Reaction-Diffusion Models and Bifurcation Theory
Lecture 3: Diffusion, advection, cross-diffusion

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Notations of vectors

- vector space $\mathbb{R}^n = \{(x_1, x_2, \cdots, x_n) : x_i \in \mathbb{R}\}$
- inner product $x \cdot y = \sum_{i=1}^{n} x_i y_i$, norm $||x|| = \sqrt{x \cdot x}$.
- function: $g : \mathbb{R}^n \to \mathbb{R}$, $g(x) = g(x_1, x_2, \cdots, x_n)$
- curve $f : \mathbb{R} \to \mathbb{R}^n$, $f(t) = (f_1(t), f_2(t), \cdot, f_n(t))$
- vector field $F : \mathbb{R}^n \to \mathbb{R}^n$, $F(x) = F(x_1, x_2, \cdots, x_n) = (F_1(x), F_2(x), \cdots, F_n(x))$

- domain (region) Ω: an open (connected) subset in $\mathbb{R}^n$
- bounded domain Ω: if $||x|| \le M$ for all $x \in \Omega$ (unbounded if not bounded)
- smooth domain Ω: the boundary $\partial\Omega$ of Ω is locally the graph of a C^k function near all $x \in \partial\Omega$ (piecewise smooth: may except a zero measure set)
- Outer normal vector on the boundary $\partial\Omega$: $n(x)$ if $\partial\Omega$ is C^1 (or piecewise C^1)

Notations of vector derivatives

1. Gradient of a function g. $\nabla g : \mathbb{R}^n \to \mathbb{R}^n$ is a vector field,
$$\nabla g(x) = grad(g) = \left(\frac{\partial g}{\partial x_1}, \frac{\partial g}{\partial x_2}, \cdots, \frac{\partial g}{\partial x_n} \right).$$
2. Hessian of a function g. $Hess\ \ g : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ is a matrix-valued function,
$$Hess\ \ g(x) = \left(\frac{\partial^2 g}{\partial x_i \partial x_j} \right)_{1\le i,j\le n}.$$
3. Jacobian of a vector field F. $Jaco\ \ F : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ is a matrix-valued function,
$$Jaco\ \ F(x) = \left(\frac{\partial F_i}{\partial x_j} \right)_{1\le i,j\le n}.$$
4. Divergence of a vector field F. $div\ \ F : \mathbb{R}^n \to \mathbb{R}$ is a function,
$$div\ \ F(x) = \sum_{i=1}^{n} \frac{\partial F_i}{\partial x_i}(x).$$ (Divergence is the trace of Jacobian)
5. Laplacian of a function g. $\Delta g : \mathbb{R}^n \to \mathbb{R}$ is a function,
$$\Delta g = div(\nabla g) = \sum_{i=1}^{n} \frac{\partial^2 g}{\partial x_i^2}(x).$$ (Laplacian is the trace of Hessian, and Laplacian is the divergence of the gradient.)
6. Others: directional derivative $\frac{\partial u}{\partial n}(x) = \nabla u \cdot n$, curl,

Divergence Theorem

Assume that Ω is a bounded smooth domain, $u, v : \overline{\Omega} \to \mathbb{R}$ are smooth.
$n(x) = (n_1(x), n_2(x), \cdots, n_n(x))$ is the outer normal vector.

- $\displaystyle\int_\Omega \frac{\partial u}{\partial x_i}(x)dx = \int_{\partial\Omega} u(x)n_i(x)dS.$
- (Divergence Theorem) $\displaystyle\int_\Omega div\ F(x)dx = \int_{\partial\Omega} F(x)\cdot n(x)dS.$
- $\displaystyle\int_\Omega \Delta u(x)dx = \int_{\partial\Omega} \nabla u(x)\cdot n(x)dS = \int_{\partial\Omega} \frac{\partial u}{\partial n}(x)dS.$
- $\displaystyle\int_\Omega \frac{\partial u}{\partial x_i}(x)v(x)dx = \int_{\partial\Omega} u(x)v(x)n_i(x)dS - \int_\Omega u(x)\frac{\partial v}{\partial x_i}(x)dx.$
- (Green's Formula) $\displaystyle\int_\Omega \Delta u(x)v(x)dx = \int_{\partial\Omega} \frac{\partial u}{\partial n}(x)v(x)dS - \int_\Omega \nabla u(x)\cdot\nabla v(x)dx.$
- (Green's Formula)
  $\displaystyle\int_\Omega \Delta u(x)v(x)dx - \int_\Omega u(x)\Delta v(x)d = \int_{\partial\Omega} \frac{\partial u}{\partial n}(x)v(x)dS - \int_{\partial\Omega} u(x)\frac{\partial v}{\partial n}(x)dS.$

Laws of science

- Law of conservation of mass, momentum and energy
- Newton's 1st, 2nd and 3rd law
- Newton's universal law of gravitation
- Law of mass action
- First order rate law

Law of conservation of mass

Chemistry: Mass is neither created nor destroyed in any ordinary chemical reaction. Or more simply, the mass of substances produced (products) by a chemical reaction is always equal to the mass of the reacting substances (reactants). [Lavoisier, 1789]

Rate of change of mass in a given space
= rate of substance moving in - rate of substance moving out

Let $u(x,t)$ be the density (concentration) of a substance. The density is defined by $u(x,t) = \lim_{n\to\infty} \dfrac{\text{population in } O_n}{\text{volume of } O_n}$, where O_n is a sequence of domains containing x, and the volume of O_n tends to zero as $n \to \infty$. ($u : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ is a function)

Let $J(x,t)$ be the flux of this substance, which is the direction of movement of the substance. ($J : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ is a vector-valued function, and for a fixed time t, it is a vector field.)

Continuity Equation for the substance: $\dfrac{\partial u(x,t)}{\partial t} = -div\ J(x,t)$
This is based on the law of mass conservation, hence it is almost always true.

First order law

Fick's law: The flux is proportional to the concentration gradient, and it goes from higher concentration to lower one. $J(x,t) = -d\nabla_x u(x,t)$.
(d is the diffusion coefficient) [Fick, 1855]

Fourier's law: the time rate of heat transfer through a material is proportional to the negative gradient in the temperature. $J(x,t) = -k\nabla_x T(x,t)$.
(k is the material's conductivity, and T is the temperature) [Fourier, 1822]
Discrete version: Newton's cooling law

Ohm's law: the strength of the current at each point in electrical conductors is proportional to the gradient of electric potential. $J(x,t) = -\sigma\nabla_x V(x,t)$.
(σ is the electric conductivity, $\rho = 1/\sigma$ is the resistance of the conductor, and V is the electric potential) [Ohm, 1827]

Darcy's law: the discharge of a fluid through a porous medium at a point is proportional to the gradient of pressure. $J(x,t) = -\dfrac{k}{\mu}\nabla_x P(x,t)$. ($k$ is the permeability of the medium, μ is the viscosity, and P is the pressure) [Darcy, 1856]

These laws were mostly observed in experiments.

Diffusion equation

Let $u(x,t)$ be the density of a substance. Then from the law of mass conservation and Fick's law, $u(x,t)$ satisfies the diffusion equation (heat equation)

$$\frac{\partial u}{\partial t}(x,t) = d\Delta_x u(x,t), \text{ or } u_t = d\Delta u.$$

More general Fick's law: $J(x,t) = -D(x)\nabla u(x,t)$, where $D(x) = (D_{ij}(x))_{1\le i,j\le n}$ is the diffusion tensor matrix. Generalized diffusion equation:

$$u_t = div(D(x)\nabla u) = div\left(\sum_{j=1}^{n} D_{1j}(x)u_{x_j}, \sum_{j=1}^{n} D_{2j}(x)u_{x_j}, \cdots, \sum_{j=1}^{n} D_{nj}(x)u_{x_j}\right)$$

Homogeneous: $D(x) = D$ (constant matrix), inhomogeneous: $D(x)$ depends on x
Isotropic: $D = I$ (identity matrix), anisotropic: $D \neq I$ (constant matrix)

Inhomogeneous anisotropic diffusion equation: $u_t = \sum_{i,j=1}^{n}\left(D_{ij}(x)u_{x_ix_j} + \frac{\partial D_{ij}(x)}{\partial x_i}u_{x_j}\right)$

Homogeneous anisotropic diffusion equation: $u_t = \sum_{i,j=1}^{n} D_{ij}u_{x_ix_j}$

Robert Brown

Having found motion in the particles of the pollen of all the living plants which I had examined, I was led next to inquire whether this property continued after the death of the plant, and for what length of time it was retained.

Robert Brown (1828)

Random walk

A walker that takes steps of length Δx to the left or right along a line, and after each Δt time units, the walker will take one step. If the walker is at location x_0 at the time t_0, then at time $t = t_0 + \Delta t$, the walker will either be at $x_{-1} = x_0 - \Delta x$ or $x_1 = x_0 + \Delta x$. Normally the chances or going left or right should be equal, thus the probability of the walker going left or right is $1/2$.

Question:
1. What is the probability of the walker at $x_k = x_0 + k\Delta x$ after n steps $(k \leq n)$?
2. What is the population density $u(x, t)$ if there are many many walkers?

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Diffusion equation: $u_t = du_{xx}$, where $d = \lim_{\Delta x \to 0, \Delta t \to 0} \dfrac{(\Delta x)^2}{2\Delta t}$

Higher dimensional random walk produces diffusion equation $u_t = d_x u_{xx} + d_y u_{yy}$, where $d_x = \lim_{\Delta x \to 0, \Delta t \to 0} \dfrac{(\Delta x)^2}{2\Delta t}$, $d_y = \lim_{\Delta y \to 0, \Delta t \to 0} \dfrac{(\Delta y)^2}{2\Delta t}$

Random walk

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Brownian motion is the random moving of particles in a fluid (a liquid or a gas) resulting from their bombardment by the fast-moving atoms or molecules in the gas or liquid. It is a continuous-time stochastic processes.
[Brown, 1827], [Bachelier, 1900], [Einstein, 1905]

The density of Brownian particles $u(x,t)$ satisfies the diffusion equation.

Solving 1-D diffusion equation

$u_t = du_{xx}, \quad x \in \mathbb{R}$

trivial solution: $u(x,t) = a + bx$ (steady state solution)

separable solution: $u(x,t) = U(t)V(x)$,
$u(x,t) = e^{-d\lambda^2 t}\cos(\lambda x)$ or $u(x,t) = e^{-d\lambda^2 t}\sin(\lambda x)$ for any $\lambda > 0$.
$u(x,t) = e^{d\lambda^2 t}e^{\lambda x}$ or $u(x,t) = e^{d\lambda^2 t}e^{-\lambda x}$ for any $\lambda > 0$.
(none of them are uniformly bounded for all $x \in \mathbb{R}$, when t is fixed)

self-similar solution: $u(x,t) = t^{-1/2}U(x/t^{1/2})$,
$u(x,t) = t^{-1/2}e^{-x^2/(4dt)}$ $\underline{\Phi(x,t) = (4\pi dt)^{-1/2}e^{-x^2/(4dt)}}$ (so $\int_{\mathbb{R}} u dx = 1$)
fundamental solution (normal distribution function with mean 0 and variance $2dt$)

traveling wave solution: $u(x,t) = U(x - ct)$,
$u(x,t) = e^{c^2 t/d}e^{-cx/d}$ for any $c \in \mathbb{R}$ (same as the 2nd separable solution)

Derivatives and integrals of any solution

$$\Phi_x(x,t) = -\frac{x}{2dt}(4\pi dt)^{-1/2}e^{-x^2/(4dt)} = -\frac{x}{2dt}\Phi(x,t)$$

$\Phi_x^{(k)}(x,t) = t^{-1}H_k(x)\Phi(x,t)$, where H_k is a Hermite polynomial.

$$\Phi_t(x,t) = (2t)^{-1}\left(\frac{x^2}{2dt} - 1\right)\Phi(x,t)$$

$\int_0^x \Phi(y,t)dy = \frac{1}{2}erf\left(\frac{x}{\sqrt{4dt}}\right)$, where $erf(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-s^2}ds$ is the error function.

Solving n-D diffusion equation

$u_t = d\Delta u, \ \ x \in \mathbb{R}^n.$

Steady state solution: $\Delta u = 0$ (harmonic functions)
the solution space is infinite dimensional (can be from any complex analytic functions)
2-D: $1, x, y, x^2 - y^2, 2xy$, harmonic polynomials, $\sin(kx)\sin(ky)$, $\sin(kx)\cos(ky)$

Liouville Theorem. Any harmonic function defined in $\mathbb{R}^n$ bounded from above or below is a constant.

separable solution: $u(x,t) = U(x)V(t)$
$d\Delta U = \lambda U$, $V' = \lambda V$ for any $\lambda \in \mathbb{R}$

self-similar solution: $u(x,t) = t^{-n/2}U(|x|/t^{1/2})$, $\underline{\Phi_n(x,t) = (4\pi dt)^{-n/2}e^{-|x|^2/(4dt)}}$

Cauchy problem: $u_t = d\Delta u, \ \ x \in \mathbb{R}^n, \ \ t > 0, \ \ u(x,0) = g(x), x \in \mathbb{R}^n.$
Solution: $u(x,t) = \displaystyle\int_{\mathbb{R}^n} \Phi(x-y,t)g(y)dy$

Diffusion is faster in lower dimensional space: let t_n be the time $\Phi_n(x,t) = A$ for some $A > 0$ and same $|x|$, then $t_n > t_m$ if $n > m$.

Boundary conditions

A partial differential equation usually has infinitely many solutions. To be well-posed, the PDE should have some boundary conditions.

Flux boundary condition:
$J(x, t) \cdot n(x) = g(x)$, $x \in \partial\Omega$ (outflow rate is $g(x)$)
Neumann boundary condition (Fick's law):
$-d\nabla u(x, t) \cdot n(x) = g(x)$, $x \in \partial\Omega$ (outflow rate is $g(x)$)
Dirichlet boundary condition:
$u(x, t) = g(x)$, $x \in \partial\Omega$ (boundary density is fixed at $g(x)$)
Robin boundary condition:
$J(x, t) \cdot n(x) = ku(x, t)$, $x \in \partial\Omega$ (outflow rate is proportional to density)
Robin boundary condition (Fick's law):
$-d\nabla u(x, t) \cdot n(x) = ku(x, t)$, $x \in \partial\Omega$ (outflow rate is proportional to density)

homogeneous: $g(x) \equiv 0$, nonhomogeneous: $g(x) \not\equiv 0$

Combined boundary condition:
$\alpha(x)d\nabla u(x, t) \cdot n(x) + (1 - \alpha(x))u(x, t) = g(x)$, $x \in \partial\Omega$, $0 \le \alpha(x) \le 1$.
Nonlinear boundary condition:

$-d\nabla u(x, t) \cdot n(x) = f(x, u(x, t))$, $x \in \partial\Omega$, for a nonlinear function f.

Mass change for boundary conditions

Mass in Ω: $\int_\Omega u(x,t)dx$

No flux boundary condition: $J(x,t)\cdot n(x) = 0$ or $-d\nabla u(x,t)\cdot n(x) = 0$:
$\frac{d}{dt}\int_\Omega u(x,t)dx = \int_\Omega u_t(x,t)dx = -\int_\Omega div(J(x,t))dx = -\int_{\partial\Omega} J(x,t)\cdot n(x)dS = 0.$
Closed system, total mass is conserved.

Homogeneous Dirichlet boundary condition: $u(x,t) = 0$:
$\frac{d}{dt}\int_\Omega u(x,t)dx = \int_\Omega u_t(x,t)dx = d\int_\Omega \Delta u(x,t)dx = d\int_{\partial\Omega} \nabla u(x,t)\cdot n(x)dS < 0$, if $u(x,t) > 0$ for $x \in \Omega$. Total mass is decreasing.

Homogeneous Robin boundary condition: $-d\nabla u(x,t)\cdot n(x) = ku(x,t)$
$\frac{d}{dt}\int_\Omega u(x,t)dx = \int_\Omega u_t(x,t)dx = d\int_\Omega \Delta u(x,t)dx = d\int_{\partial\Omega} \nabla u(x,t)\cdot n(x)dS = -k\int_{\partial\Omega} u(x,t)dS$. If $u(x,t) > 0$ for $x \in \Omega$, then the total mass is decreasing when $k > 0$ (radiation boundary condition), and the total mass is increasing when $k < 0$ (absorbing boundary condition).

Energy change for boundary conditions

No flux boundary condition: $J(x,t)\cdot n(x)=0$ or $-d\nabla u(x,t)\cdot n(x)=0$:
$$\frac{1}{2}\frac{d}{dt}\int_\Omega u^2(x,t)dx=\int_\Omega u_t u dx=d\int_\Omega u\Delta u dx=-d\int_\Omega |\nabla u|^2 dx.$$
L^2 energy is decreasing.

Homogeneous Dirichlet boundary condition: $u(x,t)=0$:
$$\frac{1}{2}\frac{d}{dt}\int_\Omega u^2(x,t)dx=\int_\Omega u_t u dx=d\int_\Omega u\Delta u dx=-d\int_\Omega |\nabla u|^2 dx.$$
L^2 energy is decreasing.

Homogeneous Robin boundary condition: $-d\nabla u(x,t)\cdot n(x)=ku(x,t)$
$$\frac{1}{2}\frac{d}{dt}\int_\Omega u^2(x,t)dx=\int_\Omega u_t u dx=d\int_\Omega u\Delta u dx=-d\int_\Omega |\nabla u|^2 dx+\int_{\partial\Omega} u(\nabla u\cdot n)dS=$$
$$-d\int_\Omega |\nabla u|^2 dx+\int_{\partial\Omega}-(k/d)\int_{\partial\Omega} u^2 dS.$$
L^2 energy is decreasing when $k>0$ (radiation boundary condition).
When $k<0$ (absorbing boundary condition)?

A system is called dissipative if the energy is decreasing. This is also a special Lyapunov function.

Boundary value problem

Let Ω be a bounded smooth domain in $\mathbb{R}^n$. Then the initial-boundary value problem

$$\begin{cases} u_t = D\Delta u + f(x), & x \in \Omega,\ t > 0, \\ u(x,t) = u_0(x) \geq 0, & x \in \Omega, \\ \alpha(x) d\nabla u(x,t) \cdot n(x) + (1-\alpha(x))u(x,t) = g(x), & x \in \partial\Omega,\ t > 0, \end{cases}$$

has a unique solution $u(x,t) \geq 0$ for $(x,t) \in \Omega \times (0,\infty)$.

For simplicity $f(x) = g(x) = 0$ (see PDE books for f, g are not 0)

Fourier series solution: $u(x,t) = u_*(x) + \displaystyle\sum_{i=1}^{\infty} c_i e^{-d\lambda_i t}\phi_i(x)$

where $u_*(x)$ is a steady state solution, $(\lambda_i, \phi_i(x))$ is the eigenvalue-eigenfunction pair satisfying
$\Delta\phi + \lambda\phi = 0,\ \ x \in \Omega,\ \ \alpha\nabla\phi \cdot n + (1-\alpha)\phi = 0, x \in \partial\Omega,$
$\displaystyle\int_\Omega \phi_i^2(x)dx = 1$, and $c_i = \displaystyle\int_\Omega \phi_i(x)u_0(x)dx$. The eigenvalues satisfy
$0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k \to \infty$.

The steady state solution $u_*(x)$ is unique, $\lambda_1 < \lambda_2$ and $\phi_1 > 0$ except for Neumann boundary condition case. Neumann case: steady state solution $u(x) = c$ (any constant), $\lambda_1 = \lambda_2$ possible since there is an eigenvalue $\lambda_0 = 0$.

1-D Eigenvalue problem

$n(x) = -1$ at left endpoint, $n(x) = 1$ at right endpoint

Dirichlet: $u'' + \lambda u = 0, \quad x \in (0, L), \quad u(0) = u(L) = 0.$
eigenvalue-eigenfunction: $\lambda_i = (i\pi/L)^2$, $u_i(x) = \sin(i\pi x/L)$, $i \in \mathbb{N}$.

Neumann: $u'' + \lambda u = 0, \quad x \in (0, L), \quad u'(0) = u'(L) = 0.$
eigenvalue-eigenfunction: $\lambda_i = (i\pi/L)^2$, $u_i(x) = \cos(i\pi x/L)$, $i \in \mathbb{N} \cup \{0\}$.

Robin: $u'' + \lambda u = 0, \quad x \in (0, L), \quad -u'(0) + ku(0) = u'(L) + ku(L) = 0.$
eigenvalue-eigenfunction: $\lambda_i = \beta_i^2$, $u_i(x) = \beta_i \cos(\beta_i x) + k \sin(\beta_i x)$, $i \in \mathbb{N}$, where β_i satisfies $\tan(\beta L) = \dfrac{2k\beta}{\beta^2 - k^2}$.

Periodic: $u'' + \lambda u = 0, \quad x \in (0, L), \quad u(0) = u(L), \ u'(0) = u'(L).$
eigenvalue-eigenfunction: $\lambda_i = (2i\pi/L)^2$, $u_i(x) = c_1 \sin(2i\pi x/L) + c_2 \cos(2i\pi x/L)$, $i \in \mathbb{N} \cup \{0\}$.
This boundary value problem can be regarded as one on a circle (with no boundary).

Rectangle, cylinder, torus

$$\begin{cases} u_t = D(u_{xx} + u_{yy}) + \lambda u, & (x, y) \in R = (0, a) \times (0, b), \ t > 0, \\ \nabla u \cdot n = 0, & (x, y) \in \partial R, \ t > 0, \\ u(x, y, 0) = u_0(x, y), & (x, y) \in R, \end{cases}$$

where $D, \lambda, a, b > 0$, and ∂R is the boundary of rectangle R.

Separation of variables: $u(x, y, t) = U(t)W(x)Z(y)$. Then

$$U'(t) = (-Dk_1 - Dk_2 + \lambda)U(t),$$
$$W''(x) + k_1 W(x) = 0, \quad x \in (0, a), \quad W'(0) = W'(a) = 0,$$
$$Z''(y) + k_2 Z(y) = 0, \quad y \in (0, b), \quad Z'(0) = Z'(b) = 0.$$

Eigenvalue-eigenfunction:

$$k_{n,m} = \frac{n^2\pi^2}{a^2} + \frac{m^2\pi^2}{b^2}, \quad V_{n,m}(x, y) = \cos\left(\frac{n\pi x}{a}\right) \cdot \cos\left(\frac{m\pi y}{b}\right).$$

Define on a rectangle. Cylinder: periodic BC on x, torus: periodic BC on x and y

2-D Eigenvalue problem

Dirichlet: $\phi_{xx} + \phi_{yy} + \lambda\phi = 0, \ \ x \in \Omega, \ \ \phi = 0, \ \ x \in \partial\Omega.$

1. Eigenvalues can be calculated for rectangle, disk (numerically), triangle (?), L-shaped (?)
2. Rayleigh quotient: $\lambda_i = \inf_{H_i} \dfrac{\int_\Omega |\nabla\phi|^2 dx}{\int_\Omega \phi^2 dx}$, where
$H_i = \{\phi \in C^2(\Omega) : \int_\Omega \phi\phi_j dx = 0, 1 \le j \le i-1, \phi(x) = 0, x \in \partial\Omega\}$.
3. If $\Omega_1 \supset \Omega_2$, then $\lambda_i(\Omega_1) < \lambda_i(\Omega_2)$.
4. For the same area (say 1), which domain Ω has the smallest first eigenvalue? [Faber, 1923], [Krahn, 1924] a disk (even for n-D) (square $2\pi^2 \approx 21.46$, rectangle $(0,a)\times(0,a^{-1})$: $(a^2+a^{-2})\pi^2$, disk $5.783\pi \approx 18.17$)
(the ball is the domain that heat is hardest to dissipate, given the same area)
5. (Can one hear the shape of a drum?) Are there two domains with same eigenvalues but different shape? [Kac, 1966], [Gordon, Webb, Wolpert, 1994] there are two such domains (no if domains are convex and analytic)

2-D Eigenvalue problem

Neumann: $\phi_{xx} + \phi_{yy} + \lambda\phi = 0, \quad x \in \Omega, \quad \nabla\phi \cdot n = 0, \quad x \in \partial\Omega.$

1. Eigenvalues can be calculated for rectangle, disk (numerically), triangle (?), L-shaped (?)
2. Rayleigh quotient: $\lambda_{i-1} = \inf_{H_i} \dfrac{\int_\Omega |\nabla\phi|^2 dx}{\int_\Omega \phi^2 dx}$, where $H_i = \{\phi \in C^2(\Omega) : \int_\Omega \phi\phi_j dx = 0, 1 \le j \le i-1\}$.
3. If $\Omega_1 \supset \Omega_2$, then $\lambda_i(\Omega_1) < \lambda_i(\Omega_2)$ may not be true. [Ni-Wang, 2007, DCDS-A], [Ni, 2011]
4. For the same area (say 1), which domain Ω has the largest first positive eigenvalue? [Szego, 1954], [Weinberger, 1956] a ball (the ball is the domain that heat can spread easiest)
5. (Where is the hottest spot) For the first positive eigenvalue $\lambda_1 > 0$, where is the maximum point of $\phi_1(x)$? Is it on the boundary? [Rauch, 1975], [Burdzy, Werner, 1999] maybe not (yes for many other domains)

Advection

Continuity Equation: $\dfrac{\partial u(x,t)}{\partial t} = -div\ J(x,t)$
Fick's law: $J(x,t) = -d\nabla u(x,t)$

Advection: $J(x,t) = V(x,t) \cdot u(x,t)$, where $V : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ is a vector field describing the velocity of the fluid.
Homogeneous flow: $V(x,t) = (v_1, v_2, \cdots, v_n)$

$$u_t = -\sum_{i=1}^{n} v_i u_{x_i}.$$

1-D advection equation (transport equation)
$u_t + au_x = 0$. Solution $u(x,t) = U(x+at)$ for any smooth (or even non-smooth) function U (traveling wave!)

Convection: convective transport is the sum of advective and diffusive transport
Advection-diffusion equation: $u_t = d\Delta u - V \cdot \nabla u$.

Advection-reaction-diffusion equation: $u_t = d\Delta u - V \cdot \nabla u + f(u)$.

1-D advection-diffusion equation

$u_t = du_{xx} - au_x$. Let $y = x - at$ and $u(x,t) = v(x - at, t)$. Then $v_t = dv_{yy}$.
Therefore all solutions of 1-D advection-diffusion equation can be obtained from 1-D diffusion equation.

separable solution: $u(x,t) = U(t)V(x - at)$,
$u(x,t) = e^{-d\lambda^2 t}\cos(\lambda(x - at))$ or $u(x,t) = e^{-d\lambda^2 t}\sin(\lambda(x - at))$ for any $\lambda > 0$.
$u(x,t) = e^{d\lambda^2 t}e^{\lambda(x-at)}$ or $u(x,t) = e^{d\lambda^2 t}e^{-\lambda(x-at)}$ for any $\lambda > 0$.
(none of them are uniformly bounded for all $x \in \mathbb{R}$, when t is fixed)

self-similar solution: $u(x,t) = t^{-1/2}U((x - at)/t^{1/2})$,
$\underline{\Phi(x,t) = (4\pi dt)^{-1/2}e^{-(x-at)^2/(4dt)}}$ (so $\int_{\mathbb{R}} u dx = 1$)
fundamental solution (normal distribution function with mean at and variance $2dt$)

traveling wave solution: $u(x,t) = U(x - ct)$,
$u(x,t) = e^{c^2 t/d}e^{-c(x-at)/d}$ for any $c \in \mathbb{R}$

Boundary value problems

All boundary conditions can be used here. But the flux is now $J = -d\nabla u + uV$, so no flux boundary condition becomes: $-d\nabla u \cdot n + uV \cdot n = 0$, $x \in \partial\Omega$.

$$\begin{cases} u_t = D\Delta u - V \cdot \nabla u + f(x), & x \in \Omega,\ t > 0, \\ u(x,0) = u_0(x) \geq 0, & x \in \Omega, \\ Bu(x,t) = g(x), & x \in \partial\Omega,\ t > 0, \end{cases}$$

For simplicity $f(x) = g(x) = 0$ (see PDE books for f, g are not 0)

Fourier series solution: $u(x,t) = u_*(x) + \displaystyle\sum_{i=1}^{\infty} c_i e^{-d\lambda_i t}\phi_i(x)$

where $u_*(x)$ is a steady state solution, $(\lambda_i, \phi_i(x))$ is the eigenvalue-eigenfunction pair satisfying

$\Delta\phi - V \cdot \nabla\phi + \lambda\phi = 0$, $x \in \Omega$, $B\phi = 0, x \in \partial\Omega$,

$\displaystyle\int_\Omega \phi_i^2(x)dx = 1$, and $c_i = \displaystyle\int_\Omega \phi_i(x)u_0(x)dx$. The eigenvalues satisfy $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k \to \infty$.

Example: chemical in a river

$$
\begin{cases}
u_t = du_{xx} - au_x - ku, & x \in (0, L),\ t > 0, \\
u(x,0) = u_0(x) \geq 0, & x \in (0, L), \\
du_x(0) - au(0) = -b, & t > 0, \\
-du_x(L) + au(L) = cu(L), & t > 0.
\end{cases}
$$

Steady state solution $u_*(x)$:
$du_{xx} - au_x - ku = 0,\ \ x \in (0, L),\ \ du_x(0) - au(0) = -b,\ \ -du_x(L) + au(L) = cu(L).$

Eigenvalue problem:
$du_{xx} - au_x - ku = -\lambda u,\ \ x \in (0, L),\ \ du_x(0) - au(0) = 0,\ \ -du_x(L) + au(L) = cu(L).$

Mass change:

$$
\frac{d}{dt}\int_0^L u(x,t)dx = \int_0^L u_t(x,t)dx = \int_0^L (du_{xx} - au_x - ku)dx
$$

$$
= (du_x - au)|_0^L - k\int_0^L u(x,t)dx = -cu(L) + b - k\int_0^L u(x,t)dx?
$$

1-D Eigenvalue problem

$n(x) = -1$ at left endpoint, $n(x) = 1$ at right endpoint

Dirichlet: $u'' - au' + \lambda u = 0, \ \ x \in (0, L), \ \ u(0) = u(L) = 0.$
eigenvalue-eigenfunction: $\lambda_i = (i\pi/L)^2 + a^2/4, \ u_i(x) = e^{ax/2} \sin(i\pi x/L), \ i \in \mathbb{N}.$

No-flux: $u'' - au' + \lambda u = 0, \ \ x \in (0, L), \ \ -u'(0) + au(0) = u'(L) - au(L) = 0.$
eigenvalue-eigenfunction: $\lambda_0 = 0, \ u_0(x) = e^{ax},$
$\lambda_i = (i\pi/L)^2 + a^2/4, \ u_i(x) = ae^{ax/2} \sin(i\pi x/L) + \frac{2i\pi}{L} e^{ax/2} \cos(i\pi x/L), \ i \in \mathbb{N}.$

Neumann: $u'' - au' + \lambda u = 0, \ \ x \in (0, L), \ \ u'(0) = u'(L) = 0.$
eigenvalue-eigenfunction:

Robin: $u'' - au' + \lambda u = 0, \ \ x \in (0, L), \ \ -u'(0) + ku(0) = u'(L) + ku(L) = 0.$
eigenvalue-eigenfunction:

Periodic: $u'' - au' + \lambda u = 0, \ \ x \in (0, L), \ \ u(0) = u(L), \ u'(0) = u'(L).$
eigenvalue-eigenfunction:
This boundary value problem can be regarded as a problem on a circle (with no boundary).

Linear growth: critical patch size

[Skellam, 1951]

$$\begin{cases} u_t = Du_{xx} + au, & x \in (0, L),\ t > 0, \\ u(t, 0) = u(t, L) = 0, & \\ u(0, x) = u_0(x), & x \in (0, L). \end{cases}$$

Solution: $u(t, x) = \sum_{i=1}^{\infty} c_i exp\left(at - d\frac{i^2\pi^2}{L^2}t\right) \sin\left(\frac{i\pi x}{L}\right)$, where

$c_i = \frac{2}{L}\int_0^L u_0(x) \sin\left(\frac{i\pi x}{L}\right) dx.$

When $a > \frac{D\pi^2}{L^2}$ or $L > \sqrt{\frac{D}{a}}\pi$, $\lim_{t\to\infty} u(t, x) = \infty$,
when $a < \frac{D\pi^2}{L^2}$ or $L < \sqrt{\frac{D}{a}}\pi$, $\lim_{t\to\infty} u(t, x) = 0$.

$L = \sqrt{\frac{D}{a}}\pi$ is called the critical patch size, as the population cannot survive if the habitat is too small (the outgoing flux wins over the growth), but the population will not only survive but thrive to an exponential growth if the habitat is large enough (growth outpaces the emigration).

Critical patch size: recent work

1. Jin, Yu; Lewis, Mark A., Seasonal influences on population spread and persistence in streams: critical domain size. SIAM J. Appl. Math. 71 (2011), no. 4, 1241-1262.
2. Berestycki, H.; Diekmann, O.; Nagelkerke, C. J.; Zegeling, P. A. Can a species keep pace with a shifting climate? Bull. Math. Biol. 71 (2009), no. 2, 399-429.
3. Artiles, W.; Carvalho, P. G. S.; Kraenkel, R. A. Patch-size and isolation effects in the Fisher-Kolmogorov equation. J. Math. Biol. 57 (2008), no. 4, 521-535.
4. Du, Yihong; Shi, Junping A diffusive predator-prey model with a protection zone. J. Differential Equations 229 (2006), no. 1, 63-91.
5. Cantrell, Robert Stephen; Cosner, Chris; Fagan, William F. Habitat edges and predator-prey interactions: effects on critical patch size. Math. Biosci. 175 (2002), no. 1, 3-55.

Linear growth: invasion speed

[Skellam, 1951]

$$\frac{\partial P}{\partial t} = D(\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}) + aP, \quad (x, y) \in \mathbb{R}^2.$$

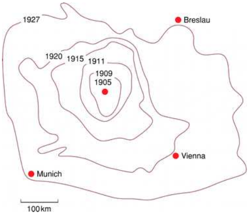
Fundamental solution: $P(x, y, t) = \frac{1}{4\pi Dt} e^{at - \frac{x^2+y^2}{4Dt}}$.

Note that $\int_{\mathbb{R}^2} P(x, y, t) dxdy = e^{at}$.

Let B_R be the ball with radius R in $\mathbb{R}^2$; we define $R(t)$ as the number such that outside of $B_{R(t)}$, the total population is always 1.

$R(t) = \sqrt{4aD}t$ (this is the front of invasion)

Spreading of muskrat

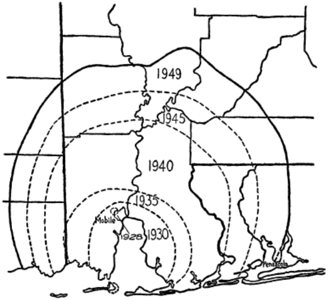


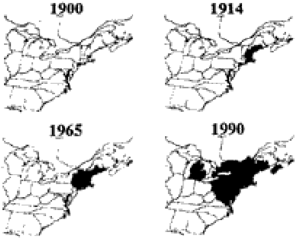
Year	1905	1909	1911	1915	1920	1927
Area (km^2)	0	5400	14000	37700	79300	201600

$$aD = \frac{119777300}{296433} \cdot \frac{1}{4\pi} = 32.15422940$$

The speed of the expansion is $R'(t) = \sqrt{4aD} = 11.34093989(km/year)$

Biological invasion





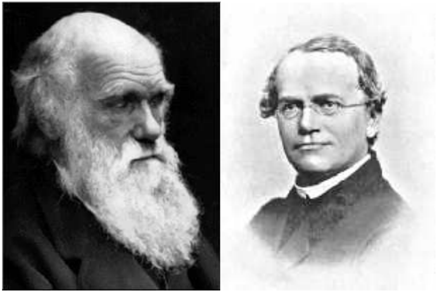
Fire ants and Gypsy moss expansions.

Genetic evolution

Darwin-Mendel's gene evolution theory assumes that the advantageous gene replaces other gene in the long run through mutations or genetic drift. Suppose that for a gene with two possible alleles: P (advantageous) and Q (non-advantageous). Then the frequency of the advantageous gene in the n-th and $n+1$-th generations is described by the Fisher-Haldane-Wright law:

$$p_{n+1} = \frac{(w_x p_n^2 + w_y p_n q_n) p_n}{w_x p_n^2 + 2 w_y p_n q_n + w_z q_n^2}, \; q_{n+1} = 1 - p_{n+1}.$$

where $w_x : w_y : w_z$ are the fitness parameters of $PP : PQ : QQ$ type genes.



Left: Charles Darwin (1809-1882), right: Gregor Mendel (1822-1884)

Fisher-Haldane-Wright equation

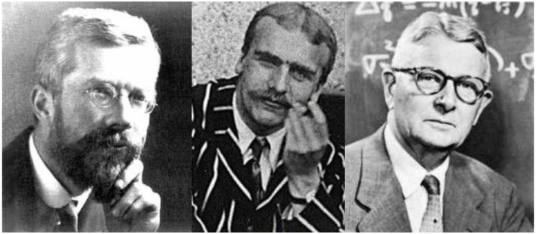
Fisher-Haldane-Wright equation can be written as

$$p_{n+1} - p_n = p_n(1-p_n)\frac{(w_x - w_y)p_n + (w_y - w_z)(1-p_n)}{w_x p_n^2 + 2w_y p_n(1-p_n) + w_z(1-p_n)^2}$$

Making the discrete process continuous, then we have

$$\frac{dp}{dt} = p(1-p)\frac{(w_x - w_y)p + (w_y - w_z)(1-p)}{w_x p^2 + 2w_y p(1-p) + w_z(1-p)^2}$$

Finally we assume that $w_z = 1$, $w_y = 1+s$, $w_x = 1+2s$ and s is a small positive number, $\frac{dp}{dt} = sp(1-p)$



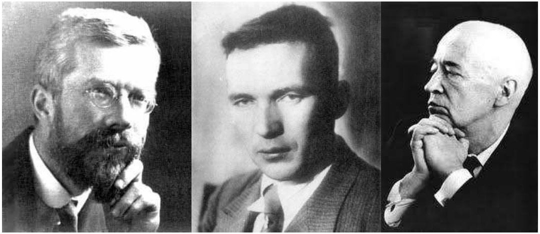
Left: Ronald Fisher (1890-1962), middle: J. B. S. Haldane (1892-1964), right: Sewall Wright (1889-1988)

Fisher-KPP equation

We have used the Fisher-Haldane-Wright Law in genetics to derive the Logistic equation. If the species also moves freely in the space, then their population density also satisfies a diffusion equation. Hence we obtain a reaction-diffusion equation assuming one dimension spatial domain:

$$\frac{\partial p}{dt} = D\frac{\partial^2 p}{\partial x^2} + sp(1-p)$$

Here $p(x,t)$ is the density function of the advantageous gene at location x and time t. This equation was first proposed by Fisher in 1937, and in the same year Soviet Union mathematicians Kolmogorov, Petrovski, Piskunov considered this nonlinear parabolic partial differential equation. They introduced the concept of traveling wave. Today this equation is called Fisher equation, KPP equation, or Fisher-KPP equation.



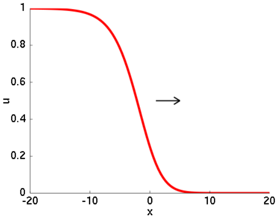
L: R. Fisher (1890-1962), M: A. N. Kolmogorov (1903-1987), R: I. G. Petrovsky (1901-1973)

Fisher-KPP traveling wave

$u_t = Du_{xx} + au(1-u)$
Let $u(t,x) = w(x-ct)$. Then w satisfies $-cw' = Dw'' + aw(1-w)$.

Look for solution of $Dw'' + cw' + aw(1-w) = 0$,
$w'(y) < 0, \quad \lim_{y\to-\infty} w(y) = 1, \quad \lim_{y\to\infty} w(y) = 0.$

Result: [Kolmogorov, Petrovski, Piskunov, 1937] For each $c \geq \sqrt{4aD}$, there exists a unique traveling wave solution. The (minimum) speed is again $\sqrt{4aD}$!



Fisher-KPP: minimal patch size

$$\begin{cases} u_t = Du_{xx} + au(1-u), & x \in (0, L),\ t > 0, \\ u(t,0) = u(t,L) = 0, & \\ u(0,x) = u_0(x), & x \in (0, L). \end{cases}$$

Result:

When $a > \dfrac{D\pi^2}{L^2}$ or $L > \sqrt{\dfrac{D}{a}}\pi$, $\lim\limits_{t\to\infty} u(t,x) = u_*(x)$, a steady state solution

when $a < \dfrac{D\pi^2}{L^2}$ or $L < \sqrt{\dfrac{D}{a}}\pi$, $\lim\limits_{t\to\infty} u(t,x) = 0$.

Wirtinger's inequality: If $u \in C^1(0,1)$ and $u(0) = u(L) = 0$, then

$$\int_0^L [u'(x)]^2 dx \le \frac{L^2}{\pi^2} \int_0^L [u(x)]^2 dx.$$

Nonlinear diffusion

Fick's law is a first order law.
Darcy law for flows in porous media: $J = -uV$, $V = -(k/\mu)\nabla p$, $p(u) = p_0 u^\gamma$

Porous medium equation: $u_t = \Delta u^{\gamma+1} = \Delta u^m$

Flow of gas in a porous medium, underground water infiltration, plasma radiation, spreading of populations, thin films under gravity

Self-similar solution: $u(x,t) = t^\alpha U(t^\beta |x|)$
$\alpha = -\dfrac{n}{2+n(m-1)}$, $\beta = -\dfrac{1}{2+n(m-1)}$, $U(z) = (C - kz^2)_+^{1/(m-1)}$, $m > 1$
(biological meaning: finite range spreading!, invasion speed: $t^{-\beta}$ ($|\beta| < 1/2$))
$\alpha = -\dfrac{n}{2-n(1-m)}$, $\beta = -\dfrac{1}{2-n(1-m)}$, $U(z) = (C + kz^2)^{-1/(1-m)}$,
$1 > m > (n-2)/n$
(biological meaning: infinite range spreading, invasion speed: $t^{-\beta}$ ($|\beta| > 1/2$))

Other nonlinear diffusion: $u_t = \Delta(F(u))$