生態模擬: 以C語言為例

Class 12

2018/06/14, 6/21

Reaction-Diffusion Models and very basic methods for their numerical solutions

12.1 How to derive reaction-diffusion model (for population dynamics)
12.2 Discretization of diffusion equation
12.3 Stability condition for discretization (skip)
12.4 Initial boundary value problems for diffusion equation
12.5 Initial boundary value problems for reaction-diffusion equation

Takeshi Miki

三木　健 (海洋研究所)

Step by step understanding of population dynamics in space

- Local population dynamics (without space)

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- Equation of continuity (mass conservation)
- Random movement of particles (diffusion)

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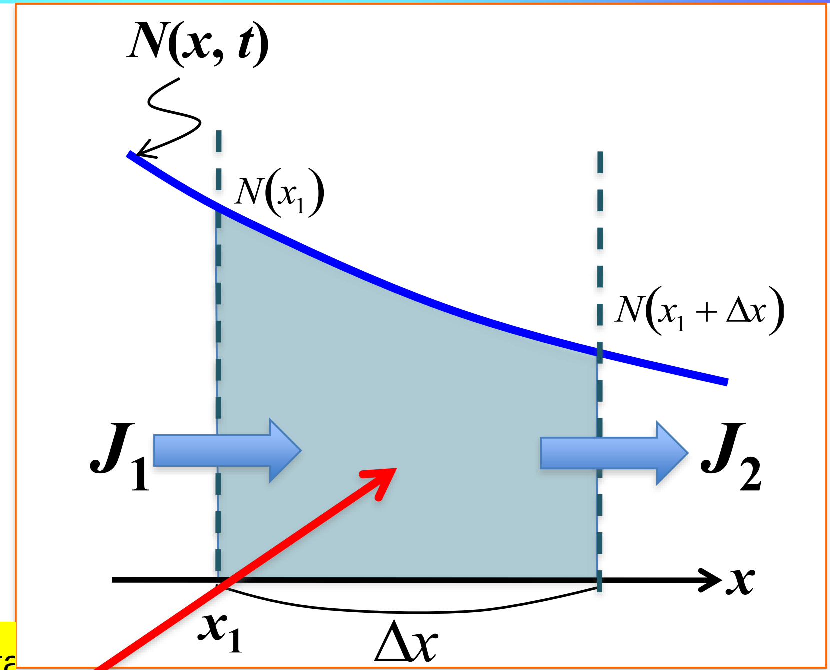
- Population dynamics in space: reaction-diffusion model

12.1 Local population dynamics (without space)

$$\underbrace{\frac{dN(t)}{dt}}_{\text{Population Growth Rate}} = \underbrace{(\text{reproduction}) - (\text{mortality})}_{\text{Local Dynamics}}$$

12.1 Equation of continuity (mass conservation)



X: Spatial axis

Delta x: aprox 0N(x1, t + delta t)* (Delta

$$N(x_1, t_1 + \Delta t) \cdot \Delta x - N(x_1, t_1) \cdot \Delta x \approx J_1 \cdot \Delta t - J_2 \cdot \Delta t$$

Temporal changes in total number of organisms in grayed region — Influx — Outflux

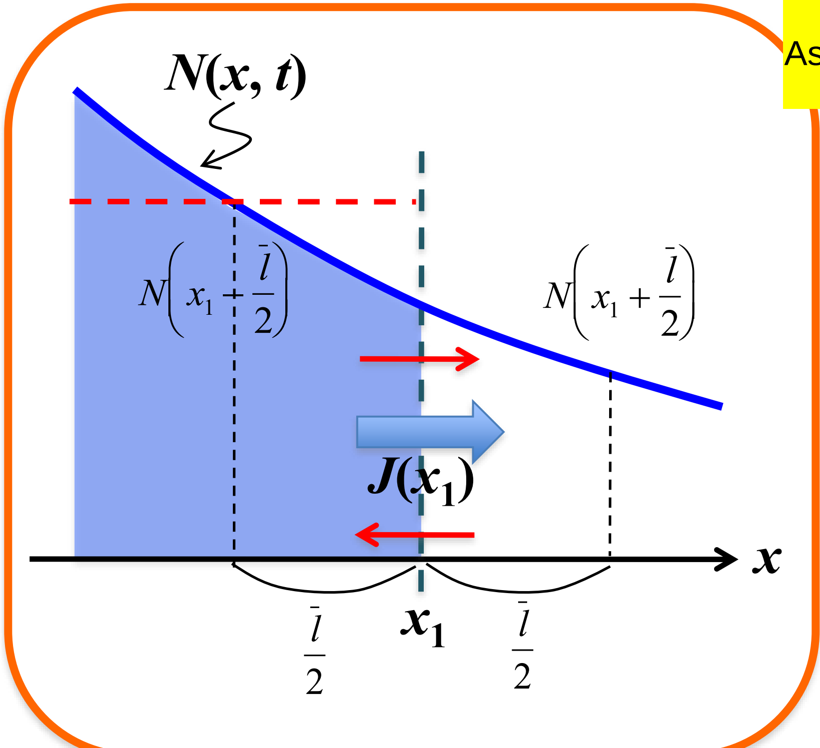
$$= \left[J(x_1) - J(x_1 + \Delta x) \right] \cdot \Delta t$$

$$\therefore \frac{\partial N}{\partial t} = -\frac{\partial J}{\partial x}$$ (Equation of continuity)

12.1 Random movement of particles (diffusion)

How to derive the flux due to diffusion

$\bar{l}$	The '**mean free path**' of a organism, defined as the average distance of movement between successive encounter events
$\overline{\Delta t}$	The average time between successive encounter events
$\bar{v} \equiv \bar{l} / \overline{\Delta t}$	The average rate of movement in short timescale when the effect of encounters can be neglected



Assumptions:Random movement of particles.No interaction betwee

$$J(x_1) \cdot \overline{\Delta t} \approx \alpha \cdot \bar{v} \cdot \overline{\Delta t} \cdot \left[N\left(x_1 - \tfrac{\bar{l}}{2}\right) - N\left(x_1 + \tfrac{\bar{l}}{2}\right) \right]$$

$$= -\alpha \cdot \bar{v} \cdot \overline{\Delta t} \cdot \left.\frac{\partial N}{\partial x}\right|_{x=x_1} \cdot \bar{l}$$

alpha: fraction of particles that moves right

$$\therefore J(x_1) = -\alpha \cdot \bar{v} \cdot \bar{l} \cdot \frac{\partial N}{\partial x} \equiv -D \frac{\partial N}{\partial x}$$

Diffusion Coefficient

12.1 Population dynamics in space: reaction-diffusion model

Local population dynamics (without space) $\boxed{\frac{dN(t)}{dt} = (reproduction) - (mortality)}$

+

- Equation of continuity (mass conservation) $\longleftrightarrow$ $\boxed{\frac{\partial N}{\partial t} = -\frac{\partial J}{\partial x}}$
- Random movement of particles (diffusion) $\longleftrightarrow$ $\boxed{J = -D\frac{\partial N}{\partial x}}$

$\downarrow$

$$\boxed{\underbrace{\frac{\partial N(x,t)}{\partial t}}_{\text{Population Growth Rate}} = \underbrace{(\text{reproduction}) - (\text{mortality})}_{\text{Local Dynamics}} + \underbrace{D\frac{\partial^2 N}{\partial x^2}}_{\text{Diffusion}}}$$

12.2 Discretization of diffusion equation

$$\frac{\partial N(x,t)}{\partial t} = D\frac{\partial^2 N}{\partial x^2} \quad \textbf{(1)}$$

Diffusion Equation

Discretization by approximation with Taylor expansion

$$N(x,t+\Delta t) \approx N(x,t) + \frac{\partial N}{\partial t}\Delta t \quad \textbf{(2)}$$

$$N(x+\Delta x,t) \approx N(x,t) + \frac{\partial N}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 N}{\partial x^2}(\Delta x)^2 \quad \textbf{(3)}$$

$$N(x-\Delta x,t) \approx N(x,t) + \frac{\partial N}{\partial x}(-\Delta x) + \frac{1}{2}\frac{\partial^2 N}{\partial x^2}(\Delta x)^2 \quad \textbf{(4)}$$

12.2 Discretization of diffusion equation

From (2),

$$\frac{\partial N}{\partial t} \approx \frac{N(x,t+\Delta t) - N(x,t)}{\Delta t} \tag{5}$$

From (3)+(4),

$$\frac{\partial^2 N}{\partial x^2} \approx \frac{N(x+\Delta x,t) - 2N(x,t) + N(x-\Delta x,t)}{(\Delta x)^2} \tag{6}$$

Substituting (5) & (6) into (1) gives

$$N(x,t+\Delta t) \approx N(x,t) + D\Delta t \frac{N(x+\Delta x,t) - 2N(x,t) + N(x-\Delta x,t)}{(\Delta x)^2} \tag{7}$$

12.2 Discretization of diffusion equation

From (2),

$$N(x,t+\Delta t) \approx N(x,t) + D\Delta t \frac{N(x+\Delta x,t) - 2N(x,t) + N(x-\Delta x,t)}{(\Delta x)^2} \quad \textbf{(7)}$$

With the following notation,

$$x_{i+1} - x_i = \Delta x$$

$$t_{j+1} - t_j = \Delta t$$

Let $n(i, j)$ as the approximation of $N(x_i, t_j)$, and then we have

$$\boxed{n(i,j+1) = n(i,j) + D\Delta t \frac{n(i+1,j) - 2n(i,j) + n(i-1,j)}{(\Delta x)^2} \qquad \textbf{(8)}}$$

12.3 Stability condition for discretization (skip)

Before thinking about stability condition, we need to think about analytical solution for the following initial boundary value problem for diffusion equation.

$$\boxed{\frac{\partial N(x,t)}{\partial t} = D\frac{\partial^2 N}{\partial x^2} \quad \textbf{(1)}}$$

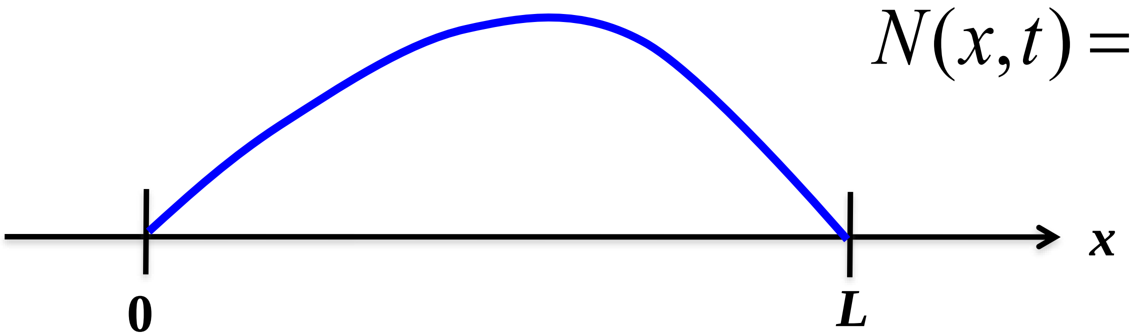
$$0 < x < L, \quad t > 0$$

(Spatial and Temporal Domain)

[Initial Conditions] $N(x,0) = N_0(x)$

[Boundary Conditions] $N(0,t) = N(L,t) = 0$

Solution should have the following form to satisfy the boundary conditions



$$N(x,t) = A(t)\cdot\sin\left(\frac{k\pi x}{L}\right) \quad \textbf{(9)}$$

***k* = 1, 2, …**

12.3 Stability condition for discretization (skip)

By substituting (9) into (1), we have

$$\frac{dA(t)}{dt} = -D\left(\frac{k\pi}{L}\right)^2 \cdot A(t)$$

$$\therefore A(t) \to 0 \quad \text{as} \quad t \to +\infty$$ **[All solutions converge to zero.]**

This characteristics of analytical solution of (1) should be kept in the numerical solution, constructed by (8).

$$\boxed{n(i, j+1) = n(i, j) + D\Delta t \frac{n(i+1, j) - 2n(i, j) + n(i-1, j)}{(\Delta x)^2} \qquad \textbf{(8)}}$$

12.3 Stability condition for discretization (skip)

$$\boxed{n(i,j+1) = n(i,j) + D\Delta t\,\frac{n(i+1,j) - 2n(i,j) + n(i-1,j)}{(\Delta x)^2}} \qquad \textbf{(8)}$$

We define

$$\Delta x = \frac{L}{M} \qquad x_i = i\Delta x = \frac{i}{M}L \qquad \boldsymbol{i = 0,\ 1,\ 2,\ \ldots,\ M}$$

Then, we can set the following numerical solution

$$n(i,j) = A_j \sin\left(\frac{i \cdot k\pi}{M}\right) \qquad \textbf{(10)}$$

,which satisfies the boundary conditions

$$n(0,j) = n(M,j) = 0$$

Substituting (10) into (8) gives

$$A_{j+1} = A_j \left\{1 - \frac{4D\Delta t}{(\Delta x)^2}\sin^2\frac{k\pi}{2M}\right\}$$

$$\sin\alpha + \sin\beta = 2\sin\frac{\alpha+\beta}{2}\cos\frac{\alpha-\beta}{2}$$

$$\cos 2\alpha = 1 - 2\sin^2\alpha$$

12.3 Stability condition for discretization (skip)

$$A_{j+1} = A_j \left\{ 1 - \frac{4D\Delta t}{(\Delta x)^2} \sin^2 \frac{k\pi}{2M} \right\}$$

Then, the numerical solution is

$$n(i,j) = A_j \sin\left(\frac{i \cdot k\pi}{M}\right) = A_0 \left\{ 1 - \frac{4D\Delta t}{(\Delta x)^2} \sin^2 \frac{k\pi}{2M} \right\}^j \cdot \sin\left(\frac{i \cdot k\pi}{M}\right)$$

Therefore, to keep the characteristics of convergence,

$$\lim_{j \to +\infty} n(i,j) = 0 \Leftrightarrow \left| 1 - \frac{4D\Delta t}{(\Delta x)^2} \sin^2 \frac{k\pi}{2M} \right| < 1$$

It gives

$$\boxed{\frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2} \Leftrightarrow \Delta t < \frac{1}{2D}(\Delta x)^2} \quad \textbf{(11)}$$

[stability condition for discretization]

12.3 Stability condition for discretization (skip)

$$\frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2} \Leftrightarrow \Delta t < \frac{1}{2D}(\Delta x)^2 \qquad \textbf{(11)}$$

[stability condition for discretization]

Time Interval (Δt) should be smaller with higher spatial resolution (smaller Δx) and with higher diffusion coefficient (D).

WHY??

$$N(x,t+\Delta t) \approx N(x,t) + D\Delta t \frac{N(x+\Delta x,t) - 2N(x,t) + N(x-\Delta x,t)}{(\Delta x)^2} \qquad \textbf{(7)}$$

12.4 Initial boundary value problems for diffusion equation

Let's go back to the original diffusion equation

$$\boxed{\frac{\partial N(x,t)}{\partial t} = D\frac{\partial^2 N}{\partial x^2} \qquad \textbf{(1)}}$$

$$0 < x < L, \quad t > 0$$

[Initial Conditions] $N(x,0) = N_0(x)$ (No needs to explain)

[Boundary Conditions]

boundary doesn't change with timeParticles 'die' on boundar

[Dirichlet boundary condition] (= fixed boundary condition)

$$N(0,t) = a, N(L,t) = b \qquad \left(\text{e.g. } \underline{N(0,t) = N(L,t) = 0}\right)$$

[Neumann boundary condition]

$$\frac{\partial}{\partial x}N(0,t) = a, \frac{\partial}{\partial x}N(L,t) = b$$

Especially when a = b = 0, it is called 'zero flux boundary' or 'reflecting boundary condition'

12.4 Initial boundary value problems for diffusion equation

How to translate boundary conditions to numerical algorism?

[Boundary Conditions]

[Dirichlet boundary condition] (= fixed boundary condition)

$$N(0,t) = N(L,t) = 0$$

$$\Rightarrow \quad n(0,j) = n(M,j) = 0 \quad (= n(-i,j) = n(M+i,j)) \qquad \textbf{(12)}$$

[Reflecting boundary condition] (skip)

$$\frac{\partial}{\partial x} N(0,t) = a, \frac{\partial}{\partial x} N(L,t) = b$$

$$\Rightarrow \begin{cases} \dfrac{n(1,j) - n(-1,j)}{\Delta x} = 2 \cdot a + O\left((\Delta x)^2\right) \\ \dfrac{n(M+1,j) - n(M-1,j)}{\Delta x} = 2 \cdot b + O\left((\Delta x)^2\right) \end{cases} \qquad \textbf{(13)}$$

Remark $\quad N(x \pm \Delta x) = N(x,t) \pm N_x(x,t) \cdot \Delta x + (1/2) N_{xx}(x,t) \cdot (\Delta x)^2 + O\left((\Delta x)^3\right)$

12.4 Initial boundary value problems for diffusion equation

Let's numerically solve (1) with <u>fixed boundary</u> condition and following settings

$$\boxed{\frac{\partial N(x,t)}{\partial t} = D\frac{\partial^2 N}{\partial x^2} \qquad D=1, \quad 0<x<L=10.0, \quad t>0}$$

$$\Delta x = \frac{L}{M} = \frac{10.0}{100} = 0.1$$

$$\Delta t = \frac{1}{5}\cdot\frac{1}{2D}(\Delta x)^2 = \frac{1}{5}\frac{1}{2}(0.1)^2 = 1.0e-3 < \frac{1}{2D}(\Delta x)^2$$

[Initial Conditions]

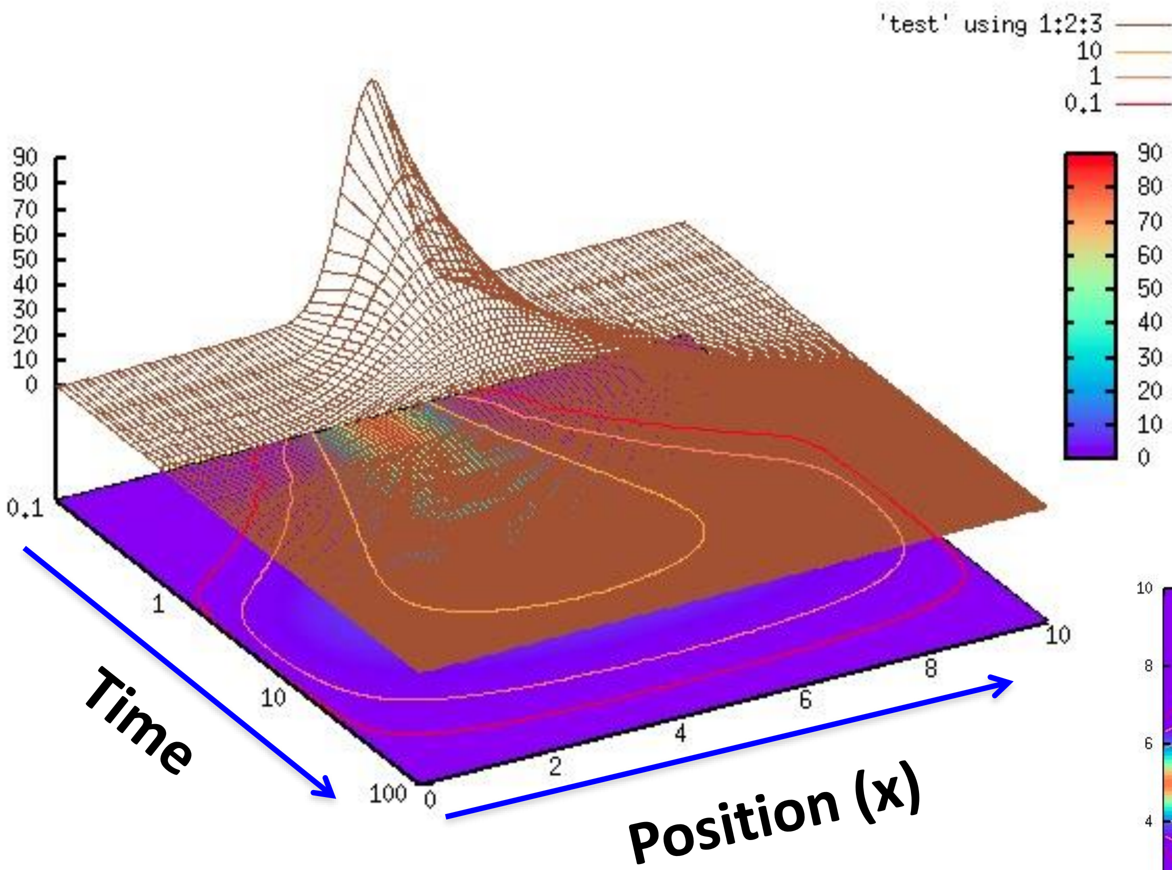
$$n(i,0) = \begin{cases} 0 & \text{if } i \neq M/2 = 50 \\ N_0 = 10^3 & \text{if } i = M/2 = 50 \end{cases}$$

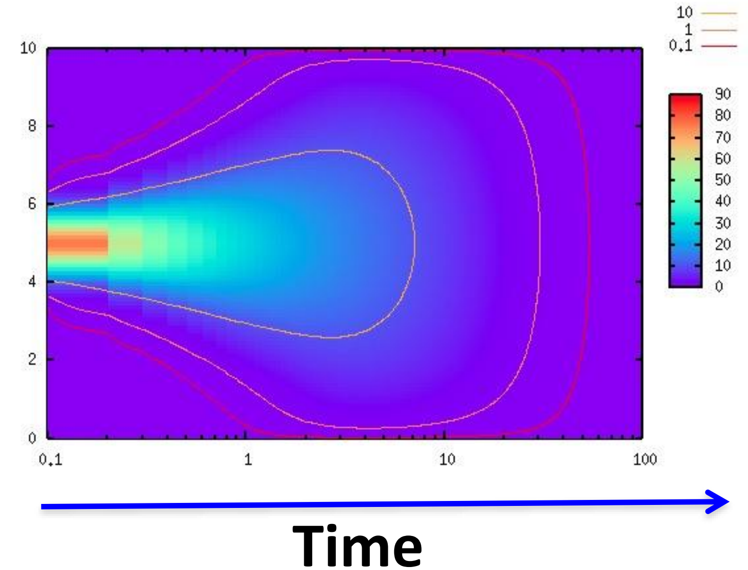
[Boundary Conditions]

$$n(0,j) = n(M,j) = 0.0 = n(-1,j) = n(M+1,j)$$

12.4 Initial boundary value problems for diffusion equation

Let's numerically solve (1) with <u>fixed boundary</u> condition





$$n(i, j) \to 0$$

12.4 Initial boundary value problems for diffusion equation

Let's numerically solve (1) with <u>reflecting boundary</u> condition and following settings

$$\frac{\partial N(x,t)}{\partial t} = D\frac{\partial^2 N}{\partial x^2} \qquad D=1, \quad 0<x<L=10.0, \quad t>0$$

$$\Delta x = \frac{L}{M} = \frac{10.0}{100} = 0.1$$

$$\Delta t = \frac{1}{5}\cdot\frac{1}{2D}(\Delta x)^2 = \frac{1}{5}\frac{1}{2}(0.1)^2 = 1.0e-3 < \frac{1}{2D}(\Delta x)^2$$

[Initial Conditions]

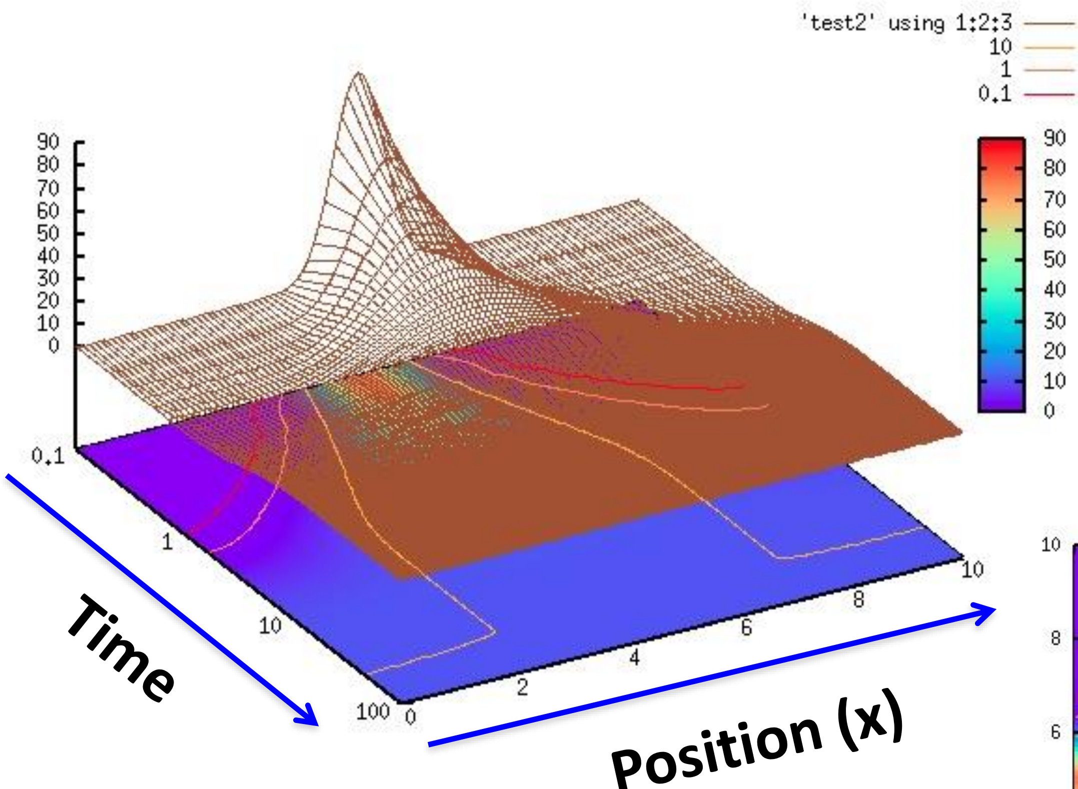
$$n(i,0) = \begin{cases} 0 & \text{if } i \neq M/2 = 50 \\ N_0 = 10^3 & \text{if } i = M/2 = 50 \end{cases}$$

[Boundary Conditions]

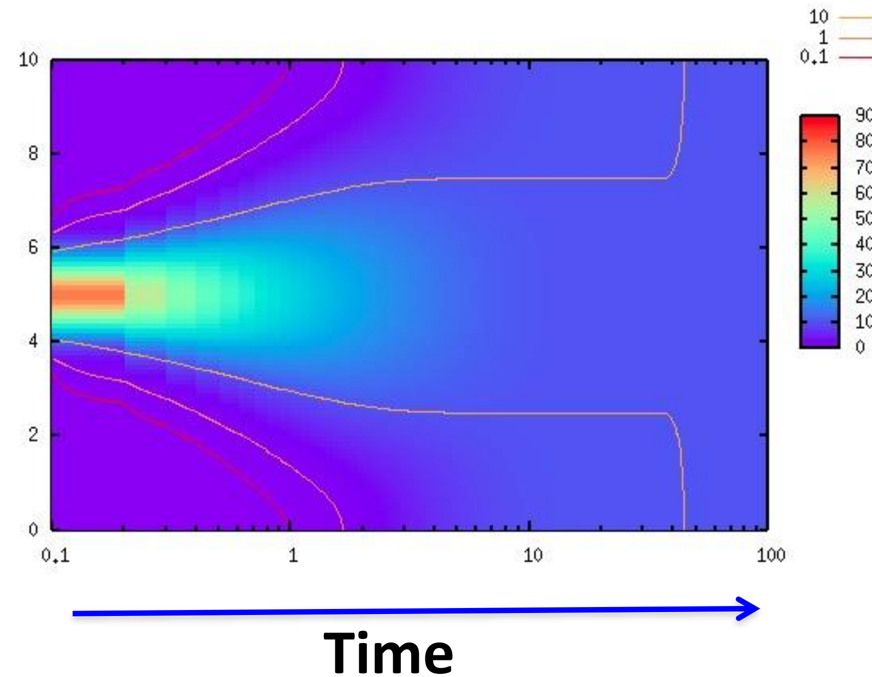
$$n(-1,j) = n(1,j), n(M+1,j) = n(M-1,j)$$

12.4 Initial boundary value problems for diffusion equation

Let's numerically solve (1) with reflecting boundary condition



$$n(i,j) \to 10$$



12.4 How to save the results into text file for graphics

Tips for R

```
library(scatterplot3d)
test_data<-read.csv("test_contour.csv")



#A simple 3d scatter plot
scatterplot3d(test_data)

#Preparation for contour plot
x<-0:2
y<-0:4
#need to prepare z data as the matrix
test_data2<-read.csv("test_contour2.csv")
class(test_data2)
test_data2<-as.matrix(test_data2)  #change data.frame to matrix

contour(x, y, test_data2)
image(x,y,test_data2, col=terrain.colors(100))
```

12.5 Initial boundary value problems for reaction-diffusion equation

$$\boxed{\frac{\partial N(x,t)}{\partial t} = f(N) + D\frac{\partial^2 N}{\partial x^2} \quad \textbf{(14)}}$$

$$0 < x < L, \quad t > 0$$

(Spatial and Temporal Domain)

[Initial Conditions] $N(x,0) = N_0(x)$

[Boundary Conditions] $N(0,t) = N(L,t) = 0$

We can use the following discretization for space

$$\frac{\partial^2 N}{\partial x^2} \approx \frac{N(x+\Delta x,t) - 2N(x,t) + N(x-\Delta x,t)}{(\Delta x)^2} \quad \textbf{(6)}$$

$$x_{i+1} - x_i = \Delta x$$

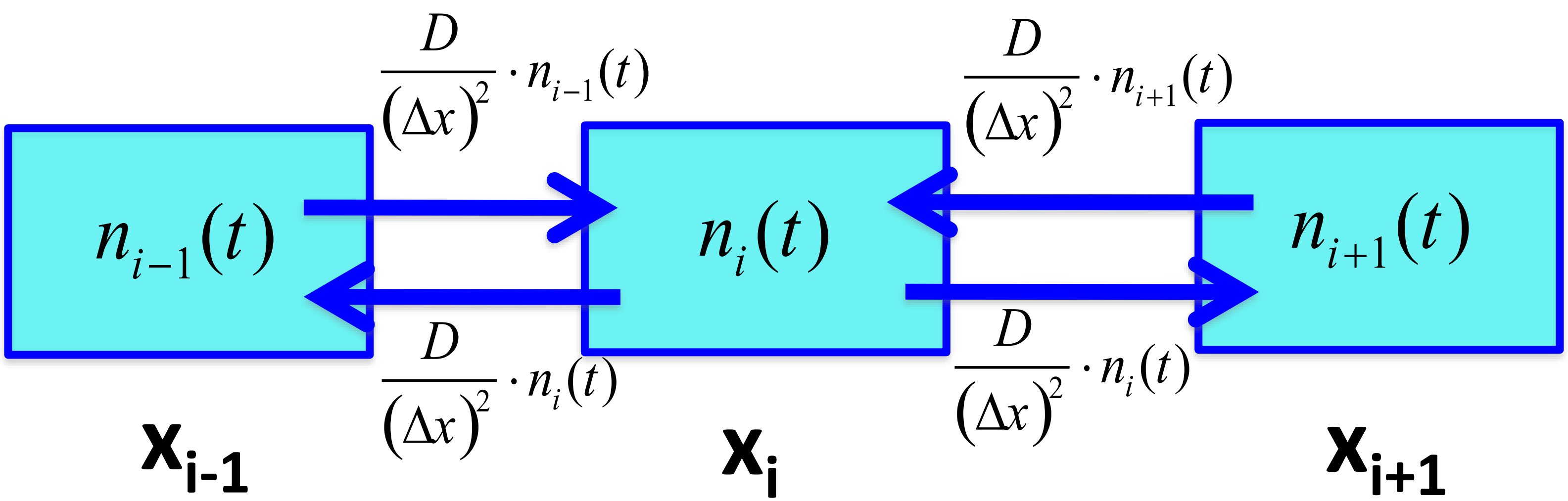
Let $n_i(t)$ as the approximation of $N(x_i$, t), and then we have

12.5 Initial boundary value problems for reaction-diffusion equation

$$\boxed{\frac{dn_i(t)}{dt} = f(n_i) + \frac{D}{(\Delta x)^2}\left[n_{i+1}(t) - 2n_i(t) + n_{i-1}(t)\right] \quad i = 1, 2, \ldots} \quad \textbf{(15)}$$

Now, we convert a reaction-diffusion model (PDE) into a set of ODE.

Then you can use any discretization methods in ODE (e.g. 4th order Runge-Kutta) for numerically solving (15).



Let's numerically solve the following exponential growth model.

$$\boxed{\frac{\partial N(x,t)}{\partial t} = rN(x,t) + D\frac{\partial^2 N(x,t)}{\partial x^2} \quad D=1, \quad 0<x<L=10.0, \quad t>0}$$

[Fixed Boundary Conditions]

$$N(0,t)=0, N(L,t)=0$$

[Initial Conditions]

$$n(i,0)=\begin{cases} 0 & \text{if } i \neq M/2=50 \\ N_0>0 & \text{if } i = M/2=50 \end{cases}$$

Confirm that population goes extinct if *r* is so small that the following condition is satisfied:

$$L < \pi\sqrt{\frac{D}{r}}$$

12.5 Final Homework

Let's numerically solve the following exponential growth model.

$$\frac{\partial N(x,t)}{\partial t} = rN(x,t) + D\frac{\partial^2 N(x,t)}{\partial x^2} \quad D=1, \quad 0<x<L=10.0, \quad t>0$$

[Fixed Boundary Conditions]

$$N(0,t)=0, N(L,t)=0$$

[Initial Conditions]

$$n(i,0) = \begin{cases} 0 & \text{if } i \neq M/2 = 50 \\ N_0 > 0 & \text{if } i = M/2 = 50 \end{cases}$$

[Spatial discritization]

$$\Delta x = \frac{L}{M} = \frac{10.0}{100} = 0.1$$

Plot the spatio-temporal dynamics of the population in two cases: (1) leading to extinction with small r and (2) leading to exponential growth with large r.