CS520: PDE difference methods (Ch. 3)

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Outline

- Semi-discretization
  - Discretizing derivatives
  - Staggered meshes and finite volumes
  - Handling boundary conditions
- Full discretization
  - Order, stability and convergence
  - General stability

SPATIAL SEMI-DISCRETIZATION

- Consider the linear initial-value PDE

$$\begin{aligned} u_t &= \mathcal{L}u + q, \qquad \mathbf{x} \in \Omega,\ t > 0 \\ u(0,x) &= u_0(x). \end{aligned}$$

- Discretizing on a mesh in space, obtain

$$\begin{aligned} \frac{d}{dt} v_j(t) &= \sum_{i=-l}^{r} \alpha_i v_{j+i}(t) \\ v_j(0) &= u_0(x_j), \quad 1 \le j \le J. \end{aligned}$$

- Leads to a method of lines (MOL), for which techniques from Chapter 2 may be applied.

Spatial semi-discretization: example

- A diffusion problem

$$\begin{aligned} u_t &= u_{xx} + q(x,u), \\ u(0,x) = u_0(x), \qquad & u(t,0) = g_0(t), \ u(t,1) = g_1(t). \end{aligned}$$

- Discretize in space using a uniform mesh width h, obtaining ($l = r = 1$ and $v_j(0) = u_0(jh)$)

$$\frac{dv_j}{dt} = \frac{v_{j+1} - 2v_j + v_{j-1}}{h^2} + q(x_j, v_j), \qquad j = 1, \ldots, J.$$

- Use boundary conditions to close the system, setting $v_0(t) = g_0(t), \ v_{J+1}(t) = g_1(t)$.
- Obtain a mildly stiff initial-value ODE system of size J.

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Difference operator notation

Use the following difference operator notation in space or time:

$$\begin{aligned} D_+ u_j &= u_{j+1} - u_j \quad \text{Forward} \\ D_- u_j &= u_j - u_{j-1} \quad \text{Backward} \\ D_0 u_j &= u_{j+1} - u_{j-1} \quad \text{Long centered} \\ \delta u_j &= u_{j+1/2} - u_{j-1/2} \quad \text{Short centered} \\ \mu u_j &= (u_{j+1/2} + u_{j-1/2})/2 \quad \text{Short average} \\ E u_j &= u_{j+1} \quad \text{Translation.} \end{aligned}$$

Difference operator identities:

$$D_+ = E - I, \; D_- = I - E^{-1},$$
$$D_+ D_- = D_- D_+ = \delta^2,$$
$$\mu^2 = 1 + \delta^2/4, \quad \mu\delta = D_0/2,$$
$$\partial_x = h^{-1} \log E$$

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Formulae for first derivative

- u_x, one-sided:

$$
\begin{aligned}
u_x &= \frac{1}{h}\left(D_+ - \frac{1}{2}D_+^2\right)u + \mathcal{O}(h^2) \\
&= \frac{1}{h}(u_{j+1} - u_j) - \frac{1}{2h}(u_{j+2} - 2u_{j+1} + u_j) + \mathcal{O}(h^2)
\end{aligned}
$$

- Just the first term above leads to the 1st order forward difference.
- u_x, symmetric, centred:

$$
\begin{aligned}
u_x &= \frac{D_0}{2h}\left(I - \frac{1}{6}D_+D_-\right)u + \mathcal{O}(h^4) \\
&= \frac{1}{2h}(u_{j+1} - u_{j-1}) - \frac{1}{12h}(u_{j+2} - 2u_{j+1} + 2u_{j-1} - u_{j-2}) + \mathcal{O}(h^4)
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- Just the first term above leads to the 2nd order centred difference.

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Formulae

- u_{xx}, symmetric, centred:

$$u_{xx} = \frac{1}{h^2}\left(\delta^2 - \frac{1}{12}\delta^4\right) u + \mathcal{O}(h^4).$$

- Just the first term above leads to the 2nd order centred difference.
- Implicit schemes for discretizing derivatives exist as well, e.g. to obtain 4th order accurate 3-point formulae.
- For explicit scheme, need polynomial of degree l for lth derivative. So, at least $l+1$ points must be used. If exactly $l+1$ points are used, the scheme is compact. *This is a desirable property.*

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Compact schemes

In general, we want as narrow a discretization stencil as possible, because:

- Generally, boundary conditions are more easily incorporated.
- Occasionally, unwanted spurious solution behaviour is avoided.

  e.g., for $u_x = \frac{u_{j+1} - u_{j-1}}{2h}$, consider a sinusoidal fluctuation

  $$\{u_j\} = 0, 1, 0, -1, 0, 1, 0, -1, \ldots .$$

  Then on a coarser mesh consisting of only the odd mesh points, u_x is approximated by identically 0.

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Staggered meshes

To avoid using long differences, consider unknowns corresponding to different solution components to be located at different meshes: It's all in our head

Example: diffusion equation in 1D

$$u_t = (a(x)u_x)_x + q(t,x), \quad x \in \Omega, \; t \ge 0.$$

Do not write $(au_x)_x = au_{xx} + a_x u_x$! Define flux $w = au_x$ and discretize:

$$a(x_{j+1/2})\frac{v_{j+1} - v_j}{h} = w_{j+1/2},$$
$$\frac{dv_j}{dt} = \frac{w_{j+1/2} - w_{j-1/2}}{h} + q(t, x_j).$$

Eliminating w-values yields the semi-discretization

$$\frac{dv_j}{dt} = h^{-1}\left[a(x_{j+1/2})\frac{v_{j+1} - v_j}{h} - a(x_{j-1/2})\frac{v_j - v_{j-1}}{h}\right] + q(t, x_j).$$

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Integrate then discretize (finite volume)

- Write the diffusion equation as

$$
\begin{aligned}
u_x &= a(x)^{-1} w, \\
u_t &= w_x + q(t,x).
\end{aligned}
$$

- Integrating first equation from x_j to x_{j+1} and using midpoint, obtain

$$v_{j+1} - v_j = h a_{j+1/2}^{-1} w_{j+1/2}.$$

- Integrating second equation from $x_{j-1/2}$ to $x_{j+1/2}$ and using midpoint, obtain

$$v_j' = h^{-1} \left(w_{j+1/2} - w_{j-1/2} \right) + q_j(t).$$

- Substituting, obtain

$$v_j' \equiv \frac{dv_j}{dt} = h^{-2} \left[a_{j+1/2} \left(v_{j+1} - v_j \right) - a_{j-1/2} \left(v_j - v_{j-1} \right) \right] + q_j(t).$$

When is this important?

The finite volume approach becomes important when one of the following occurs:

- The function $a(x)$ has discontinuities.
- The function $q(t, x)$ is a point source, i.e., a δ-function, in x.
- We wish to extend the discretization to a nonuniform spatial mesh.

Discontinuous coefficients

$$\frac{dv_j}{dt} = h^{-1}\left[a_{j+1/2}\frac{v_{j+1}-v_j}{h} - a_{j-1/2}\frac{v_j - v_{j-1}}{h}\right] + q(t, x_j).$$

As before, but how should $a_{j+1/2}$ be defined?

Harmonic averaging: define $a_{j+1/2}$ by

1. integrating $u_x = a^{-1}(x)w$, and
2. discretizing (note w is smoother than a and u_x):

$$\text{ideally } a_{j+1/2} = h\left[\int_{x_j}^{x_{j+1}} a^{-1}dx\right]^{-1}$$

$$\text{often must use } a_{j+1/2} = \left[\frac{a_j^{-1} + a_{j+1}^{-1}}{2}\right]^{-1}$$

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Point source

If

$$q(t,x) = \delta(x - x_*), \quad x_{i_*-1/2} \le x_* < x_{i_*+1/2}$$

where

$$q(t,x) = 0 \text{ if } x \neq x_*, \quad \int_\Omega q(t,x)dx = 1,$$

then integrating as before, orbtain

$$\frac{dv_j}{dt} = h^{-1}\left[a_{j+1/2}\frac{v_{j+1}-v_j}{h} - a_{j-1/2}\frac{v_j - v_{j-1}}{h}\right] + hq_j(t)$$

$$q_j(t) = \begin{cases} 1 & \text{if } i = i_*, \\ 0 & \text{otherwise} \end{cases}.$$

More than one space variable

- Discretization principles such as compactness, staggered meshes, and integrate-then-discretize are extended also to 2D and 3D.
- Mesh subintervals are now replaced by mesh cells in 2D or 3D.
- Not everything extends smoothly and effortlessly!
- Consider examples in 2D.

Anisotropic diffusion in 2D

$$u_t = (au_x)_x + (au_y)_y + q \equiv \nabla \cdot (a\boldsymbol{\nabla} u) + q$$

on a square domain $\Omega: \ 0 \le x, y \le 1$.

- If a is constant, easy:

$$\frac{dv_{i,j}}{dt} = \frac{a}{h^2}[-4v_{i,j} + v_{i-1,j} + v_{i+1,j} + v_{i,j-1} + v_{i,j+1}] + q_{i,j}, \quad 1 \le i,j \le J$$

- More generally, rewrite as 1st order system

$$\begin{aligned} u_t &= w^x_x + w^y_y + q = \nabla \cdot \mathbf{w} + q, \\ \mathbf{w} &= a\boldsymbol{\nabla} u. \end{aligned}$$

Integrate first DE over a control volume

$$\frac{dv_{i,j}}{dt} = h^{-1}[w^x_{i+1/2,j} - w^x_{i-1/2,j} + w^y_{i,j+1/2} - w^y_{i,j-1/2}] + q_{i,j}.$$

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Anisotropic diffusion in 2D cont.

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$$w^x_{i+1/2,j} = \int_{y_{j-1/2}}^{y_{j+1/2}} w^x(x_{i+1/2}, y)dy, \quad 1 \le i,j \le J.$$

- For 2nd eqn, e.g. $u_x = a^{-1}w^x$, ($\mathbf{w} = (w^x, w^y)$), integrate in x, but where in y?!
- Obtain

$$\frac{dv_{i,j}}{dt} = h^{-2}[a_{i+1/2,j}(v_{i+1,j} - v_{i,j}) - a_{i-1/2,j}(v_{i,j} - v_{i-1,j}) + a_{i,j+1/2}(v_{i,j+1} - v_{i,j}) - a_{i,j-1/2}(v_{i,j} - v_{i,j-1})] + q_{i,j},$$

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Example: isotropic denoising

- An image is polluted by noise, resulting in $u_0(x, y)$.
- Want to denoise it, i.e., recover u – something close to the original (unavailable) image.
- Isotropic diffusion: Solve

$$\begin{aligned} u_t &= u_{xx} + u_{yy}, \\ u(0, x, y) &= u_0(x, y), \end{aligned}$$

for appropriate t not too small and not too large!
- Difficulty: image edges are indiscriminantly smoothed, too. (Recall integration of heat equation starting with a step function, Fig. 1.4.)

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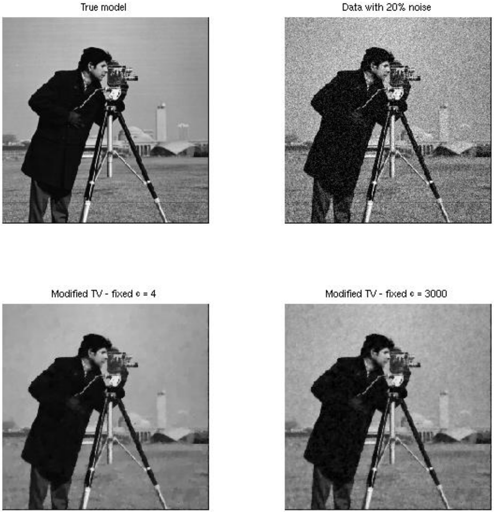
Instance: camera man



Anisotropic denoising

- Smooth only in directions where u does not vary too abruptly!
- One way: total variation (TV).

$$u_t = \nabla \cdot \left(\frac{\nabla u}{|\nabla u|} \right),$$
$$u(0,x,y) = u_0(x,y).$$

- "Like before" with

$$a = a(u) = 1 \,/\, |\nabla u|, \quad \text{where } |\nabla u| = \sqrt{u_x^2 + u_y^2}.$$

(The latter expression is modified in regions where u is very flat.)

- Common choice

$$a_{i+1/2,j} = a_{i,j+1/2} = h\left[(u_{i+1,j} - u_{i,j})^2 + (u_{i,j+1} - u_{i,j})^2 \right]^{-1/2}.$$

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Boundary conditions (BC)

- In 1D

$$\begin{aligned} u_t &= u_{xx}, \qquad 0 \le x \le 1,\ t > 0, \\ & u(0,x) = u_0(x). \end{aligned}$$

Dirichlet BC: $u(t,1) = g_1(t)$
Neumann BC: $\frac{\partial u}{\partial x}(t,0) = g_0(t)$.

- Discretization:

$$\begin{aligned} \frac{dv_j}{dt} &= \frac{v_{j+1} - 2v_j + v_{j-1}}{h^2}, \qquad j = 0, 1, \ldots, J, \\ v_{J+1} &= g_1(t), \\ \frac{v_1 - v_{-1}}{2h} &= g_0(t). \end{aligned}$$

- How to handle the ghost unknown v_{-1}?

Boundary conditions (BC)

- In 1D

$$\begin{aligned} u_t &= u_{xx}, \qquad 0 \le x \le 1,\ t > 0, \\ & u(0,x) = u_0(x). \end{aligned}$$

Dirichlet BC: $u(t,1) = g_1(t)$
Neumann BC: $\frac{\partial u}{\partial x}(t,0) = g_0(t)$.

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Handling Neumann BC

- Concentrate on Numann BC at the left interval end:

$$\frac{dv_0}{dt} = \frac{v_1 - 2v_0 + v_{-1}}{h^2},$$
$$\frac{v_1 - v_{-1}}{2h} = g_0(t).$$

- Eliminate ghost unknown: $v_{-1} = v_1 - 2hg_0(t)$. Substitute into difference eqn at $j = 0$:

$$\frac{dv_0}{dt} = \frac{2v_1 - 2v_0 - 2hg_0(t)}{h^2}.$$

- Alternatively, do not eliminate: solve differential-algebraic equations DAE in time.

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Boundary conditions in 2D

- Consider example: simplest heat equation

$$u_t = u_{xx} + u_{yy}.$$

- Dirichlet, boundary part of grid: extend directly.
- Neumann, boundary part of grid: extend in finite volume fashion. (Often in practice BC is on the flux, w.)
- More complex boundaries: interpolate locally.

Natural and essential BC

- Consider Ritz formulation of elliptic PDE

$$\min_u \int_\Omega \left[a|\nabla u|^2 + bu^2 - 2uq\right] dxdy,$$

$a(x,y) > 0,\ b(x,y) \geq 0.$

- Necessary condition for minimum are the Euler-Lagrange equations

$$\begin{aligned} -\nabla \cdot (a\nabla u) + bu &= q, \quad \text{in } \Omega, \\ \frac{\partial u}{\partial n}|_{\partial\Omega} &= 0. \end{aligned}$$

So Neumann BC are natural!

- More generally, given Neumann (natural) conditions on part of the boundary and Dirichlet (essential) on the rest, in the functional minimization formulation only the essential BC must be explicitly imposed.

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Natural and essential BC cont.

- Can discretize first and only then optimize:

$$\min_v \sum_{i,j=0}^{J} \frac{1}{2}[a_{i+1/2,j}(v_{i+1,j} - v_{i,j})^2 + a_{i+1/2,j+1}(v_{i+1,j+1} - v_{i,j+1})^2$$
$$+ \quad a_{i,j+1/2}(v_{i,j+1} - v_{i,j})^2 + a_{i+1,j+1/2}(v_{i+1,j+1} - v_{i+1,j})^2]$$
$$+ \quad \frac{h^2}{4} \sum_{i,j=0}^{J} [b_{i,j} v_{i,j}^2 - 2q_{i,j} v_{i,j} + b_{i+1,j} v_{i+1,j}^2 - 2q_{i+1,j} v_{i+1,j}$$
$$+ \quad b_{i,j+1} v_{i,j+1}^2 - 2q_{i,j+1} v_{i,j+1} + b_{i+1,j+1} v_{i+1,j+1}^2 - 2q_{i+1,j+1} v_{i+1,j+}$$

- Necessary conditions - equate gradient to $\mathbf{0}$: obtain previous 5-point discretization plus Neumann BC automatically.
- Essential BC are used to move known boundary values to right hand side of linear system.
- Advantage: the obtained matrix is symmetric positive definite!

Natural and essential BC cont.

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$$
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Outline

- Semi-discretization
  - Discretizing derivatives
  - Staggered meshes and finite volumes
  - Handling boundary conditions
- Full discretization
  - Order, stability and convergence
  - General stability

Full discretization

- Explicit one-step scheme

$$v_j^{n+1} = \sum_{i=-l}^{r} \beta_i v_{j+i}^n .$$

- Can write this in (potentially infinite) matrix-vector notation

$$v^{n+1} = Qv^n$$

- Implicit one-step scheme

$$\sum_{i=-l}^{r} \gamma_i v_{j+i}^{n+1} = \sum_{i=-l}^{r} \beta_i v_{j+i}^n ,$$

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$$Q_1 v^{n+1} = Q_0 v^n$$

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Order of accuracy

Local truncation error:

$$\tau(t,x) = k^{-1}\left[\sum_{i=-l}^{r} \gamma_i u(t+k, x+ih) - \sum_{i=-l}^{r} \beta_i u(t, x+ih)\right].$$

Pretend grid function v is defined at every point. Difference method is

- accurate of order (p_1, p_2) if

$$\|\tau(t)\| = \|\tau(t,\cdot)\| \le c(t)\,(k^{p_1} + h^{p_2})$$

- consistent if $\|\tau(t)\| \to 0$ as $k, h \to 0$.

Example: heat equation

For heat equation $u_t = u_{xx}$, discretize in space by centred $\mathcal{O}(h^2)$ scheme. Next, discretize in time:

- Forward Euler

$$\frac{1}{k}(v_j^{n+1} - v_j^n) = \frac{1}{h^2}(v_{j+1}^n - 2v_j^n + v_{j-1}^n)$$

  – order $(1,2)$.

- Crank-Nicolson: apply trapezoidal

$$\frac{1}{k}(v_j^{n+1} - v_j^n) = \frac{1}{2h^2}(v_{j+1}^{n+1} - 2v_j^{n+1} + v_{j-1}^{n+1} + v_{j+1}^n - 2v_j^n + v_{j-1}^n)$$

  – order $(2,2)$ and better stability properties, but *implicit*: must solve a tridiagonal linear system at each time step.

- Backward Euler? – at first glance, combines worst of both worlds, but...

Same methods using operator notation

Set $\mu = k/h^2$.

Forward Euler:

$$v_j^{n+1} = v_j^n + \mu D_+ D_- v_j^n$$

Trapezoidal (CN):

$$v_j^{n+1} = v_j^n + \frac{\mu}{2} D_+ D_- (v_j^n + v_j^{n+1})$$

Backward Euler:

$$v_j^{n+1} = v_j^n + \mu D_+ D_- v_j^{n+1}$$

Stability and convergence

Method is

- *stable* if there are constants $\tilde{K}$ and $\tilde{\alpha}$ such that

$$\|v(t)\| \le \tilde{K} e^{\tilde{\alpha} t} \|v(0)\|.$$

- *convergent* if

$$u(t,x) - v(t,x) \to 0, \qquad k, h \to 0.$$

Lax Equivalence Theorem:
If the linear evolutionary PDE is well-posed and the difference method is consistent then

$$\text{convergence} \iff \text{stability}.$$

In fact, if the method is stable then the solution error inherits the order of accuracy.

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General linear stability

- Generally, with $Q = Q_1^{-1} Q_0$, can write

$$v^{n+1} = Q(nk, h)v^n = \cdots = \Pi_{l=0}^{n} Q(lk, h)v^0 = \mathcal{S}_{k,h}(t_{n+1}, 0)v^0.$$

- The stability condition is

$$\|\Pi_{l=0}^{n} Q(lk, h)\| \le \tilde{K} e^{\tilde{\alpha} nk} \qquad \forall n, k,\ nk \le t_f.$$

- If Q does not depend on t

$$\|Q(h)^n\| \le \tilde{K} e^{\tilde{\alpha} nk}.$$

- This is satisfied if for all k and h small enough,

$$\|Q\| \le e^{\tilde{\alpha} k} = 1 + O(k).$$

Low order terms

- Difficult in general to show that $\|Q^n\| \leq \bar{K}$. Fortunately, can sometimes ignore lower order derivatives:
- Theorem: *If the scheme*

$$v^{n+1} = \hat{Q} v^n$$

is stable and $\tilde{Q}$ *is a bounded operator then the scheme*

$$v^{n+1} = (\hat{Q} + k\tilde{Q}) v^n$$

is stable as well.

- Good for $u_t = u_x + b(x)u$ and for $u_t = u_{xx} + bu$, but not for $u_t = u_{xx} + au_x$.

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