\frac{\partial \alpha}{\partial t}(z, t) = [\lambda c - \frac{\partial c}{\partial t}] + \frac{\partial c}{\partial t} = \lambda c(z + vt, t) = \lambda \alpha(z, t).
\]

we have thus reduced to the case \( v = 0 \) for \( \alpha \)!

so, \( \alpha(z, t) = e^{\lambda t} \alpha(z, 0) \)

therefore, substituting back:

\[
c(x, t) = \alpha(x - vt, t) = e^{\lambda t} \alpha(x - vt, 0)
\]

conclude:

\[
c(x, t) = e^{\lambda t} f(x - vt)
\]

as claimed (writing \( f(z) := \alpha(z, 0) \))

thus all solutions *traveling waves*,

with decay or growth depending on the sign of \( \lambda \)
E.g. \((\nu = 3; \lambda = 0 \text{ and } \lambda < 0 \text{ respectively}; \ t = 0, 1, 2)\)
*Chemotaxis*: movement in response to chemoattractants/repellants
best-studied example: *E. coli*
given “potential” function $V = V(x)$:
concentration of food (chemical; friends or foes), at location $x$

suppose:  *population attracted to where $V$ is larger*

(if $V$ has negative values, movement towards larger values =
movement away from $V$ large in absolute value, = repulsion)

more precisely: individuals move at any given time *in the direction*
in which $V(x)$ *increases the fastest when taking a small step,*
and with a velocity that is proportional to this increase

(other choices are: maximum speed; fixed speed; . . . )
Review gradient descent/ascent

From multivariate calculus: $V(x + \Delta x) - V(x)$ maximized in the direction of its gradient.

Proof: need to find a direction, i.e., unit vector "$u$", so that $V(x + hu) - V(x)$ is maximized, for any small stepsize $h$.

Take a linearization (Taylor expansion) for $h > 0$ small:

$$V(x + hu) - V(x) = [\nabla V(x) \cdot u] h + o(h)$$

So average change in $V$ when taking a small step:

$$\frac{1}{h} \Delta V = \nabla V(x) \cdot u + O(h) \approx \nabla V(x) \cdot u$$

Conclude: maximum value is obtained precisely when the vector $u$ is picked in the same direction as $\nabla V$.

Thus direction of movement given by gradient of $V$.

Magnitude of vector $\frac{1}{h} \Delta V \approx \nabla V(x)$

So, for chemotaxis: velocity proportional to $\nabla V(x)$.
Chemotaxis equation

\[ J(x, t) = \alpha c(x, t) \nabla V(x) \]

for some \( \alpha \), so (ignoring reaction or transport effects):

\[
\frac{\partial c}{\partial t} = - \text{div} (\alpha c \nabla V) \quad \text{or:} \quad \frac{\partial c}{\partial t} + \text{div} (\alpha c \nabla V) = 0
\]

and in particular, in the special case of dimension one:

\[
\frac{\partial c}{\partial t} = - \frac{\partial (\alpha c V')}{\partial x} \quad \text{or, equivalently:} \quad \frac{\partial c}{\partial t} + \frac{\partial (\alpha c V')}{\partial x} = 0
\]

and therefore, using the product rule for \( x \)-derivatives:

\[
\frac{\partial c}{\partial t} = -\alpha \frac{\partial c}{\partial x} V' - \alpha c V''
\]
Diffusion

Fick’s Law (1855): diffusion due to movement from higher to lower concentration regions:

\[ J(x, t) \propto -\nabla c(x, t) \]

e.g. movement of particles in a solution, where proportionality constant depends on sizes of molecules (solvent and solute) and temperature

or diffusion across membranes, where constant depends on permeability and thickness as well

physical explanation of diffusion is probabilistic: thermal motion of individual particles due to environment (e.g., molecules of solvent) constantly “kicking” the particles

** see java applet **

“smoothing” effect if no additional constraints
in small $\Delta t$, particles jump right or left, equal probs
half of the $p_1$ particles in first box move right; other half move left
similarly for the $p_2$ particles in second box
(assume jumps big enough, particles exit respective box)
net number of particles (counting rightward as positive) through
segment proportional to $\frac{p_1}{2} - \frac{p_2}{2}$,
proportional roughly to $c(x, t) - c(x + \Delta x, t)$, and in turn to $-\frac{\partial c}{\partial x}$
[argument not really correct: what is velocity of particles?]
Diffusion (heat) equation

\[ J(x, t) = -D \nabla c(x, t), \] for some constant \( D \)

(diffusion coefficient)

from \( \frac{\partial c}{\partial t} = -\text{div} \ J \), conclude:

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

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

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

[notation \( \nabla^2 \): divergence can be thought of as “dot product by \( \nabla \)” so “\( \nabla \cdot (\nabla c) \)” is written as \( \nabla^2 c \)

note that the equation is just:

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

in dimension one