MATH60025 Computational PDEs

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Transcribed by a muppet from Sesame Street

1 Info

Office Hours: HXLY 734

LeVeque, Randall J., Finite difference methods for ordinary and partial differential equations: steady-state and time-dependent problems.

Smith, G.D., Numerical solution of partial differential equations: Finite difference methods.

Contents:

- Introduction: How can we solve PDEs on a computer? Finite Difference Methods. Basic types of PDEs. Well-posedness and the importance of Boundary Conditions.
- Parabolic equations: Explicit and Implicit Schemes. Maximum principle and analysis.
- Elliptic equations: Iterative methods: How can they be made faster? Jacobi, Gauss-Seidel, relaxation techniques. Multigrid methods and motivation and implementation.
- Hyperbolic equations: characteristics, upwinding, Lex-Wendroff schemes. Non-reflecting boundary conditions, perfectly matched layers.
- Combinations, Extensions and Applications: *e.g.*advection/diffusion and Navier-Stokes

2 Brief motivation

Wave equation: u is a function of x and t. The notation u_t denotes the partial derivative with respect to t whilst holding all other variables (in this case, x) constant. c is a fixed real constant, known as the wave speed. If it's positive, information progresses in a certain direction over time. If it's negative, it goes in the other direction.

$$u_t + cu_x = 0 \tag{2.1}$$

There's also a second order form:

$$u_{tt} - c^2 u_{xx} = 0 \tag{2.2}$$

This represents data that can propogate in both directions at the same time. Or in higher dimensions:

$$u_{tt} - c^2 \nabla^2 u = 0 \tag{2.3}$$

Burgers equation:

$$u_t + cuu_x = 0 \tag{2.4}$$

and its viscous counterpart. The new term is known as a diffusion or viscosity term. The equation represents a sort of competition between the shock term cuu_x and the smoothing term vu_{xx}.

$$u_t + cuu_x = vu_{xx} \tag{2.5}$$

Recall that this equation has some interesting behaviour: it can generate discontinuities, or shocks. Diffusion/heat equation. κ represents the thermal conductivity. Again, we may generalise this equation to higher dimensions by replacing the u_{xx} term with the laplacian:

$$u_t = \kappa u_{xx} \tag{2.6}$$

$$u_t = \kappa \nabla^2 u \tag{2.7}$$

Laplace/Poisson equation:

$$\nabla^2 u = 0 \tag{2.8}$$

$$\nabla^2 u = f \tag{2.9}$$

Laplace's equation is a special case of Poisson's equation, when the inhomogenous term f is equal to zero.

Maxwell's equations: electromagnetism:

$$\nabla \cdot \tag{2.10}$$

Black-Scholes Model (Finance):

Navier-Stokes Equations: no, absolutely not.

2.1 Finite differences in 1D and 2D and so on

Lets suppose we want a function on an interval $[a, b]$. Well too bad. We're on a computer so we can only get a set of points, with a discretisation of gap $h = \frac{b-a}{N-1}$ between points.

In a 2D and so on, we approximate on a mesh of some kind.

Now that we have a finite approximation, what are the derivatives?

$$\frac{\mathrm{d}u}{\mathrm{d}x}, \frac{\partial u}{\partial x_1} \tag{2.11}$$

$$1 \tag{2.12}$$

Well, we are going to use finite differences. Just truncate the definition of the derivative with a small, finite h instead. Could be forward finite difference, backward finite difference, central finite difference.

How to derive those formulas? Just use the Taylor series.

Definition 2.1. Forward difference: $\Delta x_n = x_{n+1} - xn$
Backward difference: $\nabla x_n = x_n - xn - 1$
Averaging operator: $\mu x_n = \frac{1}{2}(x_{n+\frac{1}{2}} + x_{n-\frac{1}{2}})$
Central difference:
Central difference:

You can do the same thing with 2nd order derivatives, etc. Have fun.

Alternatively, use the method of undetermined coefficients.

Solve $u_x = ux > 0$ and $u(0)$ with finite difference.

3 2 points

2 point formulae: Forward Difference: order h accuracy. Backward Difference: order h accuracy as well. Central difference: order h^2 accuracy.

Second order: $[1, -2, 1]$ order h^2 accuracy.

Finite differences formula via Lagrange interpolation: 1: interpolation of the data point by a polynomial of appropriate degree

2:Exact differentiation of the polynomial interpolant and 3: Evaluation of the differentiated interpolant at the desired grid point.

4 boundary condition stuff

Types of boundary conditions (again): Dirichlet boundary condition: $u(x) = a$ also known as setting the value of u at the boundary. Neumann boundary condition: $\frac{\mathrm{d}u}{\mathrm{d}n} = a$ also known as setting the value of the normal derivative. In one dimension, this is just $\frac{\mathrm{d}u}{\mathrm{d}x}$. Robin/Mixed boundary condition: could be $\frac{\mathrm{d}u}{\mathrm{d}x} + \gamma u = g$. Mixture, as it literally says.

5 Finite partial derivatives

We have a grid instead of a set of points. (image to be drawn :D) Discretise:

$$\frac{\partial^2}{\partial x \partial y} = \frac{\partial}{\partial x}\frac{\partial}{\partial y} \tag{5.1}$$

And individually replace the new partial derivatives with their 1D approximations to get the result.

6 Classification of 2nd order Quasi-linear PDEs in 2 variables

There are 3 main categories of problems:

- Equilibrium - BVP
- Eigenvalue (not covered in this course)
- Propogation - IVP

For example, an equilibrium problem could be solving the Poisson equation in some domain D. We would then specify the conditions on the outer boundary $e.g. u = g$ on ∂D. In more complicated problems, you could specify the normal derivative on the boundary instead (recall Dirichlet and Neumann conditions).

If the domain D is bounded, this is called an interior problem. There are also ones in unbounded domains, which is generally much harder to deal with.

Boundary value problems are generally **Elliptic PDEs**.

In contrast, a propogation problem are generally initial value problems, where you specify some initial state and have some constraints along the way.

Comparison: if you change a bit of the boundary condition in an Elliptic PDE, the change is felt instantly everywhere inside of the domain. In constrast, if you change a bit of the initial data, the change isn't felt until some time when the information has time to travel.

There are two classes of propogation problems: **Parabolic and Hyperbolic PDEs**.

6.1 Well-posedness of PDEs

Solution exists, solution is unique, solution function varies continuously based on the initial data.

6.2 wt

Basic first order PDE

$$\alpha u_x + \beta u_y = g(x, y) \tag{6.1}$$

First order PDE.

$$u_{xx} - u_{yy} + bu_x + cu_y = g(x, y, u) \tag{6.2}$$

Second order PDE.

Semilinear, Quasilinear, aaaaaaaaaaa etc. etc. etc.

Consider a general second order PDE

$$au_{xx} + bu_{xy} + c_{yy} = f \tag{6.3}$$

where

$$f = du_x + eu_y + hu + g \tag{6.4}$$

the *abc* are functions of x, y, u, u_x, u_y so that we remain at least quasilinear.

Suppose we know u, u_x, u_y along some curve in xy space. Then from a point p we move a small vector displacement dx, dy. Can we continue the solution to the new point q?

$$du = u_x dx + u_y dy \tag{6.5}$$

$$d(u_x) = u_{xx} dx + u_{xy} dy \tag{6.6}$$

$$d(u_y) = u_{xy} dx + u_{yy} dy \tag{6.7}$$

Along with the PDE, we end up with 3 equations which can be solved in a matrix form. You end up with

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{b \pm \sqrt{b^2 - 4ac}}{2a} \tag{6.8}$$

Be careful: the sign of b is not $-b$ as in the usual quadratic formula! If there are 2 real roots, it is hyperbolic. If there is 1 root, it is parabolic. Else if there is no real roots it is elliptic.

7 Heat Equation

$$u_t = u_{xx} \tag{7.1}$$

Explicit method: initial value problem.

$$u_n^{i+1} = ru_{n-1}^i + (1 - 2r)u_n^i + ru_{n+1}^i \tag{7.2}$$

Maximum principle Analysis: $O(k)$, $O(h^2)$. A log graph of the errors should be a linear line, with a slope of 1. If you kept the timestep fixed but reduced the spatial errors, the linear line would have slope 2.

Fourier Stability Analysis: $r \leq \frac{1}{2}$.

Let's solve a 3D problem now.

$$u_t = u_{xx} + u_{yy} \tag{7.3}$$

Your 100 data points in x, and 100 data points in y becomes 10000 points which you have to march in time. It gets worse with more dimensions, but still within reachability. Still limited by $r \leq \frac{1}{2}$.

7.1 Implicit Method

Approximate $u_t \approx \frac{u_n^{i+1} - u_n^i}{k}$. $u_{xx} \approx \frac{u_{n-1}^{i+1} - 2u_n^{i+1} + u_{n+1}^{i+1}}{h^2}$. This is $O(k), O(h^2)$.

Scheme 2: we can keep u_t as before but change u_{xx} to be the average of the finite difference between the explicit and implicit methods. Effectively the midpoint of the solution. Since the scheme. This is $O(k^2), O(h^2)$, called the theta method, where $\theta = \frac{1}{2}$. We can change $\theta = 0$, which is the explicit method, and $\theta = 1$ which is the implicit scheme described before. (Technically speaking, theta method is an implicit scheme, since it contains a bit of the future terms.)

8 Nonlinear BVP equation

$$u_t = u_{xx} + f(u) \tag{8.1}$$

- Explicit approach:

$$\frac{u_n^{j+1} - u_n^j}{k} = \frac{u_{n+1}^j - 2u_n^j + u_{n-1}^j}{h^2} + f(u_n^j) \tag{8.2}$$

  with $r \leq \frac{1}{2}$.

- $\theta = \frac{1}{2}$
$$u_n^{j+1} - u_n^j = \frac{1}{2} r \left(s^2 u_n^j + s^2 u_n^{j+1} \right) + \frac{1}{2} k \left(f(u_n^j) + f(u_n^{j+1}) \right) \tag{8.3}$$
nonlinear terms f can be approximated with taylor series, which has linearised it.

Boundary conditions: Dirichlet conditions: impose values on field. Neumann conditions: impoves values of normal derivative instead. Periodic conditions suppose you have a PDE on an interval $[a, b]$. The periodic condition is $u(a) = u(b)$ and $u_x(a) = u_x(b)$ matching derivatives as well. How to do this?

If we discretise, name the points $u[1]$ and $u[n]$. Then $u[1] = u[n]$. We also have $u[2] = u[n+1]$ even though point $n+1$ doesn't actually exist. Similarly $u[-1] = u[n-1]$. Once we have this, we can impose the finite difference on either side to be the same to impose the second boundary condition.

9 Multigrid Methods

We wish to solve $A_F u_F = b_F$ on a fine grid, and we have a coarse grid with half the points on each axis at our disposal.

- Gauss-Seidel sweeps on F to get rid of the short waves, obtaining an approximation u_F.
- Calculate the residual $r_F = A_F u_F - b_F$
- transfer to the coarse grid C using a restriction operator to find r_C.
- On the coarse grid, we calculate the error z_C where $A_C z_C = r_C$ quickly since it's coarse.
- Interpolate this back into z_F
- modify the fine estimate by taking the new estimate as $u_F + z_F$
- repeat. This new iteration will have a few short wave errors, which will be filtered out by the first step.

10 Hyperbolic PDEs

Fourier mode:
$$u_k^n = \hat{u} e^{i(n\omega\Delta t + \alpha k \Delta x)} \tag{10.1}$$

11 Systems of PDEs

Let us have a matrix A which is constant, and consider the PDE
$$u_t + A u_x = 0 \tag{11.1}$$
We 'd like to generalise the upwinding method to this problem. Diagonalise A into a form $A = SDS^{-1}$.

Then let us have $u = Sv$. Thus v satisfies
$$(v_i)_t + \lambda_i (v_i)_x = (S^{-1} * \mathbf{d})_i \tag{11.2}$$

12 Lax-Wendroff method