Ordinary and partial differential equations

Victor Eijkhout

335/394 fall 2011

ODEs and PDEs

Time-evolving phenomena: IVP (Initial Value Problem), usually Ordinary Differential Equations

Space-constraint phenomena: BVP (Boundary Value Problem), usually Partial Differential Equations

Ordinary Differential Equations

Numerical treatment of differential equations

Initial value problem: $u'(t) = f(t, u(t)), \qquad u(0) = u_0, \qquad t > 0$

Boundary value problem:
$u''(x) = f(x), \qquad x(0) = x_0, x(1) = x_1, \qquad x \in [0, 1]$

General assumption: f has higher derivatives.

IVP stability: solutions corresponding to different u_0 values converge as $t \to \infty$. Criterium:

$$\frac{\partial}{\partial u} f(t, u) = \begin{cases} > 0 & \mathit{unstable} \\ = 0 & \mathit{neutrallystable} \\ < 0 & \mathit{stable} \end{cases}$$

Simple example: $f(t, u) = -\lambda u$, then $u(t) = u_0 e^{-\lambda t}$;
stable if $\lambda > 0$

proof

Let u^* s.t. $f(u^*) = 0$, then $u(t) \equiv u^*$ is a solution of $u' = f(u)$,

Write solutions as $u(t) = u^* + \eta(t)$, then

$$\begin{aligned} \eta' &= u' = f(u) = f(u^* + \eta) = f(u^*) + \eta f'(u^*) + O(\eta^2) \\ &= \eta f'(u^*) + O(\eta^2) \end{aligned}$$

Ignoring the second order terms, this has the solution

$$\eta(t) = e^{f'(u^*)t}$$

which means that the perturbation will damp out if $f'(u^*) < 0$.

Finite difference approximation

We turn the continuous problem into a discrete one, by looking at finite time/space steps.

Assume all functions are sufficiently smooth, and use Taylor series:

$$u(t+\Delta t) = u(t) + u'(t)\Delta t + u''(t)\frac{\Delta t^2}{2!} + u'''(t)\frac{\Delta t^3}{3!} + \cdots$$

This gives for u':

$$u'(t) = \frac{u(t+\Delta t) - u(t)}{\Delta t} + O(\Delta t^2)$$

So we approximate

$$u'(t) \approx \frac{u(t+\Delta t) - u(t)}{\Delta t}$$

and the "truncation error" is $O(\Delta t^2)$.

Finite differences 2

How does this help? In $u' = f(t,u)$ substitute

$$u'(t) \to \frac{u(t+\Delta t) - u(t)}{\Delta t}$$

giving

$$\frac{u(t+\Delta t) - u(t)}{\Delta t} = f(t, u(t))$$

or

$$u(t+\Delta t) = u(t) + \Delta t\, f(t, u(t))$$

Let $t_0 = 0$, $t_{k+1} = t_k + \Delta t = \cdots = (k+1)\Delta t$, $u(t_k) = u_k$:

$$u_{k+1} = u_k + \Delta t\, f(t_k, u_k)$$

Discretization
'Explicit Euler' or 'Euler forward'.

Does this compute something close to the true solution?
'Discretization error'

Some error analysis

Local Truncation Error: assume computed solution is exact at step k, how wrong will we be at step $k+1$?

$$\begin{aligned} u(t_{k+1}) &= u(t_k) + u'(t_k)\Delta t + u''(t_k)\frac{\Delta t^2}{2!} + \cdots \\ &= u(t_k) + f(t_k, u(t_k))\Delta t + u''(t_k)\frac{\Delta t^2}{2!} + \cdots \\ u_{k+1} &= u_k + f(t_k, u_k)\Delta t \end{aligned}$$

So

$$\begin{aligned} L_{k+1} &= u_{k+1} - u(t_{k+1}) \\ &= u_k - u(t_k) + f(t_k, u_k) - f(t_k, u(t_k)) - u''(t_k)\frac{\Delta t^2}{2!} + \cdots \\ &= -u''(t_k)\frac{\Delta t^2}{2!} + \cdots \end{aligned}$$

Global error: $E_k \approx \Sigma_k L_k = k\Delta t \frac{\Delta t^2}{2!} = O(\Delta t)$: First order method

An Euler forward example

Consider $f(t,u) = -\lambda u$, exact solution $u(t) = u_0 e^{-\lambda t}$;
stable if $\lambda > 0$

Explicit Euler scheme

$$u_{k+1} = u_k - \Delta t \lambda u_k = (1 - \lambda \Delta t) u_k = (1 - \lambda \Delta t)^k u_0$$

Then

$$\begin{aligned} & u_k \to 0 \text{ as } k \to \infty \\ \Leftrightarrow\ & |1 - \lambda \Delta t| < 1 \\ \Leftrightarrow\ & -1 < 1 - \lambda \Delta t < 1 \\ \Leftrightarrow\ & -2 < -\lambda \Delta t < 0 \\ \Leftrightarrow\ & 0 < \lambda \Delta t < 2 \\ \Leftrightarrow\ & \Delta t < 2/\lambda \end{aligned}$$

Conditionally stable

Implicit Euler

Or 'Euler backward':

$$u(t-\Delta t) = u(t) - u'(t)\Delta t + u''(t)\frac{\Delta t^2}{2!} + \cdots$$

so

$$u'(t) = \frac{u(t) - u(t-\Delta t)}{\Delta t} + u''(t)\Delta t/2 + \cdots$$

Compute $u'(t) = f(t, u(t))$ as

$$\begin{aligned} & \frac{u(t) - u(t-\Delta t)}{\Delta t} = f(t, u(t)) \\ \Rightarrow \quad & u(t) = u(t-\Delta t) + \Delta t f(t, u(t)) \\ \Rightarrow \quad & u_{k+1} = u_k + \Delta t f(t_{k+1}, u_{k+1}) \end{aligned}$$

Implicit equation for u_{k+1}!

Let $f(t, u) = -u^3$, then $u_{k+1} = u_k - \Delta t u_{k+1}^3$
needs nonlinear solver

Stability of Implicit Euler

Again the $f(t,u) = -\lambda u$ example:

$$\begin{aligned} u_{k+1} &= u_k - \lambda\Delta t u_{k+1} \\ (1+\lambda\Delta t)u_{k+1} &= u_k \\ u_{k+1} &= \left(\frac{1}{1+\lambda\Delta t}\right) u_k = \left(\frac{1}{1+\lambda\Delta t}\right)^k u_0 \end{aligned}$$

If $\lambda > 0$ (stable equation), then $u_k \to 0$ for all values of λ and Δt: unconditionally stable.

Pro: larger time steps possible, no worries
Con: implicit equation needs to be solved

Higher order methods

Runge-Kutta
Adams-Bashforth
Crank-Nicholson

Boundary value problems

Consider $u''(x) = f(x, u, u')$ for $x \in [a, b]$ where $u(a) = u_a$, $u(b) = u_b$ in 1D and

$$-u_{xx}(\bar{x}) - u_{yy}(\bar{x}) = f(\bar{x}) \text{ for } x \in \Omega = [0, 1]^2 \text{ with } u(\bar{x}) = u_0 \text{ on } \delta\Omega. \quad (1)$$

in 2D.

Approximation of 2nd order derivatives

Taylor series (write h for δx):

$$u(x+h) = u(x) + u'(x)h + u''(x)\frac{h^2}{2!} + u'''(x)\frac{h^3}{3!} + u^{(4)}(x)\frac{h^4}{4!} + u^{(5)}(x)\frac{h^5}{5!} + \cdots$$

and

$$u(x-h) = u(x) - u'(x)h + u''(x)\frac{h^2}{2!} - u'''(x)\frac{h^3}{3!} + u^{(4)}(x)\frac{h^4}{4!} - u^{(5)}(x)\frac{h^5}{5!} + \cdots$$

Subtract:

$$u(x+h) + u(x-h) = 2u(x) + u''(x)h^2 + u^{(4)}(x)\frac{h^4}{12} + \cdots$$

so

$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} - u^{(4)}(x)\frac{h^4}{12} + \cdots$$

Numerical scheme:

$$-\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} = f(x, u(x), u'(x))$$

(2nd order PDEs are very common!)

This leads to linear algebra

$$-\frac{u(x+h)-2u(x)+u(x-h)}{h^2} = f(x,u(x),u'(x))$$

Equally spaced points on $[0,1]$: $x_k = kh$ where $h = 1/n$, then

$$-u_{k+1} + 2u_k - u_{k-1} = h^2\, f(x_k, u_k, u'_k) \quad \text{for } k = 1,\ldots,n-1$$

Written as matrix equation:

$$\begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} h^2 f_1 + u_0 \\ h^2 f_2 \\ \vdots \end{pmatrix}$$

Matrix properties

- Very sparse, banded
- Symmetric (only because 2nd order problem)
- Sign pattern: positive diagonal, nonpositive off-diagonal (true for many second order methods)
- Positive definite (just like the continuous problem)

Initial Boundary value problem

Heat conduction in a rod $T(x,t)$ for $x \in [a,b]$, $t > 0$:

$$\frac{\partial}{\partial t} T(x,t) - \alpha \frac{\partial^2}{\partial x^2} T(x,t) = q(x,t)$$

- Initial condition: $T(x,0) = T_0(x)$
- Boundary conditions: $T(a,t) = T_a(t)$, $T(b,t) = T_b(t)$
- Material property: $\alpha > 0$ is thermal diffusivity
- Forcing function: $q(x,t)$ is externally applied heating.

The equation $u''(x) = f$ above is the steady state.

Discretization

Space discretization: $x_0 = a$, $x_n = b$, $x_{j+1} = x_j + \Delta x$
Time discretiation: $t_0 = 0$, $t_{k+1} = t_k + \Delta t$
Let T_j^k approximate $T(x_j, t_k)$

Space:

$$\frac{\partial}{\partial t} T(x_j, t) - \alpha \frac{T(x_{j-1}, t) - 2T(x_j, t) + T(x_{j+1}, t)}{\Delta x^2} = q(x_j, t)$$

Explicit time stepping:

$$\frac{T_j^{k+1} - T_j^k}{\Delta t} - \alpha \frac{T_{j-1}^k - 2T_j^k + T_{j+1}^k}{\Delta x^2} = q_j^k$$

Implicit time stepping:

$$\frac{T_j^{k+1} - T_j^k}{\Delta t} - \alpha \frac{T_{j-1}^{k+1} - 2T_j^{k+1} + T_{j+1}^{k+1}}{\Delta x^2} = q_j^{k+1}$$

Computational form: explicit

$$T_j^{k+1} = T_j^k + \frac{\alpha\Delta t}{\Delta x^2}(T_{j-1}^k - 2T_j^k + T_{j+1}^k) + \Delta t q_j^k$$

This has an explicit form:

$$\underset{\sim}{T}^{k+1} = \left(I + \frac{\alpha\Delta t}{\Delta x^2}\right)\underset{\sim}{T}^k + \Delta t \underset{\sim}{q}^k$$

Computational form: implicit

$$T_j^{k+1} - \frac{\alpha\Delta t}{\Delta x^2}(T_{j-1}^k - 2T_j^k + T_{j+1}^k) = T_j^k + \Delta t q_j^k$$

This has an implicit form:

$$\left(I - \frac{\alpha\Delta t}{\Delta x^2}K\right)\underset{\sim}{T}^{k+1} = \underset{\sim}{T}^k + \Delta t\underset{\sim}{q}^k$$

Needs to solve a linear system in every time step

Stability of explicit scheme

Let $q \equiv 0$; assume $T_j^k = \beta^k e^{i\ell x_j}$; for stability we require $|\beta| < 1$:

$$\begin{aligned}
T_j^{k+1} &= T_j^k + \frac{\alpha \Delta t}{\Delta x^2}(T_{j-1}^k - 2T_j^k + T_{j+1}^k) \\
\Rightarrow \beta^{k+1} e^{i\ell x_j} &= \beta^k e^{i\ell x_j} + \frac{\alpha \Delta t}{\Delta x^2}(\beta^k e^{i\ell x_{j-1}} - 2\beta^k e^{i\ell x_j} + \beta^k e^{i\ell x_{j+1}}) \\
\Rightarrow \beta &= 1 + 2\frac{\alpha \Delta t}{\Delta x^2}[\frac{1}{2}(e^{i\ell \Delta x} + e^{-\ell \Delta x}) - 1] \\
&= 1 + 2\frac{\alpha \Delta t}{\Delta x^2}(\cos(\ell \Delta x) - 1)
\end{aligned}$$

$$\frac{\beta^{k+1}}{\beta^k} = 1 + 2\frac{\alpha\Delta t}{\Delta x^2}(\cos(\ell\Delta x) - 1)$$

To get $|\beta| < 1$:

- $2\frac{\alpha\Delta t}{\Delta x^2}(\cos(\ell\Delta x) - 1) < 0$: automatic
- $2\frac{\alpha\Delta t}{\Delta x^2}(\cos(\ell\Delta x) - 1) > -2$: needs $2\frac{\alpha\Delta t}{\Delta x^2} < 1$, that is

$$\Delta t < \frac{\Delta x^2}{2\alpha}$$

big restriction on size of time steps

Stability of implicit scheme

$$
\begin{aligned}
T_j^{k+1} - \frac{\alpha\Delta t}{\Delta x^2}(T_{j_1}^{k+1} - 2T_j^{k+1} + T_{j+1}^{k+1}) &= T_j^k \\
\Rightarrow \beta^{k+1}e^{i\ell\Delta x} - \frac{\alpha\Delta t}{\Delta x^2}(\beta^{k+1}e^{i\ell x_{j-1}} - 2\beta^{k+1}e^{i\ell x_j} + \beta^{k+1}e^{i\ell x_{j+1}}) &= \beta^k e^{i\ell x_j}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow \beta^{-1} &= 1 + 2\frac{\alpha\Delta t}{\Delta x^2}(1 - \cos(\ell\Delta x)) \\
\beta &= \frac{1}{1 + 2\frac{\alpha\Delta t}{\Delta x^2}(1 - \cos(\ell\Delta x))}
\end{aligned}
$$

Noting that $1 - \cos(\ell\Delta x) > 0$, the condition $|\beta| < 1$ always satisfied: method always stable.

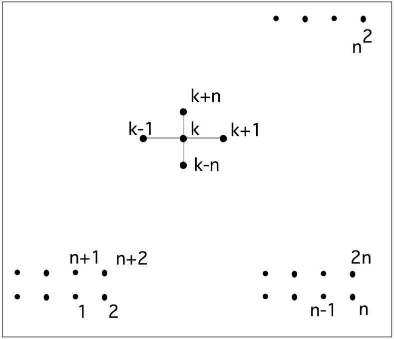
Sparse matrix in 2D case

Sparse matrices so far were tridiagonal: only in 1D case.

Two-dimensional: $-u_{xx} - u_{yy} = f$ on unit square $[0,1]^2$

Difference equation:

$$4u(x,y) - u(x+h,y) - u(x-h,y) - u(x,y+h) - u(x,y-h) = h^2 f(x,y)$$



Sparse matrix from 2D equation

$$
\left(\begin{array}{ccccc|ccccc|cc}
4 & -1 & & & \emptyset & -1 & & & & \emptyset & & \\
-1 & 4 & 1 & & & & -1 & & & & & \\
 & \ddots & \ddots & \ddots & & & & \ddots & & & & \\
 & & \ddots & \ddots & -1 & & & & \ddots & & & \\
\emptyset & & & -1 & 4 & \emptyset & & & & -1 & & \\
\hline
-1 & & & & \emptyset & 4 & -1 & & & & -1 & \\
 & -1 & & & & -1 & 4 & -1 & & & & -1 \\
 & \uparrow & \ddots & & & \uparrow & \uparrow & \uparrow & & & & \uparrow \\
 & k-n & & & & k-1 & k & k+1 & & -1 & & k+n \\
 & & & & -1 & & & & -1 & 4 & & \\
\hline
 & & & & & \ddots & & & & & \ddots &
\end{array}\right)
$$