

1 Non-Flat Mutation Rates INITIAL

$$\bar{r}\dot{x}_i = u_i r_{i-1} x_{i-1} + x_i (r_I (1 - u_{i+1}) - \bar{r})$$

$$r = \text{const.}$$

$$\dot{\rho}_i = u_i \rho_{i-1} - \rho_i u_{i+1}$$

$$\begin{aligned} \dot{\rho}(x, t) &= u(x) \rho(x - \Delta x, t) - \rho(x, t) u(x + \Delta x, t) \\ &= u(x) \left(\rho(x) - \Delta x \frac{\partial \rho}{\partial x} + \Delta x^2 \frac{\partial^2 \rho}{\partial x^2} \right) - \rho(x, t) \left(u(x) + \Delta x \frac{\partial u}{\partial x} + \Delta x^2 \frac{\partial^2 u}{\partial x^2} \right) \end{aligned}$$

$$\Delta x = 1$$

$$\dot{\rho}(x, t) = -u \frac{\partial \rho}{\partial x} + u \frac{\partial^2 \rho}{\partial x^2} - \rho \left(\frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial x^2} \right)$$

Collecting up some terms.

$$\dot{\rho} = -\frac{\partial}{\partial x}(\rho u) + u \frac{\partial^2 \rho}{\partial x^2} - \rho \frac{\partial^2 u}{\partial x^2}$$

Fourier transform convention

$$\tilde{\rho} = \int_{-\infty}^{\infty} \rho e^{-ikx} dx \quad (1)$$

$$\dot{\rho} = -\int \frac{\partial}{\partial x}(\rho u) e^{-ikx} dx + \int u \frac{\partial^2 \rho}{\partial x^2} e^{-ikx} dx - \int \rho \frac{\partial^2 u}{\partial x^2} e^{-ikx} dx$$

$$\begin{aligned} \int \frac{\partial}{\partial x}(\rho u) e^{-ikx} dx &= [e^{-ikx} \rho u]_{-\infty}^{\infty} - \int (-ik) \rho u e^{-ikx} dx \\ &= ik \int \rho u e^{-ikx} dx \end{aligned}$$

Applying the convolution theorem:

$$\begin{aligned} F(f \cdot g) &= F(f) * F(g) \\ f * g &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(y) f(x - y) dy \end{aligned}$$

Need to prove these.

Applying this to the new differential equation.

$$\dot{\rho} = -ik(\mathcal{F}(\rho) * \mathcal{F}(u)) + (\mathcal{F}(u) * \mathcal{F}(\frac{\partial^2 \rho}{\partial x^2})) - (\mathcal{F}(\rho) * \mathcal{F}(\frac{\partial^2 u}{\partial x^2}))$$

Using what we know for the differentials and Fourier bits.

$$\dot{\tilde{\rho}} = -ik(\tilde{\rho} * \tilde{u}) + (\tilde{u} * (-k^2)\tilde{\rho}) - (\tilde{\rho} * (-k^2)\tilde{u})$$

We can take out the factors of k^2 .

$$\begin{aligned}\dot{\tilde{\rho}} &= -ik(\tilde{\rho} * \tilde{u}) - k^2((\tilde{u} * \tilde{\rho}) + (\tilde{\rho} * \tilde{u})) \\ &= (-ik - 2k^2)(\tilde{\rho} * \tilde{u})\end{aligned}$$

Convolution is commutative.

Chose a simple $u = \cos(\frac{\pi}{2M}x)$.

$$\begin{aligned}\tilde{u} &= \int \cos(\frac{\pi}{2M}x) e^{-ikx} dx \\ &= \frac{1}{2} \int (e^{\frac{i\pi}{2M}x} + e^{-\frac{i\pi}{2M}x}) e^{-ikx} dx \\ &= \frac{1}{2} \left(\delta(k - \frac{\pi}{2M}) + \delta(k + \frac{\pi}{2M}) \right)\end{aligned}$$

Convolution of a delta function just returns the same function with the variable shifted.

$$f(x) * \delta(x \pm a) = f(x \pm a) \quad (2)$$

$$\begin{aligned}\tilde{\rho} * \tilde{u} &= \tilde{\rho} * \frac{1}{2} \left(\delta(k - \frac{\pi}{2M}) + \delta(k + \frac{\pi}{2M}) \right) \\ &= \frac{1}{2} \left(\tilde{\rho}(k - \frac{\pi}{2M}) + \tilde{\rho}(k + \frac{\pi}{2M}) \right)\end{aligned}$$

Combining everything in one.

$$\dot{\tilde{\rho}} = -\frac{(ik + k^2)}{2} \left(\tilde{\rho}(k - \frac{\pi}{2M}) + \tilde{\rho}(k + \frac{\pi}{2M}) \right)$$

Improved

$$\begin{aligned}
\dot{\rho} &= u\rho(x - \Delta x) - \rho u(x + \Delta x) \\
&= u \left(\rho(x) - \Delta x \frac{\partial \rho}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 \rho}{\partial x^2} \right) - \rho \left(u(x) + \Delta x \frac{\partial u}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} \right) \\
&= -u \frac{\partial \rho}{\partial x} \Delta x + u \frac{\Delta x^2}{2} \frac{\partial^2 \rho}{\partial x^2} - \Delta x \rho \frac{\partial u}{\partial x} - \frac{\Delta x^2}{2} \rho \frac{\partial^2 u}{\partial x^2}
\end{aligned}$$

Introduce a new scaled variable $\hat{u} = u(x) \cdot \Delta x$.

$$\dot{\rho} = -\hat{u} \frac{\partial \rho}{\partial x} + \frac{\Delta x}{2} \hat{u} \frac{\partial^2 \rho}{\partial x^2} - \rho \frac{\partial \hat{u}}{\partial x} - \frac{\Delta x}{2} \rho \frac{\partial^2 \hat{u}}{\partial x^2}$$

This collapses down into our old equation with an additional term.

$$\dot{\rho} = -\hat{u} \frac{\partial \rho}{\partial x} + \frac{\Delta x}{2} \hat{u} \frac{\partial^2 \rho}{\partial x^2} - \rho \left(\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} \right)$$

In the limit $\Delta x \rightarrow 0$ we get the normal advection equation

$$\lim_{\Delta x \rightarrow 0} \dot{\rho} = -\frac{\partial(\rho \hat{u})}{\partial x} \quad (3)$$

2 Numerically Solving the PDE

Start with the PDE and initial condition.

$$\dot{\rho} = -\hat{u} \frac{\partial \rho}{\partial x} + \frac{\Delta x}{2} \hat{u} \frac{\partial^2 \rho}{\partial x^2} - \rho \left(\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} \right) \quad (4)$$

$$\rho(x, 0) = \delta(x - x_0) \quad (5)$$

We discretise with $x_i = ih$ and $t_j = jk$.

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \frac{\rho(x_i, t_{j+1}) - \rho(x_i, t_j)}{k} \\ \frac{\partial \rho}{\partial x} &= \frac{\rho(x_{i+1}, t_j) - \rho(x_i, t_j)}{h} \\ \frac{\partial^2 \rho}{\partial x^2} &= \frac{\rho(x_{i+1}, t_j) - 2\rho(x_i, t_j) + \rho(x_{i-1}, t_j)}{h^2} \end{aligned}$$

Inserting these into the PDE

$$\begin{aligned} \frac{\rho(x_i, t_{j+1}) - \rho(x_i, t_j)}{k} &= -\hat{u} \left(\frac{\rho(x_{i+1}, t_j) - \rho(x_i, t_j)}{h} \right) + \frac{\hat{u} \Delta x}{2} \left(\frac{\rho(x_{i+1}, t_j) - 2\rho(x_i, t_j) + \rho(x_{i-1}, t_j)}{h^2} \right) \\ &\quad - \rho(x_i, t_j) f(\hat{u}', \hat{u}'', \Delta x) \\ f(\hat{u}', \hat{u}'', \Delta x) &= \left(\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} \right) \end{aligned}$$

$$\begin{aligned} \rho(x_i, t_{j+1}) &= \rho - \frac{\hat{u}k}{h} (\rho(x_{i+1}, t_j) - \rho) + \frac{\hat{u} \Delta x k}{2h^2} (\rho(x_{i+1}, t_j) - 2\rho + \rho(x_{i-1}, t_j)) - k\rho f \\ &= \rho \left(1 + \frac{\hat{u}k}{h} - \frac{\hat{u} \Delta x k}{h^2} - kf \right) + \frac{\hat{u} \Delta x k}{2h^2} \rho(x_{i-1}, t_j) + \rho(x_{i+1}, t_j) \left(\frac{\hat{u} \Delta x k}{2h^2} - \frac{\hat{u}k}{h} \right) \\ &= \rho \left(1 + \frac{\hat{u}k}{h} \left(1 - \frac{\Delta x}{h} \right) - k \left(\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} \right) \right) + \frac{\hat{u} \Delta x k}{2h^2} \rho(x_{i-1}, t_j) + \rho(x_{i+1}, t_j) \left(\frac{\Delta x}{2h} - 1 \right) \frac{\hat{u}k}{h} \end{aligned}$$

Can then solve this the normal computational way.

3 PDE Analysis

$$\dot{\rho} = -\hat{u} \frac{\partial \rho}{\partial x} + \frac{\Delta x}{2} \hat{u} \frac{\partial^2 \rho}{\partial x^2} - \rho \left(\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} \right) \quad (6)$$

Re-arrange this to the standard form.

$$\frac{\Delta x \hat{u}}{2} \frac{\partial^2 \rho}{\partial x^2} - \hat{u} \frac{\partial \rho}{\partial x} - \frac{\partial \rho}{\partial t} - \rho \left(\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} \right) = 0$$

Classification of this PDE is based on the coefficients of the double derivatives.

$$\Delta(x, y) = 0^2 - 0^2 = 0$$

As there are no terms with the cross derivative and no terms with the second differential of t , the determinate is zero and the equation is parabolic.

4 Mutation Function analysis

We are free to chose a function for the mutation rate.

$$\dot{\rho} = -\hat{u} \frac{\partial \rho}{\partial x} + \frac{\Delta x}{2} \hat{u} \frac{\partial^2 \rho}{\partial x^2} - \rho \left(\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} \right) \quad (7)$$

The degree of freedom comes in the last term, so we define a function for ease of notation.

$$\mathcal{U}(x, \hat{u}, \hat{u}^{(n)}) = \frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} \quad (8)$$

4.1 $\mathcal{U} = \hat{u}$

By setting the function equal to the mutation function then it can be taken as a common factor from all the terms in the PDE.

$$\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} = \hat{u}$$

\hat{u} is just a function of x , therefore this is a linear, second order differential equation with auxillary equation;

$$\lambda = \frac{-1 \pm \sqrt{1 + 2\Delta x}}{\Delta x},$$

therefore, is has solutions

$$\hat{u} = A \exp \left(\left(-\frac{1}{\Delta x} + \frac{\sqrt{1 + 2\Delta x}}{\Delta x} \right) x \right) + B \exp \left(- \left(\frac{1}{\Delta x} + \frac{\sqrt{1 + 2\Delta x}}{\Delta x} \right) x \right)$$

A and B are constants that determine the scale of mutation probabilities.

4.2 $\mathcal{U} = \text{polynomial}$

$$\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} = \sum_{-\infty}^{\infty} c_n x^n$$

$$v = \frac{\partial \hat{u}}{\partial x}$$

$$v + \frac{\Delta x}{2} \frac{\partial v}{\partial x} = \sum_{-\infty}^{\infty} c_n x^n$$

This has complimentary function (correct phrase?)

$$v = Be^{-\frac{2}{\Delta x}x}$$

Trial form for the particular integral;

$$\begin{aligned} v(x) &= Be^{-\frac{2}{\Delta x}x} + \sum c_\alpha x^\alpha \\ v' &= \frac{-2B}{\Delta x}e^{-\frac{2}{\Delta x}x} + \sum \alpha c_\alpha x^{\alpha-1} \end{aligned}$$

$$\begin{aligned} Be^{-\frac{2}{\Delta x}x} + \sum c_\alpha x^\alpha + \frac{\Delta x}{2} \left(\frac{-2B}{\Delta x}e^{-\frac{2}{\Delta x}x} + \sum \alpha c_\alpha x^{\alpha-1} \right) &= \sum_{-\infty}^{\infty} c_n x^n \\ \sum c_\alpha x^\alpha + \frac{\Delta x}{2} \sum \alpha c_\alpha x^{\alpha-1} &= \sum_{-\infty}^{\infty} c_n x^n \\ \sum c_\alpha x^\alpha + \frac{\Delta x}{2} \sum (\alpha+1) c_{\alpha+1} x^\alpha &= \sum_{-\infty}^{\infty} c_n x^n \end{aligned}$$

From orthogonality of the powers

$$c_\alpha + \frac{\Delta x}{2}(\alpha+1)c_{\alpha+1} = c_n$$

OR

$$\begin{aligned} c_\alpha + \frac{\Delta x}{2} \frac{\alpha c_\alpha}{x} &= c_n \\ c_\alpha &= \frac{c_n}{1 + \frac{\Delta x \alpha}{2x}} \end{aligned}$$

So the full solution is

$$v(x) = Be^{-\frac{2x}{\Delta x}} + \sum \frac{c_n x^n}{1 + \frac{\Delta x n}{2x}}$$

Unwinding the substitution

$$\begin{aligned} \frac{\partial \hat{u}}{\partial x} &= Be^{-\frac{2x}{\Delta x}} + \sum \frac{c_n x^n}{1 + \frac{\Delta x n}{2x}} \\ \hat{u} &= -\frac{B\Delta x}{2}e^{-\frac{2x}{\Delta x}} + \int \sum \frac{2c_n x^{n+1}}{2x + \Delta x n} dx \end{aligned}$$

Testing by differentiation and subbing back in.

$$\begin{aligned}
\hat{u} &= -\frac{B\Delta x}{2}e^{-\frac{2x}{\Delta x}} + \int \sum \frac{2c_n x^{n+1}}{2x + \Delta x n} dx \\
\hat{u}' &= Be^{-\frac{2x}{\Delta x}} + \sum \frac{2c_n x^{n+1}}{2x + \Delta x n} \\
\hat{u}'' &= \frac{-2B}{\Delta x}e^{-\frac{2x}{\Delta x}} + \sum \left(\frac{2c_n(n+1)x^n}{(2x + \Delta x n)} - \frac{4c_n x^{n+1}}{(2x + \Delta x n)^2} \right) \\
\hat{u}' + \frac{\Delta x}{2}\hat{u}'' &= \sum \frac{2c_n x^{n+1}}{2x + \Delta x n} + \frac{\Delta x}{2} \left(\sum \left(\frac{2c_n(n+1)x^n}{(2x + \Delta x n)} - \frac{4c_n x^{n+1}}{(2x + \Delta x n)^2} \right) \right)
\end{aligned}$$

In the limit of $\Delta x \rightarrow 0$ this is correct.

Example

$$\begin{aligned}
\frac{\partial \hat{u}}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 \hat{u}}{\partial x^2} &= \sum_{-\infty}^{\infty} c_n x^n \\
\sum_{-\infty}^{\infty} c_n x^n &= x \\
c_n &= \begin{cases} 1 & n = 1 \\ 0 & n \neq 1 \end{cases} \\
\hat{u} &= -\frac{B\Delta x}{2}e^{-\frac{2x}{\Delta x}} + \int \sum \frac{2c_n x^{n+1}}{2x + \Delta x n} dx \\
&= -\frac{B\Delta x}{2}e^{-\frac{2x}{\Delta x}} + \int \left(\frac{2x^2}{2x + \Delta x} \right)
\end{aligned}$$

4.3 FKPP Methods

"Wave of Advance of Advantageous Genes" Ronald Fisher.

$$\dot{\rho} = -\hat{u} \frac{\partial \rho}{\partial x} + \frac{\Delta x \hat{u}}{2} \frac{\partial^2 \rho}{\partial x^2} - \rho \left(\frac{\partial u}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 u}{\partial x^2} \right)$$

We want a wave solution, travelling at speed v , therefore $\frac{\partial \rho}{\partial t} = -v \frac{\partial \rho}{\partial x}$

$$\frac{\Delta x \hat{u}}{2} \rho'' + (v - \hat{u}) \rho' - \rho \left(u' + \frac{\Delta x}{2} u'' \right) = 0 \quad (9)$$

There is no explicit x dependence in the equation, therefore we can write the concentration as the derivative of another function.

$$\begin{aligned} g &= -\frac{d\rho}{dx} \\ \frac{\partial g}{\partial x} &= -\frac{\partial^2 \rho}{\partial x^2} \\ \frac{\partial^2 \rho}{\partial x^2} &= g \frac{\partial g}{\partial \rho} \end{aligned}$$

$$\frac{\Delta x \hat{u}}{2} g \frac{\partial g}{\partial \rho} + (v - \hat{u})(-g) - \rho \left(\frac{\partial u}{\partial x} + \frac{\Delta x}{2} \frac{\partial^2 u}{\partial x^2} \right) = 0 \quad (10)$$

$$\lim_{\rho \rightarrow 0} \frac{g}{\rho} = \omega$$

$$\frac{\partial g}{\partial \rho} = \omega$$

$$\frac{\hat{u} \Delta x}{2} \omega^2 + (v - \hat{u})(-\omega) - \left(\hat{u}' + \frac{\Delta x}{2} \hat{u}'' \right) = 0 \quad (11)$$

By examining the determinant of this quadratic equation we can arrive at an equation for v .

$$\begin{aligned} (v - \hat{u})^2 - 4 \frac{\hat{u} \Delta x}{2} \left(- \left(\hat{u}' + \frac{\Delta x}{2} \hat{u}'' \right) \right) &\geq 0 \\ v^2 - 2v\hat{u} + \hat{u}^2 + 2\hat{u}\Delta x \left(\hat{u}' + \frac{\Delta x}{2} \hat{u}'' \right) &\geq 0 \\ v^2 - 2v\hat{u} + \hat{u}^2 + 2\hat{u}\Delta x \left(\hat{u}' + \frac{\Delta x}{2} \hat{u}'' \right) &= C \\ C &\geq 0 \end{aligned}$$

$$v^2 - 2v\hat{u} + \hat{u}^2 + 2\hat{u}\Delta x \left(\hat{u}' + \frac{\Delta x}{2}\hat{u}'' \right) - C = 0$$

$$\begin{aligned} v &= 2\hat{u} \pm \sqrt{4\hat{u}^2 - 4 \left(\hat{u}^2 + 2\hat{u}\Delta x \left(\hat{u}' + \frac{\Delta x}{2}\hat{u}'' \right) - C \right)} \\ &= 2\hat{u} \pm \sqrt{-8\hat{u}\Delta x \left(\hat{u}' + \frac{\Delta x}{2}\hat{u}'' \right) + 4C} \end{aligned}$$

As the velocity is a physical quantity, this gives us some constraints on the function inside the square brackets.

$$C - 2\hat{u}\Delta x \left(\hat{u}' + \frac{\Delta x}{2}\hat{u}'' \right) \geq 0 \quad (12)$$

This gives us an ODE for \hat{u} :

$$\hat{u}\Delta x \left(\hat{u}' + \frac{\Delta x}{2}\hat{u}'' \right) + D = 0$$

Where D is just the redefining of the constant.

This is very non linear and doesn't have an analytic solution.

NEED TO SOLVE IT NUMERICALLY.