COMPUTATIONAL APPROACHES

IN MATHEMATICAL ECOLOGY

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LECTURE 3: Numerical solution of partial differential equations

The outline

- Ecological problem: monitoring insects movement
- Mathematical problem: the initial-boundary-value problem (IBVP) for the diffusion equation
- The $1 - D$ case: finite difference discretization of the second order IBVP
- The $2 - D$ case: finite difference method for the diffusion IBVP

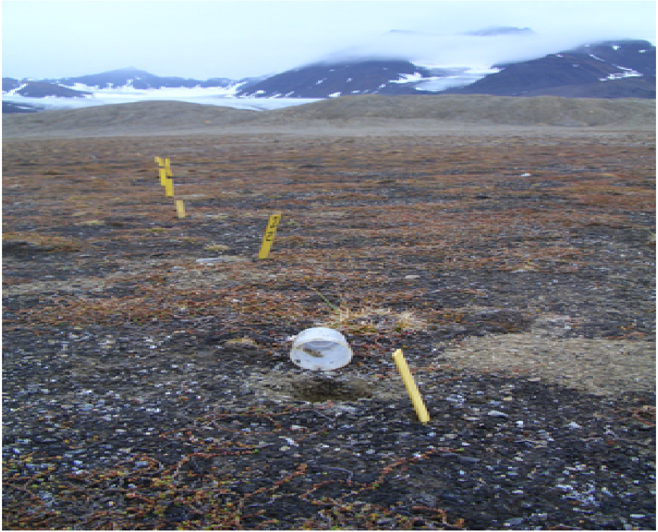
Ecological problem:

monitoring insects movement

Problem statement

- Monitoring of pest insects is an important part of the integrated pest management.
- Interpretation of trap counts remains a challenging problem.
- *How is the number of insects caught over a fixed time related to the insects population density?*
- A mean-field mathematical model of insect trapping is based on the diffusion equation.

A single trap



The road map

- Learn how to solve the diffusion equation in a $2-D$ domain.
- Learn how to reconstruct trap counts from the solution $u(x, y)$ to the diffusion equation.
- Compare the trap counts obtained from the solution $u(x, y)$ to the diffusion equation with field data.
- Vary the parameters in the diffusion equation to reach good agreement between numerical data and field data. That will give you the density $u(x, y)$ as required.

Skills required

- Solve the diffusion equation in a $2-D$ domain:

  approximation of the spatial terms – lecture 3
  approximation of the temporal term – lecture 2
  approximation of the boundary conditions – lecture 3

- Reconstruct trap counts from the solution $u(x, y)$ to the diffusion equation:

  approximation of the flux – interpolation, lecture 1
  calculation of trap counts – numerical integration, lecture 1

- Error analysis, validation, verification – lectures 1, 2, 3

One-dimensional problem: mathematical model

$$\frac{\partial u(x,t)}{\partial t} = D\,\frac{\partial^2 u(x,t)}{\partial x^2}\,,$$

where $u(x,y)$ is the insects population density, D is the diffusion coefficient.

The initial condition: $u(x,0) \;=\; U_0, \quad \text{for } 0 < x < L.$

The boundary conditions:

$$u(0,t) \;=\; 0\,, \quad \frac{\partial u(L,t)}{\partial x} \;=\; 0.$$

Why is a $1-D$ model important?

- It is easy to understand basic concepts behind the numerical method in the $1-D$ case.
- It is easy to design a computer program for a $1-D$ model.
- The exact solution is available: we can validate and verify the program and results.
- Predictions for a $2-D$ solution can be made based on $1-D$ results.

One-dimensional problem: trap counts

- The solution $u(x,t)$ is given by the following infinite series:

$$u(x,t) \;=\; \frac{4U_0}{\pi}\sum_{k=0}^{\infty}\frac{1}{(2k+1)}\sin\left(\frac{(2k+1)\pi x}{2L}\right)\exp\left(-\frac{(2k+1)^2\pi^2 Dt}{4L^2}\right).$$

- The corresponding trap count over time t is

$$\Delta U(t) \;=\; \int_0^t j(\tau)d\tau\ ,$$

where $j(t)$ is the absolute value of the population density flux through the trap boundary,

$$j(t) \;=\; D\left|\frac{\partial u(x,t)}{\partial x}\right|_{x=0}.$$

$$j(t) \;=\; \frac{2DU_0}{L}\sum_{k=0}^{\infty}\exp\left(-\frac{(2k+1)^2\pi^2 Dt}{4L^2}\right).$$

One-dimensional problem: trap counts

$$\Delta U(t) \;=\; \frac{8LU_0}{\pi^2}\sum_{k=0}^{\infty}\frac{1}{(2k+1)^2}\left[1-\exp\left(-\frac{(2k+1)^2\pi^2 Dt}{4L^2}\right)\right].$$

- In the large-time limit $\Delta U(t) \to LU_0$, i.e. all insects are trapped.
- The trap count can be approximated as

$$\Delta U(t) \;\approx\; \frac{2U_0}{\sqrt{\pi}}\,\sqrt{Dt},$$

which shows a very good accuracy when either time t is sufficiently small or the domain length L is sufficiently large, or both.

References

- S.V.Petrovskii, N.B.Petrovskaya, D.Bearup. *Multiscale Approach to Pest Insect Monitoring: Random Walks, Pattern Formation, Synchronization, and Networks.* Physics of Life Reviews, 2014, doi: 10.1016/j.plrev.2014.02.001

- D. Bearup, N.B.Petrovskaya, S.V.Petrovskii. *Some Analytical and Numerical Approaches to Understanding Trap Counts Resulting from Pest Insect Immigration.* (submitted to Mathematical Biosciences)

- S.V.Petrovskii, D.Bearup, D.A.Ahmed, R.Blackshaw. *Estimating Insect Population Density from Trap Counts.* Ecological Complexity, 2012, pp.69–82.

Finite difference (FD) discretization of a one-dimensional problem

FD discretization of ODE

- The linear second-order boundary value problem:

$$y'' = p(x)y' + q(x)y + r(x), \quad a \leq x \leq b,$$

$$y(a) = \alpha, \; y(b) = \beta$$

- The underlying idea for an FD method:

– replace the first and second derivatives with their difference approximations

– hence, reduce the boundary value problem to a system of algebraic equations

Forward difference approximation of the first derivative

- The Taylor series expansion of $y(x)$ about the point x

$$y(x+h) = y(x) + h\frac{dy(x)}{dx} + \frac{h^2}{2}\frac{d^2y(\xi)}{dx^2}$$

$$\frac{dy(x)}{dx} = \frac{y(x+h)-y(x)}{h} + \frac{h}{2}\frac{d^2y(\xi)}{dx^2}$$

$$\frac{dy(x)}{dx} = \frac{y(x+h)-y(x)}{h} + O(h)$$

$$\frac{dy(x)}{dx} \approx \frac{y(x+h)-y(x)}{h} \qquad \text{forward difference}$$

- The error is

$$e = \left|\frac{dy(x)}{dx} - \frac{y(x+h)-y(x)}{h}\right| = O(h), \quad e \to 0, \text{ as } h \to 0.$$

the first order approximation

Central difference approximation of the first derivative

- The Taylor series expansion of $y(x)$ about the point x

$$y(x+h) = y(x) + h\frac{dy(x)}{dx} + \frac{h^2}{2}\frac{d^2y(x)}{dx^2} + \frac{h^3}{6}\frac{d^3y(\xi)}{dx^3}$$
$$y(x-h) = y(x) - h\frac{dy(x)}{dx} + \frac{h^2}{2}\frac{d^2y(x)}{dx^2} - \frac{h^3}{6}\frac{d^3y(\eta)}{dx^3}$$

$$\frac{dy(x)}{dx} = \frac{y(x+h) - y(x-h)}{2h} + \frac{h^2}{6}[-\frac{d^3y(\xi)}{dx^3} + \frac{d^3y(\eta)}{dx^3}]$$

$$\frac{dy(x)}{dx} = \frac{y(x+h) - y(x-h)}{2h} + O(h^2)$$
$$\frac{dy(x)}{dx} \approx \frac{y(x+h) - y(x-h)}{2h} \quad \text{central difference}$$

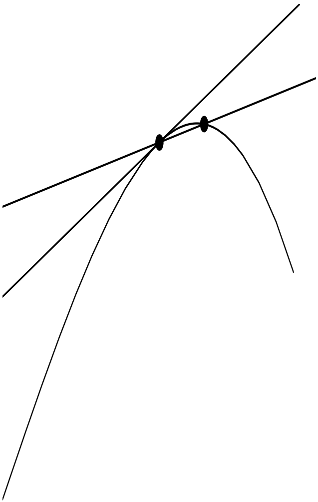
- The error is

$$e = |\frac{dy(x)}{dx} - \frac{y(x+h) - y(x-h)}{2h}| = O(h^2), \quad e \to 0, \text{ as } h \to 0.$$

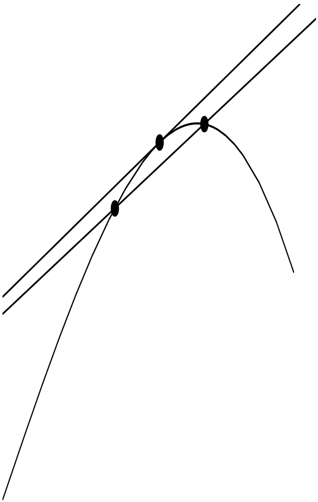
the second order approximation

A sketch of FD approximation of the first derivative

the forward (backward) difference



the central difference



FD approximation of higher order derivatives

- Let $g(x) = y'(x)$

$$\frac{d^2y(x)}{dx^2} = \frac{dg(x)}{dx} \approx \frac{g(x+h/2) - g(x-h/2)}{h}$$

$$g(x+h/2) = \frac{dy(x+h/2)}{dx} \approx \frac{y(x+h) - y(x)}{h}$$

$$g(x-h/2) = \frac{dy(x-h/2)}{dx} \approx \frac{y(x) - y(x-h)}{h}$$

$$\frac{d^2y(x)}{dx^2} \approx \frac{y(x+h) - 2y(x) + y(x-h)}{h^2}$$

- The error is

$$e = \left|\frac{d^2y(x)}{dx^2} - \frac{y(x+h) - 2y(x) + y(x-h)}{h^2}\right| = O(h^2)$$

the second order approximation

Numerical solution of the BVP by finite differences: example

$$y'' = 2,\ \ y(0) = 1,\ \ y(1) = 3$$

$$(y'' = p(x)y' + q(x)y + r(x),\ \ a \le x \le b,\ y(a) = \alpha,\ \ y(b) = \beta)$$

$Y(x) = x^2 + x + 1$ – the exact solution

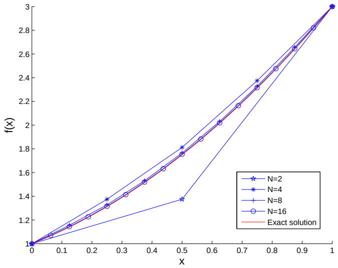
- A uniform computational grid $\mathcal{G}$ in the domain $x \in [0,1]$: $x_1 = 0$, $x_{i+1} = x_i + h$, $i = 1, \dots, N$, where $h = 1/N$ is the grid step size, and N is the number of grid subintervals
- FD discretization at grid points:

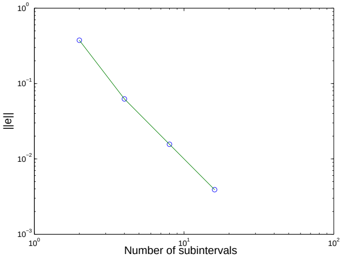
$$\frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} = 2, \quad i = 2, \dots, N \text{ – the equation}$$

$$y(x_1) = 1, \quad y(x_{N+1}) = 3 \quad \text{– the boundary conditions}$$

$$e_i = |Y(x_i) - y(x_i)| \quad \text{– the error at the point } x_i$$

Example of numerical solution





FD discretization of boundary conditions

$$y'' = p(x)y' + q(x)y + r(x), \;\; a \le x \le b, \;\; \frac{dy(a)}{dx} = \alpha, \;\; y(b) = \beta$$

- FD discretization at grid points:

$$\frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} = p(x_i)\frac{y(x_{i+1}) - y(x_{i-1})}{2h} +$$

$$q(x_i)y(x_i) + r(x_i), \quad i = 2, \ldots, N$$

$$\frac{y(x_2) - y(x_1)}{h} = \alpha, \text{ – the first order!} \quad y(x_{N+1}) = \beta$$

- We need the second order approximation of the boundary condition!

FD discretization of boundary conditions

- $$\frac{y(x_2) - y(x_0)}{h} = \alpha? \quad \text{but } x_0 \text{ does not exist!}$$
- The equation at the point x_1:

$$\frac{y_2 - 2y_1 + y_0}{h^2} = p_1 \frac{y_2 - y_0}{2h} + q_1 y_1 + r_1,$$

where $g_i \equiv g(x_i)$

- $$\frac{dy(x_1)}{dx} \approx \frac{2y_2 - (2 + q_1 h^2)y_1 - r_1 h^2}{2h + p_1 h^2} = \alpha$$

second order approximation

References

- F.B.Hildebrand. *Finite-Difference Equations and Simulations.* Prentice-Hall, Englewood Cliffs, New Jersey, 1968.
- H.Levy and F.Lessman. *Finite Difference Equations.* Dover, New York, 1992.
- D.Richtmeyer and K.W.Morton. *Difference Methods for Initial Value Problems.* Wiley, New York, 1967.
- M.Spiegel. *Calculus of Finite Differences and Differential Equations.* New York: McGraw-Hill, 1971.

Numerical solution

of a $1 - D$ diffusion equation

The one-dimensional problem

$$\frac{\partial u(x,t)}{\partial t} = D\,\frac{\partial^2 u(x,t)}{\partial x^2}\ ,$$

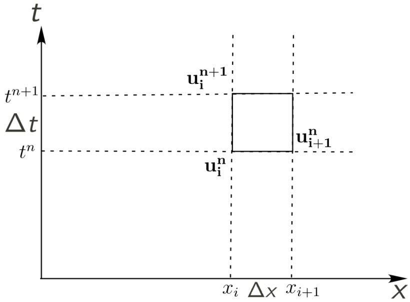
where $u(x, y)$ is the insects population density, D is the diffusion coefficient.

The initial condition: $u(x, 0) \;=\; U_0, \quad \text{for } 0 < x < L.$

The boundary conditions:

$$u(0,t) \;=\; 0\ , \qquad \frac{\partial u(L,t)}{\partial x} \;=\; 0.$$

FD discretization of the diffusion equation



- a uniform grid in the domain $x \in [0, L]$, $h = L/N$
- a uniform grid in the domain $t \in [0, T]$, $\Delta t = T/M$

FD discretization of the diffusion equation

A finite difference discretization scheme:

$$\frac{1}{\tau}(u_i^{n+1} - u_i^n) = \Lambda[u_i^n],$$

where the discrete operator Λ is

$$\Lambda[v_i] = \frac{D}{h^2}(v_{i+1} - 2v_i + v_{i-1}).$$

Boundary conditions

$$u_1^{n+1} = 0, \qquad \text{for } x = 0,$$

$$u_{N+1}^{n+1} = u_{N+1}^n + \frac{2\tau D}{h^2}(u_N^n - u_{N+1}^n), \qquad \text{for } x = L.$$

Initial condition

$$u_i^0 = U_0, \quad i = 2, \ldots, N.$$

Importance of accurate BC approximation

Nodes per unit length	3	5	9	11	21
1st order ($\times 10^{-4}$)	359	183	92.4	74.1	37.2
2nd order ($\times 10^{-4}$)	0.949	0.288	0.110	0.194	0.100

Maximum relative error obtained in the $1 - D$ system for 1st order and 2nd order approximation of the boundary condition at the external boundary.

Stability of the FD scheme

$$\frac{1}{\tau}(u_i^{n+1} - u_i^n) = \Lambda[\sigma u_i^{n+1} + (1-\sigma)u_i^n],$$

$$\Lambda[v_i] = \frac{D}{h^2}(v_{i+1} - 2v_i + v_{i-1}).$$

The weight parameter σ defines a type of the scheme:

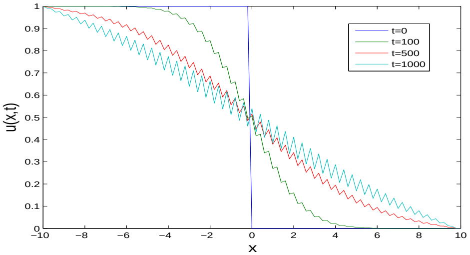
The weight $\sigma = 1$ – an implicit (therefore unconditionally stable) scheme.

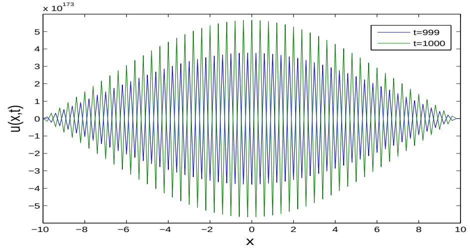
The weight $\sigma = 0$ – an explicit scheme.

Stability condition (CFL):

$$\frac{D\tau}{h^2} \leq \frac{1}{2}.$$

Examples of instability





Implicit and semi-implicit FD schemes

- Fully implicit scheme (backward difference)

$$\frac{1}{\tau}(u_i^{n+1} - u_i^n) = \Lambda[u_i^{n+1}] = \frac{D}{h^2}(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1})$$

- Unconditionally stable scheme

- Higher computational cost (matrix inversion at each time step)

- The order of approximation is $O(\tau + h^2)$

Implicit and semi-implicit FD schemes

- Crank-Nicolson scheme

$$\frac{1}{\tau}(u_i^{n+1} - u_i^n) = \Lambda[\frac{1}{2}u_i^{n+1} + \frac{1}{2}u_i^{n+1}],$$

$$\Lambda[v_i] = \frac{D}{h^2}(v_{i+1} - 2v_i + v_{i-1}).$$

- Unconditionally stable scheme

- Higher computational cost (matrix inversion at each time step)

- The order of approximation is $O(\tau^2 + h^2)$

Calculation of trap counts

- The trap count over time t is

$$\Delta U(t) \;=\; \int_0^t j(\tau) d\tau \;,$$

where $j(t)$ is the absolute value of the population density flux through the trap boundary,

$$j(t) \;=\; D \left| \frac{\partial u(x,t)}{\partial x} \right|_{x=0} .$$

First order approximation (for any fixed $t = t_n$):

$$\frac{du(x_i)}{dx} = \frac{u_{i+1} - u_i}{h} + O(h).$$

Calculation of trap counts: second order approximation

$$j(x) \approx D\left|\frac{du(x)}{dx}\right|$$

$$u(x) \approx p_k(x) = a_0 + a_1 x + a_2 x^2$$

$$j(0) \approx D|a_1|$$

We have

$$p(0) = a_0 = u_1, \quad p(h) = a_0 + a_1 h + a_2 h^2 = u_2,$$
$$p(2h) = a_0 + 2a_1 h + 4a_2 h^2 = u_3$$

As $u_1 = 0$, the approximation of the flux is given by

$$j(0) \approx \frac{D}{2h}|4u_2 - u_3|.$$

Calculation of trap counts

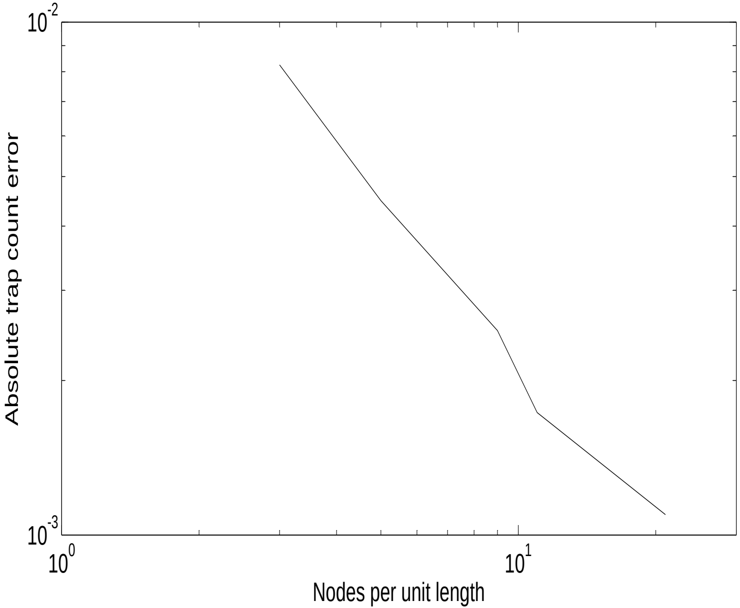
$$j(0) \approx \frac{D}{2h}|4u_2 - u_3|.$$

- The total number of insects $\Delta U^{n,n+1}$ crossing the trap boundary between time t_n and t_{n+1} is obtained as $\Delta U^{n,n+1} = j(0)\tau$ (the midpoint rule of integration).

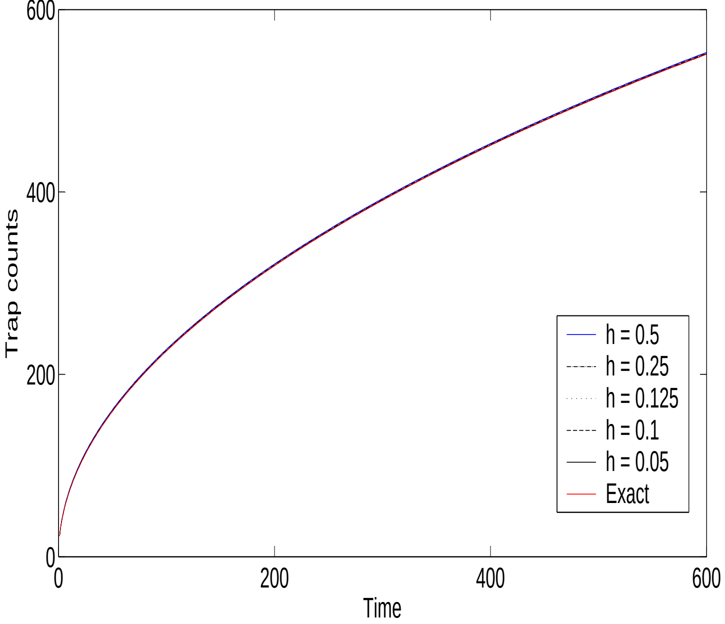
- The cumulative trap count $\Delta U(t_{n+1}) = \Delta U^{n+1}$ at time t_{n+1} is then computed by adding this value to that obtained at the previous time t_n:

$$\Delta U^{n+1} = \Delta U^n + \Delta U^{n,n+1}.$$

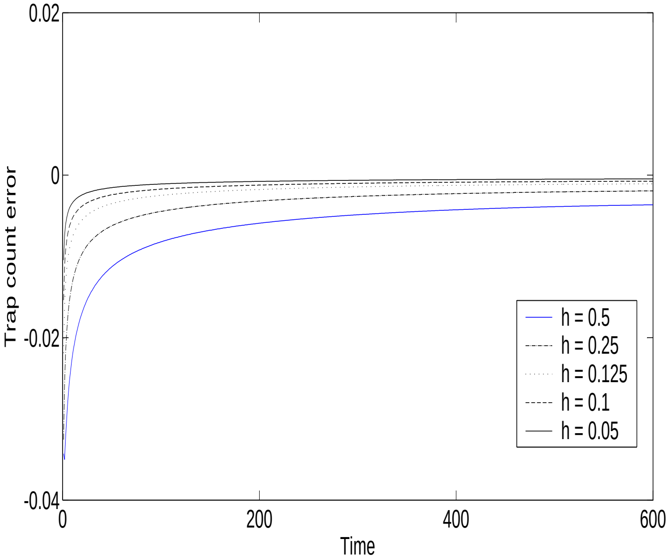
Validation of computations



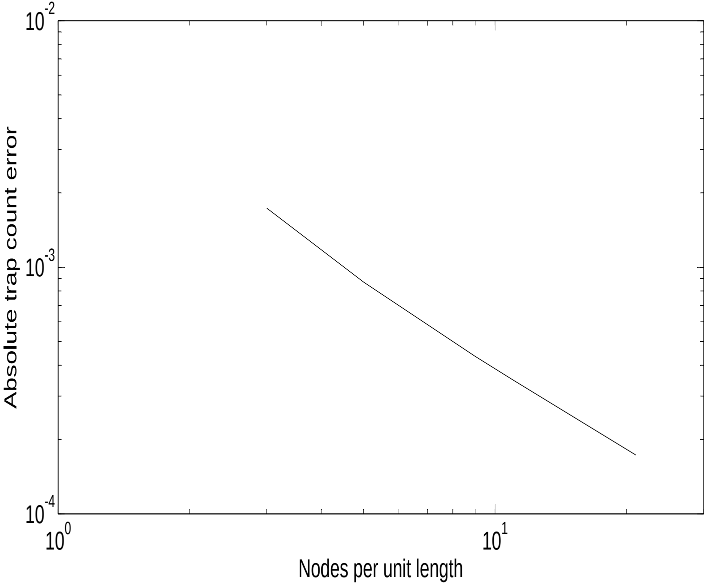
Validation of computations



Validation of computations



Validation of computations



References

- S.V.Petrovskii, N.B.Petrovskaya, D.Bearup. *Multiscale Approach to Pest Insect Monitoring: Random Walks, Pattern Formation, Synchronization, and Networks.* Physics of Life Reviews, 2014, doi: 10.1016/j.plrev.2014.02.001
- J.C.Strikwerda. *Finite Difference Schemes and Partial Differential Equations.* Brooks/Cole Publishing, Pacific Grove, CA, 1989.
- J.W. Thomas. *Numerical Partial Differential Equations.* Springer-Verlag, NY, 1995.

Finite difference discretization

of a $2-D$ diffusion equation

The 2-D diffusion model

Equation:

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right).$$

Boundary condition at the trap boundary:

$$u(x, y, t) = 0 \quad \text{for any} \;\; (x, y) \in \partial S.$$

Boundary condition at the external boundary:

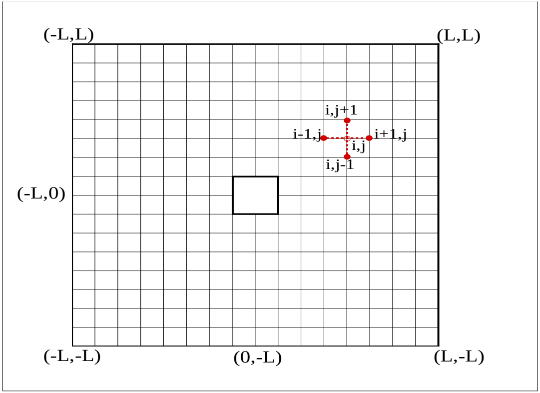
$$\frac{\partial u(x, y, t)}{\partial \mathbf{n}} = 0 \quad \text{at} \;\; \partial\Omega.$$

Initial condition:

$$u(x, y, t) = U_0 > 0 \;\; \text{for any} \;\; (x, y) \in \Omega_s.$$

2-D computational grid

- a uniform grid in the domain $x \in [-L, L]$, $h = L/Nm$
- a uniform grid in the domain $y \in [-L, L]$, $h = L/Nm$
- a uniform grid in the domain $t \in [0, T]$, $\Delta t = T/M$



FD discretization of the $2-D$ problem

Let $u_{ij}^n \equiv u(x_i, y_j, t_n)$ and $u_{ij}^{n+1} \equiv u(x_i, y_j, t_{n+1})$.

FD discretization of the equation:

$$\frac{1}{\tau}(u_{ij}^{n+1} - u_{ij}^n) = (\Lambda_1 + \Lambda_2)[u_{ij}^n],$$

where

$$\Lambda_1[v_{ij}] = \frac{D}{h^2}(v_{i+1,j} - 2v_{ij} + v_{i-1,j}),$$

$$\Lambda_2[v_{ij}] = \frac{D}{h^2}(v_{i,j+1} - 2v_{ij} + v_{i,j-1}).$$

FD discretization of the 2-D problem

The boundary condition at the trap boundary:

$$u_{ij}^{n+1} = 0,$$

for $i = i_I, j = j_I, \ldots, j_{II}$ (the left boundary of the trap),
$i = i_{II}, j = j_I, \ldots, j_{II}$ (the right boundary of the trap),
$j = j_I, i = i_I, \ldots, i_{II}$ (the bottom boundary of the trap),
$j = j_{II}, i = i_I, \ldots, i_{II}$ (the top boundary of the trap)

The boundary condition at the external boundary $x = 0$:

$$\frac{h^2}{\tau D}\left(u_{1,j}^{n+1} - u_{1,j}^{n}\right) + 4u_{1,j+1}^{n} - 2u_{2,j}^{n} - u_{1,j+1}^{n} - u_{1,j-1}^{n} = 0,$$

for $j = 2, \ldots, 2Nm$ (similar b.c. at the rest of the external boundary)

The initial condition:

$$u_{ij}^{0} = U_0, \quad i = 1, 2, \ldots, 2Nm + 1, \; j = 1, 2, \ldots, 2Nm + 1.$$

2-D challenges

- Increasing complexity of programming
- Time consuming computation: 1 node = 1 second $\rightarrow N$ seconds (a $1 - D$ problem) vs. $N * N$ seconds (a $2 - D$ problem)
- Geometry challenges:
  - discretization at the corners;
  - a curvilinear boundary is a realistic option (unstructured grids, finite element discretization);

References

- G. Gordon, G.D.Smith. *Numerical Solution of Partial Differential Equations: Finite Difference Methods.* Oxford University Press, 1985.
- K.W.Morton, D.F.Mayers. *Numerical Solution of Partial Differential Equations. An Introduction.* Cambridge, Cambridge University Press, 1994.
- D. Bearup, N.B.Petrovskaya, S.V.Petrovskii. *Some Analytical and Numerical Approaches to Understanding Trap Counts Resulting from Pest Insect Immigration.* (submitted to Mathematical Biosciences)

More examples of PDEs in ecology: reaction-diffusion equations

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + f(u, x, y).$$

Reaction-diffusion equations describe the following ecological phenomena (see the ref. below)

- the existence of a minimal patch size necessary to sustain a population
- the propagation of wavefronts corresponding to biological invasions
- the formation of spatial patterns in the distributions of populations in homogeneous environments

C.Cosner. *Reaction-diffusion equations and Ecological Modeling.* *in Tutorials in Mathematical Biosciences IV: Evolution and Ecology, Avner Friedman (ed.), Springer, 2008*

Course overview:

anything else?

Topics for self-study: numerical linear algebra

- Matrix computations
- Solving linear systems of algebraic equations
- Finding eigenvalues