III. Population Dynamics in Spatially Extended Systems

A. Spatial range expansion

1. Diffusion equation

If individuals perform random walk, then the local density \( f(\vec{r},t) \) evolves according to the diffusion equation

\[
\frac{\partial f}{\partial t} = D \nabla^2 f(\vec{r},t) ; \text{ boundary condition: } f(\vec{r},t) = 0 \\
\text{ initial condition: } f(\vec{r},0) = N_0 \delta^3(\vec{r})
\]

(i.e., \( N_0 \) individuals placed in a small volume at \( t=0 \))

\[
p(\vec{r},t) = \frac{N_0}{(4\pi D t)^{3/2}} e^{-\frac{\vec{r}^2}{4Dt}}
\]

plot along x-axis

\[ x = \text{ the width of the density distribution expands} \]

\[ \langle x^2 \rangle = \int d^3r \ x^2 \ p(\vec{r},t) = 2Dt ; \quad W \sim \sqrt{Dt} \]

\[ \Rightarrow \ \int d^3r \ p(\vec{r},t) = N_0 \, \text{ unchanged} \]
2. Range expansion for growing population

- Logistic growth of well-mixed population
  \[
  \frac{dp}{dt} = rs(1 - s/s^*)
  \]
- Allow random spatial movement
  Starting from localized initial spatial dist \( p(0) \)
- Study in 1d for illustration

\[
\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p}{\partial x^2} + rp(1 - p/s^*)
\]

Fisher–Kolmogorov Equation (1937)
Dimensionsless form: \( u = s/p, \quad \tau = rt, \quad \xi = \frac{x}{\sqrt{Dt}} \)

\[
\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial \xi^2} + u(1 - u)
\]

a) Look for propagating soln:

\[ u(\xi, \tau) = y(\xi - c\tau) \quad v = c\sqrt{D} \]

\[
\frac{dy}{d\xi} = \frac{\partial u}{\partial \xi} = \frac{\partial^2 u}{\partial \xi^2} + c \frac{dy}{d\xi} + y(1 - y) = 0
\]

\[ \Rightarrow \text{What is the propagating speed } c \text{ or } v = c\sqrt{D} \]
\[ \text{find } c \text{ such that } y(z) > 0 \text{ exist} \]
with \( y(z \rightarrow -\infty) = 1, y(z \rightarrow \infty) = 0. \)

- Can visualize ③ as Newton's eqn of motion for a "particle" at "position" \( y \) at "time" \( z \)

\[ \frac{d^2 y}{dz^2} = -c \frac{dy}{dz} - y(1-y) \]

friction: \( F(y) = -\frac{dU}{dy} \)

\[ U(y) = \frac{y^2}{2} - \frac{y^3}{3} \]

- Expect two types of motion:
  - If "friction" \( c \) is small, get "damped oscillation" around \( y=0 \)
    (unphysical since \( y \) cannot be -ve)
  - If friction \( c \) suff large (over damped), then expect \( y(z) > 0 \)

\( \Rightarrow \) a range of allowed \( c \)?
**Quantify the above conditions by doing linear stability analysis around \( y = 0 \) (front):**

For \( y < 1 \), \( \frac{d^2 y}{dz^2} = -c \frac{dy}{dz} - y \).

Let \( y = y_0 e^{\lambda z} \), \( \lambda^2 - c \lambda + 1 = 0 \).

\[
\lambda = \frac{c \pm \sqrt{c^2 - 4}}{2} \rightarrow \begin{cases} \frac{c \pm i\sqrt{4-c^2}}{2} & c < 2 \\ > 0 & c \geq 2 \end{cases}
\]

\(-\) damped osc if \( c < 2 \); \( \rightarrow \) Stable if \( c \geq 2 \)

\( \Rightarrow \) propagating soln exist for \( c \geq 2 \)

- For \( c \geq 2 \), \( y = A e^{\lambda_+ z} + B e^{\lambda_- z} \) (since \( \lambda_- < \lambda_+ \))

\[
u(3, t) = y(3-ct) \propto e^{-\lambda_-(3-ct)}
\]

\[
= e^{-\lambda_+ - \frac{c-x}{2\sqrt{D}t}} = e^{-k(x-uc)}
\]

*allowed speed:* \( u = c \sqrt{D} \geq 2 \sqrt{D} \)

*steepness of front:*

\[
\kappa = \frac{\lambda}{\sqrt{D}} = \sqrt{D} \left( \frac{c}{2} - \frac{1}{2\sqrt{D}} \right) \leq \sqrt{D}
\]

For \( c \gg 2 \), \( \frac{c}{2} - \frac{1}{2\sqrt{D}} = \frac{c}{2} (1 - \frac{1}{2\sqrt{D}}) \approx \frac{c}{4} \Rightarrow \kappa \approx \frac{c}{4} \).

\( \Rightarrow \) broader front for faster prop.
b) Selection of propagating speed

In general, propagating speed \( c \) can depend on the initial profile \( U(z, 0) \).

- Examine the soln at the front

\( U^2 \) term can be neglected at front

\[
\frac{\partial u}{\partial t} = u + \frac{u^2}{2} \frac{\partial u}{\partial z}
\]

Suppose \( u(0, t) \) is \( U(z, 0) \). \( \lim_{z \to \infty} U(z, 0) = u_0 e^{-\lambda z} \)

For \( t > 0 \), look for traveling soln

\[
U(z, t) = u_0 e^{-\lambda(z - ct)}
\]

Then \( \lambda c = 1 + \lambda^2 \)

\[
\Rightarrow \quad c = \lambda + \frac{1}{\lambda}
\]

\[
\frac{dc}{d\lambda} = 1 - \frac{1}{\lambda^2}
\]

\[
\frac{d^2 c}{d\lambda^2} = \frac{2}{\lambda^3} > 0
\]

\( \Rightarrow \) at most one min

\[
\frac{dc}{d\lambda} = 0 \quad \Rightarrow \quad \lambda^2 = 1
\]

\( \Rightarrow \quad c(\lambda^*) = 2 \)

\( \Rightarrow \) speed depends on steepness of ini profile (A)
Stability of propagating front with different slopes

[Heuristics given below: formal solve via stability analysis]

\[ e^{-(\xi/c)} \ (\lambda=1) \quad \text{Sharply declining init cond} \]
\[ \rightarrow C = 2 \quad \rightarrow C = \text{Cmin} = 2 \]

Marginal stability

The above does not apply to broader init cond.

Thus for any init cond \( U(\xi,0) \)

such that \( U(\xi,0) = 0 \) for \( \xi > \xi_0 \)

(i.e. Init pop confined to a certain region \( \xi < \xi_0 \))

then eventually the speed of the front

approaches \( C = \text{Cmin} = 2 \) or \( v = 2\sqrt{D(C)} \).

[Validation for motile bacteria population, Cremer 2019]

\[ u \sim e^{-\lambda (\xi - 2c)} \quad \lambda(c=2) = 1 \]

K = steepness \( K = \lambda \frac{[D]}{[V]} = \frac{[D]}{[V]} \)
3. Trigger wave:

\[ u = \text{"order parameter" of a bistable system} \]

\[ \frac{du}{dt} = r \left( u (a - u) \right) (u - b) \]

\[ g(u) = - \frac{2u}{3u} \]

E.g. Magnetization (ferromagnet)

Mitotic wave, Chromosome mod...

Spatially coupled dynamics:

\[ \frac{2u}{\delta t} = \frac{\partial^2 u}{\delta x^2} + r \left( u (a - u) \right) (u - b) \]

\[ -a < c \cdot t ; \frac{\delta x}{\delta t} = \frac{\partial u}{\partial x} \rightarrow \frac{2u}{\delta t} = \frac{\partial^2 u}{\partial x^2} + u (a - u) \left( u - b \right) \]

Propagation from stable to metastable phase ("trigger wave")

\[ u(\xi, t) = g \left( \xi - c \cdot t \right) \]

\[ \Rightarrow \frac{\partial^2 y}{\partial z^2} = -c \frac{\partial y}{\partial z} - y (a - y) (y - b) \]

\[ f(y) = -\frac{du}{dy} \]

Note: \( f = -f \), fictitious dynamics always from stable to metastable phase

Mechanical analogy: a ball rolling down from \( a \), move pass \( a \), and stop exactly at \( b \).
"dissipation energy", proportional to \( c \),

must be exactly equal to \( \Delta U \equiv U(a) - U(b) \)

(unique criterion for prop. speed \( c \))

\[
\frac{d^2y}{dz^2} = -c \left( \frac{dy}{dz} \right)^2 - \frac{dy}{dz} \frac{dy}{dz}
\]

\[
\int_{-\infty}^{\infty} dz \left( \frac{dy}{dz} \right)^2 = -c \int_{-\infty}^{\infty} dz \left( \frac{dy}{dz} \right)^2 - \int_{-\infty}^{\infty} dz \frac{dy}{dz}
\]

\[
= (y')^2 \bigg|_{-\infty}^{\infty} = 0
\]

\[
c \cdot \int_{-\infty}^{\infty} dz \left( \frac{dy}{dz} \right)^2 = U(-\infty) - U(\infty) = U(a) - U(b)
\]

\[
\Rightarrow \quad c \propto U(a) - U(b),
\]

thermodynamic potential \( U(a) - U(b) = -\Delta G \)

is the driving force for propagation.
Analysis of trigger wave dynamics:

\[
\frac{dv}{dt} = \frac{d^2 v}{dz^2} + (u-u_1) \cdot (u_2-u)(u-u_3)
\]

let \( u(z,t) = y(z-c t) \)

\[L = \frac{d^2 y}{dz^2} + c \frac{dy}{dt} + (y-u_1) \cdot (u_2-y)(y-u_3) = 0\]

\[f(y) = -f(y) = \frac{dy}{dy}\]

Solve: try \( \frac{dy}{dz} = \alpha \cdot (y-u_1) \cdot (y-u_3) \cdot \frac{h(y)}{h(y)} \)

\[
\frac{d^2 y}{dz^2} = \frac{dy}{dz} \cdot \frac{dy}{dy} = \frac{dy}{dz} \cdot \alpha \cdot (y-u_1+y-u_3)
\]

\[
= \alpha^2 (y-u_1)(y-u_3) \cdot (2y-u_1-u_3)
\]

\[-L(u) = (y-u_1)(y-u_3) \cdot \left[ \alpha^2 (2y-u_1-u_3) + c\alpha + (u_2-y) \right]
\]

\[-[ ] = 0 \rightarrow 2\alpha^2 = 1 \quad \Rightarrow \quad \alpha = \pm \frac{1}{\sqrt{2}}
\]

\[
\alpha^2 (u_1+u_3) = c\alpha + u_2
\]

\[
c = \frac{1}{2\alpha} (u_1+u_3-2u_2)
\]

\( y(z) \) from direct integration:

\[
\frac{dy}{dz} = \alpha \cdot (y-u_1)(y-u_3)
\]

\[
\rightarrow y(z) = \frac{u_3+u_1}{1+e^{\alpha (u_3-u_1)(z-z_0)}}
\]

\( z_0 \) is arbitrary shift of \( z \)-axis

\[
= \frac{u_1+u_3}{2} + \frac{u_1-u_3}{2} \tanh \left[ \frac{\alpha}{2} (u_3-u_1)(z-z_0) \right]
\]
boundary condition: \( y(z \to -\infty) = u_3 \quad \forall \quad d > 0 \), \( y(z \to +\infty) = u_1 \).

\[ C = \frac{1}{\sqrt{2}} (u_1 + u_3 - 2u_2) \]

\( \Rightarrow \) propagation to the right if \( \frac{u_1 + u_3}{2} > u_2 \),

left if \( \frac{u_1 + u_3}{2} < u_2 \).

Direction of propagation:

\( U(u_3) - U(u_1) = \int_{u_1}^{u_3} f(y) \, dy = \int_{u_1}^{u_3} (y - u_1)(u_2 - y)(y - u_3) \)

\[ = -\frac{1}{12} (u_3 - u_1)^2 \left[ (u_2 - u_1)^2 - (u_3 - u_1)^2 \right] \]

\[ = \frac{1}{12} (u_3 - u_1)^2 (u_1 + u_3 - 2u_2) \]

\( \geq 0 \) for \( u_3 > u_1 \).

\[ C = \frac{6u_2}{(u_3 - u_1)^2} \left[ U(u_3) - U(u_1) \right] \]

propagation from stable to metastable state

\( \Rightarrow \) Why does the system know about metastability even though the dynamics is deterministic?

existence of Lyapunov function

\( Z[u] = \int dx \left[ \frac{1}{2} \nabla^2 u^2 - U(u) \right] \)

\( \frac{\partial u}{\partial t} = -\frac{\delta}{\delta u(x,t)} Z[u] \)

Can show \( \frac{\partial Z}{\partial t} < 0 \) except when \( u \) solves PDE.