Modelling movement in space

Population-level description

\[ n(x,t) \text{ pop. dens. at point } x \text{ and time } t. \]
\[ J(x,t) \text{ pop. flux } \]
\[ \int_{x_0}^{x} n(\xi,t) \, d\xi \text{ number of particles between points } x_0 \text{ and } x \text{ at time } t. \]

Ignoring births and deaths, we have

\[ \partial_t \int_{x_0}^{x} n(\xi,t) \, d\xi = J(x_0,t) - J(x,t). \]

Differentiation with respect to \( x \) gives:

\[ \partial_t n(x,t) = - \partial_x J(x,t) \] (1-dim balance equation)

How do we connect the flux \( J(x,t) \) (which is a population characteristic: number of particles passing through a given point per unit of time) to the behavior of individual particles?
Individual-level description

Partitioning of (1-dim.) space into discrete intervals of length $\Delta x$.

$N_k$: particle in interval $(k\Delta x, (k+1)\Delta x)$

Probability per unit of time of moving one interval up or down is $\alpha_k$.

$N_k \xrightarrow{\alpha_k} N_{k+1}$ (monomolecular reactions).

$N_k$: pop. density in interval of length in interval $(k\Delta x, (k+1)\Delta x)$.

$J_k$: positive flux between intervals $(k\Delta x, (k+1)\Delta x)$ and $(k+1)\Delta x, (k+2)\Delta x)$.

\[ J_k = \alpha_k \cdot n_k \Delta x - \alpha_k \cdot n_{k+1} \Delta x = -\alpha_k (\Delta x)^2 \frac{n_{k+1} - n_k}{\Delta x} \]

Let $x_\text{an}$, $J_\text{an}$ be smooth interpolating functions $R^2 \to R$ such that $x_\text{an}(k\Delta x, t) = x_k$, $J_\text{an}(k\Delta x, t) = J_k$, $n_{k+1} \geq n_k$ for all $k$ and all $t$. 
Let $\mathbf{x}_0$, $\mathbf{J}_0$, $\mathbf{n}_0$ be smooth functions from $\mathbb{R}^2$ to $\mathbb{R}$ such that

$$\mathbf{x}_0(\mathbf{k}\cdot \mathbf{x}, t) = \mathbf{x}_0$$
$$\mathbf{J}_0(\mathbf{k}\cdot \mathbf{x}, t) = \mathbf{J}_0$$
and $\mathbf{n}_0(\mathbf{k}\cdot \mathbf{x}, t) = \mathbf{n}_0$

for all $\mathbf{k}$ and all $t$, and write $\mathbf{x} = \mathbf{k}\cdot \mathbf{x}$. Then

$$\mathbf{J}_0(\mathbf{x}, t) = \mathbf{x}_0(\mathbf{x}, t)(\Delta x)^2 \frac{\mathbf{v}_0(\mathbf{x}+\Delta \mathbf{x}, t) - \mathbf{v}_0(\mathbf{x}, t)}{\Delta x}$$

Let $k \rightarrow \infty$ and $\Delta x \rightarrow 0$ such that $\Delta x$ stays constant, and assume that

$$\mathbf{x}_0(\mathbf{x}, t)(\Delta x)^2 \rightarrow D(x, t) \quad \text{(some given func.)}$$
$$\mathbf{J}_0(\mathbf{x}, t) \rightarrow \mathbf{J}(x, t) \quad \text{and} \quad \mathbf{n}_0(\mathbf{x}, t) \rightarrow \mathbf{n}_0(x, t).$$

Then

$$\mathbf{J}(x, t) = -D(x, t) \frac{\partial}{\partial x} \mathbf{v}(x, t) \quad \text{(Fick's Law).}$$

Fick's law describes diffusion on the population level, which corresponds to the uncorrelated random walk on the individual level.

$D(x, t)$ is called the diffusion coefficient.
Interpretation of the diffusion coefficient in terms of individual behavior.

Back to discretized space ...(p.2).

Expected distance travelled per unit of time is

$$\Delta x \cdot x_k - \Delta x \cdot x_k = 0.$$ 

Expected distance\(^2\) travelled per unit of time is

$$\langle \Delta x \rangle^2 \cdot x_k + (-\Delta x)^2 \cdot x_k = 2 \langle \Delta x \rangle^2 x_k.$$ 

Taking the limit \( k \to \infty \), \( \Delta x \to 0 \) as previously, we find that

$$2D(x,t) = \text{Expected distance}^2 \text{ travelled}$$

$$2D(x,t) = \frac{\text{per unit of time}}.$$ 

If \( D(x,t) \) is independent of \( x \) and \( t \), then the average position of a particle does not change with time and the variance grows linearly with time with rate \( 2D \).

Hence, the standard deviation of the distribution of a particle's position grows \( \sqrt{2D \cdot \text{time}} \).
**Diffusion-reaction equations.**

\[ J(x,t) = -D(x,t) \partial_x u(x,t) \]

(Fick's Law).

**Population equation:**

\[ \partial_t n = \partial_x \left( D \partial_x n \right) + \text{(local reactions)} \]

(Reaction-diffusion equation).

\( \text{N.B. The local reactions describe birth, death and i-state transitions as modelled by mono- and bimolecular reactions.} \)

\[ \begin{align*}
\partial_x k &= \partial_x (D_k \partial_x k) + \beta k (1 - \frac{R}{K}) - \frac{\beta RC}{1 + \beta TR} \\
\partial_x c &= \partial_x (D_c \partial_x c) + \frac{\beta RC}{1 + \beta TR} - \delta c
\end{align*} \]

**Example.** (Resource-consumer)

see previous lectures for mechanistic underpinning

const. death rate for consumer

Holling II func. resp.

logistic growth of resource

diffusion


Boundary conditions

Frequently encountered boundary conditions

* Constant concentration boundary

\[ u(0, t) = u_0 \geq 0 \quad \forall t. \]

Special case: absorbing boundary

\[ u(0, t) = 0 \quad \forall t. \]

* Constant flux boundary

Case of diffusion: \( \frac{\partial}{\partial x} n(0, t) = \text{const.} \quad \forall t. \)

Special case: reflecting boundary

\[ \frac{\partial}{\partial x} u(0, t) = 0 \quad \forall t. \]

Formulating the bud conditions in year of the model formulation...
Example

\[ 21\% O_2 \]

- oxygen conc. \( c \)
- fish density \( n \)
- dissolved \( O_2 \) in equil. with atmospheric \( O_2 \)
- at bottom oxygen is absorbed in detritus layer.

\[ \frac{\partial c}{\partial t} = D_c \frac{\partial^2 c}{\partial x^2} - \beta c n \]  
( oxygen consumption by fish )

\[ \frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} \]

**oxygen**

\[ c(0, t) = c_o > 0 \quad \forall t \]  
(const. conc. bnd)

\[ c(L, t) = 0 \quad \forall t \]  
(absorbing bnd).

**init.**

\[ n(x, 0) = \begin{cases} \frac{\partial n(0, t)}{\partial t} = 0 \quad \forall t \\ \frac{\partial n(L, t)}{\partial t} = 0 \quad \forall t \end{cases} \]  
(reflecting bnds for fish).
Generalizations to k-dim space

\[ x = (x_1, ..., x_k), \quad J = (J_1, ..., J_k) \]

\[ \left( x_0, x_1, ..., x_k \right) \text{ pop density.} \] (2-dim case:

\[ \text{total no of particles is} \]
\[ \iint_{x_0 x_k} n(x_1, x_2, t) \, dx_2 \, dx_1. \]

\[ \text{change in total no of particles per unit of time} \]
\[ \partial_t \iint_{x_0 x_k} n(x_1, x_2, t) \, dx_2 \, dx_1 = \]
\[ = \int_{x_0}^{x_2} J_1(x_1, x_2, t) \, dx_2 - \int_{x_2}^{x_1} J_1(x_1, x_2, t) \, dx_2 + \]
\[ + \int_{x_0}^{x_1} J_2(x_1, x_2, t) \, dx_1 - \int_{x_1}^{x_0} J_2(x_1, x_2, t) \, dx_1. \]

Differentiate with respect to \( x_1 \) and \( x_2 \)

\[ \Rightarrow \partial_t n = -\partial_{x_1} J_1 - \partial_{x_2} J_2 \] (2-dim balance equation)

Random movement on i-level

\[ J = \begin{pmatrix} \delta_{i,1} & \delta_{i,2} \\ \delta_{i,2} & \delta_{i,2} \end{pmatrix} \begin{pmatrix} \partial_{x_1} n \\ \partial_{x_2} n \end{pmatrix} \] (Fick's Law) (2-dim, space)
General k-dim. case:

\[ \partial_t u = - \nabla \cdot J \]  
(balance equation)

where \( \nabla = (\partial_x, \ldots, \partial_x) \) (del operator)

\( \nabla \cdot J = \partial_x J_x + \ldots + \partial_x J_x \) (divergence).

Diffusion given

\[ J = -D \nabla u \]  
(Fick's law)

where \( \nabla u = (\partial_x u, \ldots, \partial_x u) \) (gradient)

\[ D = \text{matrix of diffusion coefficients}. \]

\[ D = (D_{ij}) \] where \( D_{ij} \) is the expected distance travelled in \( i \) direction \( \times \) distance travelled in \( j \) direction per unit of time.

If \( D \) is constant matrix, then the covariation between \( x_i \) and \( x_j \) of the distribution of the particle's position \( x = (x_1, \ldots, x_k) \) grows at a rate \( 2D_{ij} \).
Subst. of Fick's Law into the balance equation gives

\[ \partial_t n = \nabla \cdot (D \nabla n) \]

If \( D \) is constant, this becomes

\[ \partial_t n = D \Delta n \]

where \( \Delta \) is the Laplacian:

\[ \Delta n = \nabla \cdot \nabla c = (\partial_{x_1}, \ldots, \partial_{x_k}) \cdot (\partial_{x_1} n, \ldots, \partial_{x_k} n) = \partial_{x_1}^2 n + \cdots + \partial_{x_k}^2 n. \]

(Alternative notation: \( \Delta n = \nabla^2 n \).)

Adding local reactions gives a reaction–diffusion equation

\[ \partial_t n = \nabla \cdot (D \nabla n) + \text{(local reactions)} \]