MTH 453-553 Spring 2018
Class notes

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Introduction and Overview

These notes are intended to supplement rather than replace any textbook material or material covered in lectures.
Examples will be worked out in class.

I will use material from several references

- [RJL]. R.J. LeVeque, Finite Difference Methods for ODEs and PDEs, SIAM 2007
- [IK] Isaacson, Keller, Analysis of Numerical Methods
- [QV] Quarteroni, Valli, Numerical Approximation of Partial Differential Equations, Springer, Second Ed., 1997

The purpose ... (by Richard Hamming)

- "The purpose of computing is insight, not numbers"
- "The purpose of analysis is to solve problems, not create pretty theorems"

PDE types

Consider $u = u(t, x, y, \ldots)$, or $u : \Omega \in \mathbb{R}^n \to \mathbb{R}$ which solves

$$F(u, u_t, u_x, u_y, \ldots, u_{tx}, u_{ty}, u_{tt}, u_{xx}, u_{yy}, u_{xy}, \ldots) = 0 \quad (1)$$

1. The PDE (1) must be supplemented with appropriate boundary and/or initial conditions on $\partial\Omega$. We will consider BVP, IVP, and IBVP.
2. Does the solution to (1) (with the additional conditions) exist? Is it unique? How does it depend on its data? Is the problem well-posed?
3. What is the qualitative nature of solutions and their regularity?
4. In principle, higher order PDEs can be converted to systems of lower order, but this does not help much in analysis/solving except in special circumstances.
5. Numerical methods have to honor the behavior.

Suggested review/reading: Guenter/Lee text; other MTH 621- or MTH 4/582.*

Examples of PDEs of canonical types and not

Recognize . . .

Order, linear/nonlinear, what conditions (BVP, IVP, IBVP) needed.
Application/name ?

$$u_t + au_x = 0; \;\; u_t + uu_x = 0; \;\; u_t + (\frac{u^2}{2})_x = 0; \;\; u_t + (u_x)^2 = 0 \tag{2}$$

$$-u_{xx} - u_{yy} = 0; \;\; -\Delta u = f; \tag{3}$$

$$u_t - u_{xx} = 0; \quad u_t - \nabla \cdot (k(x,y)\nabla u(x,u)) = f; \tag{4}$$

$$u_t - \nabla \cdot (k(u)\nabla u) = 0; \tag{5}$$

$$u_t + au_x - ku_{xx} = f(u), \; u_t + \nabla \cdot g(u) - \nabla \cdot (k(x,y,u)\nabla u) = f(u) \tag{6}$$

$$u_{tt} - u_{xx} = 0; \;\; u_{tt} + u_t = \Delta u \tag{7}$$

$$-\mu \Delta u = -\nabla p, \; \nabla \cdot u = 0, \;\; \text{or} \;\; u_t - u \cdot \nabla u - \mu \Delta u = -\nabla p, \; \nabla \cdot u = 0 \tag{8}$$

NOT (just) PDEs:

$$u_t + \int_0^t e^{-(t-s)} u_t(s) ds - u_{xx} = 0 \tag{9}$$

$$u_t + \int_\Omega k(x) u(x) dx - u_{xx} = 0 \tag{10}$$

What we have covered in other classes

MTH 452/552, Basic methods for BVP and IVP

- BVP solvers for $-u'' = f$:
  - Approximate as $-(D_h^2 U)_j = f_j$; apply BC, solve linear system
  - Error analysis for BVP solvers:
    Consistency & Stability ≡ Convergence
    LTE of $O(h^p)$ & Bounds for $\| A^{-1} \|_* \equiv \| E_h \|_\dagger = O(h^p)$.
  - Norm choice † depends on $*$ and p
- IVP solvers for $u' = f(t, u)$: single-step and LMM methods

What we have not covered

- Non-Dirichlet BC; higher order methods, non-uniform grids
- How to extend to BVP in $\Omega \subset \mathbb{R}^d, d > 1$; $-\nabla \cdot (K \nabla u) = f$
- How to treat IBVP, e.g., for $u_t - u_{xx} = f$
- How to solve large sparse linear systems (see MTH 451-551)

Outline of class

- Two-point BVP, general BC, variable coefficients

  Recall 4/552 material; expand the theory, implementation, and applications
- Laplace equation $-\Delta u = 0$ and more generally $-\nabla \cdot (K \nabla u) = f$
- Heat (diffusion) equation $u_t - \Delta u = f$
- Wave equation $u_{tt} - \Delta u = 0$
- Advection/transport equation $u_t + au_x = 0$
- Other: in particular, ADR $u_t + au_x - du_{xx} = f(u)$.

Methods, math/ implementation/ applications content

We will focus on FD (finite differences). However, other methods such as FE (finite elements), and spectral methods will be mentioned.

`Code templates will be provided.`

We will study, as always, consistency, stability, convergence.

Interplay of discretization in t and x will be important.

Recall the two-point BVP (MTH 452/552)

Conditions in linear two-point constant coefficient BVP

$$u'' + mu' + nu = f(x), \;\; x \in [a,b]; u(a) = u_a, u(b) = u_b \tag{11}$$

Condition $u(a) = u_a$ is known as Dirichlet condition, $u'(a) = u_b$ is known as Neumann condition, $u'(a) + Cu(a) = u_c$ is known as the Robin condition. One can also impose periodic conditions, e.g., $u(a) = u(b), u'(a) = u'(b)$. If the data equals 0, we call the BC homogeneous.

Example 2.1 (Existence and uniqueness of solutions depending on BC)

Consider $x \in [0,1]$. Find the general solution and determine if the solution exists and if it is unique.
$u'' = 0, u(0) = 0, u(1) = 0$
$u'' = 1, u(0) = 0, u(1) = 0$
$u'' = 1, u'(0) = 0, u'(1) = 0$
$u'' = 1, u(0) = 0, u'(1) = 0$
$u'' = 1, u'(0) + u(0) = 0, u'(1) = 0$
$u'' = 1, u(0) = u(1), u'(0) = u'(1)$
$u'' = u, u(0) = 0, u(1) = 0$
$u'' = u, u(0) = 0, u'(1) = 0$
$u'' = -u, u(0) = 0, u(1) = 0$

Numerical solution of two-point BVP (11)

1. Define a grid on $[a, b]$. Easiest is uniform grid $a = x_0, x_1, \dots x_M = b$. Here $h = \frac{b-a}{M}$, and $x_j = a + jh$.
2. Discretize. (Replace $u''(x)$ by $D_h^2 u(x) = \frac{u(x+h)-2u(x)+u(x-h)}{h^2}$, and other derivatives by difference quotients.)
3. Write the discrete equation to be satisfied by U^{j-1}, U^j, U^{j+1} at every interior node t_j
4. Apply BC to U^0 and U^M
5. Collect all unknowns in $U = [U^0, U^1, \dots U^{M-1}, U^M]^T$, and right-hand side in $F = [f_0, f_1, f_2, \dots f_{M-1}, f_M]^T$. The entries f_0, f_M will be given from boundary conditions.
6. Identify the coefficients in steps 2,3 as components of a matrix A
7. Solve the linear system $AU = F$

Remark 1 (MATLAB numbering)

The nodes and unknowns above are numbered from $0, 1, \dots M$. *MATLAB does not allow indexing from 0, so the unknowns in your code will likely be numbered* $U^1, \dots U^{M+1}$. *The principles remain the same.*

Example: $-u'' = f$ on $[a,b]$ with Dirichlet BC $u(a) = u_a, u(b) = u_b$

Example 2.2 (Derive and solve the discrete system of equations)

Decide on M and h, $h = \frac{b-a}{M}$.
Equation for internal nodes and boundary conditions

$$\text{Interior nodes}: \quad \frac{1}{h^2}(2U^j - U^{j-1} - U^{j+1}) = f(t_j), \quad \forall j = 1, \dots M-1 \tag{12a}$$

$$\text{Boundary nodes}: \quad U^0 = u_a, \; U^M = u_b. \tag{12b}$$

Set-up an equivalent system of equations $AU = F$ with

$$A = \frac{1}{h^2}\begin{bmatrix} h^2 & 0 & \dots & 0 & \\ -1 & 2 & -1\dots & & \\ \dots & & & & \\ \dots & & -1 & 2 & -1 \\ \dots & & & & h^2 \end{bmatrix}, \quad F = \begin{bmatrix} u_a \\ f(t_1) \\ \dots \\ f(t_{M-1}) \\ u_b \end{bmatrix}. \tag{13}$$

Solve linear system $AU = F$. In MATLAB, write `U=A\F`

Note the first and last rows in (13) correspond to the boundary conditions, and could be trivially eliminated. The numbering above is not MATLAB-like.

Code for BVP from slide 9

Numbering, again (recall Remark 1)

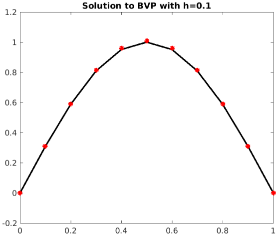
When coding, the interior nodes will be numbered $2, \dots M$, and boundary nodes will be numbered 1 (left boundary) and $M+1$ (right boundary). In particular, when we apply the Dirichlet BC, we write $U(1) = u_a; U(M+1) = u_b$, for the first and last entries of U.

```
dx = (b-a)/(M); x = (a:dx:b)'; %% use uniform grid, x is numbered from 1...M+1
%% set up the matrix and the right hand side vector
f = rhsfun(x);
A = sparse(M+1,M+1);
for j=2:M
    %% set up j'th internal row of the matrix
    A(j,j) = 2; A(j,j-1) = -1; A(j,j+1) = -1;
end
A = A / (dx*dx);
%% apply the Dirichlet b.c. to the matrix and right hand side
A (1,1) = 1; f (1) = ua;
A (M+1,M+1) = 1; f (M+1) = ub;
%% solve the linear system;
U = A \ f;
```

This code can be vectorized for faster performance

Solution to BVP from slide 9

Start assuming an exact solution $u(t) = \sin(\pi t)$.
Calculate (manufacture) $f(t) = \pi^2 \sin(\pi t)$.
Implement the code and plot ...



h	$E(h,\infty)$	$E(h,2)$
0.1	0.008265	0.058
0.05	0.00205871	0.0015
0.01	0.0000822508	0.0000582

Test convergence in L^∞ and L^2 to see that $E(h,*) = O(h^2)$ for each norm; see table.
(See below for a precise definition of norms, and convergence analysis).

Analysis of convergence of FD for BVP

Define $A_h \in \mathbb{R}^{(M-1)\times(M-1)}$ *to be the interior part of the matrix* A *from* (13).

Remark 2 (Error analysis)

Writing the error equation we find $A_h E = \tau$ *where* τ *is the vector of truncation errors* τ_j *(truncation errors on the boundary are 0). Proving convergence*

$$\| E \|_* \to 0, \quad \text{as } h \to 0 \tag{14}$$

requires proving consistency and stability.

Here $*$ *stands for the functional space in which we want to measure the error.*

- Consistency: with D_h^2, the truncation error $\tau_j \approx O(h^2)$ if $u \in C^4$
- Stability: to keep $\| E \|_* = O(h^2)$, we require $\| A_h^{-1} \|_* \leq C$.

Choosing norm

We generally like to use $*$ to be L^∞ space, but it is easier to get the bound $\| A_h^{-1} \|_{L^2}$.

Vector, matrix, function & grid function norms.

Remark 3 (Vector norms in l_p spaces)

$$\mathbb{R}^d \ni x, \quad \|x\|_p := \left(\sum_j |x_j|^p\right)^{\frac{1}{p}}, \ 1 \le p < \infty. \ \|x\|_\infty = \max_j |x_j| \,. \tag{15}$$

Remark 4 (Norms for functions and grid functions)

For functions $f : [a, b] \to \mathbb{R}$ we extend the l_p vector norms to the norms in Lebesgue spaces L^p of functions for which the integral below is well defined and finite

$$\|f\|_p = \left(\int_a^b |f(x)|^p \, dx\right)^{\frac{1}{p}}; \quad 1 \le p < \infty. \quad \|f\|_\infty = esssup_{x \in [a,b]} |f(x)| \,. \tag{16}$$

For grid functions $f : \Delta \to \mathbb{R}$ (sampled on a grid $\Delta = \{x_1, x_2, \ldots x_M\}$) with $1 \le p < \infty$, we approximate these integrals with Riemann sums

$$\|f\|_{\Delta,p} = \left(\sum_j h\,|f(x_j))|^p\right)^{\frac{1}{p}} = h^{\frac{1}{p}} \,\|[f(x_1), \ldots f(x_j) \ldots f(x_M)]^T\|_p \tag{17}$$

The text uses the same symbol $\|\cdot\|_p$ for the norms of vectors in $\mathbb{R}^d$, functions on $\mathbb{R}$, or grid functions. We will use $\|f\|_{\Delta,p}$ for grid functions.

Stability and convergence in the 2-norm

Remark 5 (Recall some matrix norms)

$$\mathbb{R}^{d\times d} \ni A, \qquad \|A\|_1 = \text{“max abs col sum”} = \max_j \sum_i |a_{ij}| \tag{18}$$
$$\mathbb{R}^{d\times d} \ni A, \qquad \|A\|_\infty = \text{“max abs row sum”} = \max_i \sum_j |a_{ij}| \tag{19}$$

The norm $\|A\|_2 = \sqrt{\rho(A^T A)}$, where the spectral radius $\rho(B)$ is the largest to magnitude eigenvalue of matrix B.
For a symmetric real matrix $\|A\|_2 = \rho(A)$.

In MTH 452-552 we proved stability of FD solution to the two-point Dirichlet BVP...

We have proved that $\|A_h^{-1}\|_p \leq C$ for $p = 2, \infty$.
From this it follows for $E = A_h^{-1}\tau$ that

$$\|E\|_{\Delta,2} = \sqrt{h}\,\|E\|_2 \leq \sqrt{h}\,\|A_h^{-1}\|_2\,\|\tau\|_2 = \sqrt{h}CO(h^2)\sqrt{M} = O(h^2) \tag{20}$$
$$\|E\|_{\Delta,\infty} = \|E\|_\infty \leq \|A_h^{-1}\|_\infty\,\|\tau\|_\infty \leq CO(h^2) = O(h^2) \tag{21}$$

Two-point BVP; Neumann boundary conditions

Consider $-u'' = f, \;\; x \in (a,b); u(a) = u_a, u'(b) = g_b$.

To discretize, we modify (12b) in (12)

$$\text{Interior}: \quad \frac{1}{h^2}(2U^j - U^{j-1} - U^{j+1}) = f(t_j), \;\; \forall j = 1, \dots M-1 \qquad (22a)$$

$$\text{Boundary}: \quad U^0 = u_a, \; (D_h^* U)_M = g_b. \qquad (22b)$$

We have to choose the difference operator $(D_h^* U)_M$.

- One-sided $(D_h^* U)_M = \frac{U^M - U^{M-1}}{h} = g_b$, which is $O(h)$ accurate
- Two-sided $(D_h^* U)_M = \frac{U^{M+1} - U^{M-1}}{2h} = g_b$, which is $O(h^2)$, but introduces an additional unknown U^{M+1} and requires an additional equation (e.g., we can write (22a) for $j = M$).
- One-sided second order approximation (recall from MTH 4/552).

After the choice is made, write the system (22) as $AU = F$.

When choosing D_h^*, note: if one can ensure that the system $AU = F$ has a symmetric matrix A, (i) proofs of stability in L^2 are much easier, and (ii) iterative linear solvers for sparse systems "like" spd A.

Variable coefficients

Consider $-(ku')' = f, x \in (a,b), u(a) = u_a, -(ku')(b) = q_b$.

Do it right

1. It is a BAD idea to apply the product rule to this problem.
2. Instead, we first discretize $(D_h U)_{j\pm 1/2}$ at each point $x_{j\pm 1/2}$, calculate $k(x_{j\pm 1/2})(D_h U)_{j\pm 1/2}$, and apply D_h again.

The analogue of (22a) is now

$$-\frac{1}{h}\left(k(x_{j+1/2})\frac{U^{j+1}-U^{j}}{h} - k(x_{j-1/2})\frac{U^{j}-U^{j-1}}{h}\right) = f(x_j) \qquad (23)$$

Next we discretize the flux condition $-(ku')(b) = q_b$ with, say, one-sided approximation.
Finally we set up the system $AU = F$, and solve.

Ex.: Attempt LTE analysis assuming $k(x)$ is smooth. Also, write the linear system to be solved