<u>6.003 R</u> Feb 10, 2010

Looking forword.. In Pset #2 there are some problems on numerical methods and analysis. The plan here is to begin talking about numerical methods. There are lots of reasons to do this:

(1) Numerical methods are becoming more important since computer are more powerful

(2) Numerical methods provide a connection between CT and DT worlds

(3) We can understand numerical methods from 6.003 signals and systems point of view.

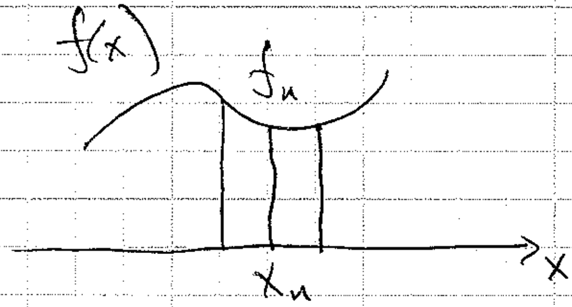
Approach in this recitation:

(a) Think about discretization

(b) Second-order differential equation with simple 3-pt differencing

(c) Noumerov differencing

Look at uniform grid to start with



$$f(x_n) \longleftrightarrow f_n \longleftrightarrow f[n]$$

$\uparrow$ CT (or space) $\qquad$ $\uparrow$ Numerical $\qquad$ $\uparrow$ 6.003 DT

<u>Discretization</u>

We would like to approximate $\frac{d^2f}{dx^2} = f''$

Use Taylor series expansions

$$f_{n+1} = f(x_{n+1}) = f_n + h f_n' + \frac{h^2}{2} f_n'' + \frac{h^3}{3!} f_n''' + \cdots$$

$$f_{n-1} = f(x_{n-1}) = f_n - h f_n' + \frac{h^2}{2} f_n'' - \frac{h^3}{3!} f_n''' + \cdots$$

$$f_{n+1} - 2f_n + f_{n-1} = h^2 f_n'' + 2\frac{h^4}{4!} f_n^{IV} + 2\frac{h^6}{6!} f_n^{VI} + \cdots$$

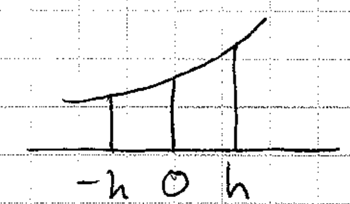
$$\left(\frac{d^2f}{dx^2}\right)_{x_n} = f_n'' = \frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} - \frac{h^2}{12} f_n^{IV} \ldots$$

2ND derivative — 3 pt discretization — Numerical error

How good is this ?

let $f(x) = e^x \quad \frac{df}{dx} = e^x \quad \frac{d^2f}{dx^2} = e^x$

Lets compute $\frac{d^2f}{dx^2}$ at $x=0$ using 3-pt formula



$$f_n'' \approx \frac{e^h - 2 + e^{-h}}{h^2}$$

let $h = 0.1$

$$= \frac{e^{0.1} - 2 + e^{-0.1}}{0.1^2} = 1.00083 \ldots$$

Thinking about the error..

$$\frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} = f_n'' + \frac{h^2}{12} f_n^{IV} + \ldots$$

$0.000833 \ldots$ — 1

So, we can understand the error

Can we do better?

Try $f''_n = A f_{n+2} + B f_{n+1} + C f_n + D f_{n-1} + E f_{n-2}$

$$
\begin{aligned}
&= A \left[f_n + (2h) f'_n + \frac{(2h)^2}{2!} f''_n + \frac{(2h)^3}{3!} f'''_n + \frac{(2h)^4}{4!} f^{IV}_n + \cdots \right] \\
&+ B \left[f_n + h f'_n + \frac{h^2}{2!} f''_n + \frac{h^3}{3!} f'''_n + \frac{h^4}{4!} f^{IV}_n \cdots \right] \\
&+ C \; f_n \\
&+ D \left[\quad \right] \\
&+ E \left[\quad \right]
\end{aligned}
$$

Get constraints

$$A + B + C + D + E = 0$$

$$2A + B - D - 2E = 0$$

$$2h^2 A + \frac{h^2}{2} B + \frac{h^2}{2} D + 2h^2 E = 1$$

$$\vdots$$

Solve and get

$$f''_n = \frac{-f_{n+2} + 16 f_{n+1} - 30 f_n + 16 f_{n-1} - f_{n-2}}{12 h^2} + O(h^4)$$

This is a centered 5 pt scheme

Lets see how good it is...

$$f(x) = e^x \quad \text{again}$$

$$\left(\frac{d^2f}{dx^2}\right)_0 \approx \frac{-e^{2h} + 16e^{h} - 30 + 16e^{-h} - 2e^{-2h}}{12h^2}$$

let $h = 0.1$ get $0.9999988\ldots$

$$= 1 - 1.1121\ldots \times 10^{-6}$$

This is great, and it seems we can do better with more points (although in practice you eventually lose because computers keep only finite number of digits).

Next, lets try a differential equation

$$\frac{d^2f}{dx^2} + k^2 f = g$$

$\Big\downarrow$ discretize

$$\frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} + k^2 f_n = g_n$$
$$+ O(h^2)$$

Can solve this on a computer...

Think $f[n+1] = 2f[n] - f[n-1] - (hk)^2 f[n]$
$- h^2 g[n]$

Like to understand how good the answer is.
Look at simpler problem that ~~and~~ we know the answer to...

$$\frac{d^2f}{dx^2} + k^2 f = 0$$

$$f(x) = A e^{ikx} + B e^{-ikx}$$

Can we solve the finite difference equation?

Try $f_n = e^{jkx_n}$

$$\frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} + k^2 f_n = 0$$

$$\frac{e^{jkx_{n+1}} - 2e^{jkx_n} + e^{jkx_{n-1}}}{h^2} + k^2 e^{jkx_n} = 0$$

$$\frac{e^{jkh} - 2 + e^{-jkh}}{h^2} + k^2 = 0$$

$$\frac{2\cos kh - 2}{h^2} + k^2 = 0$$

$$\cos(kh) = 1 - \frac{(kh)^2}{2}$$

if kh is small, then

$$kh = \text{Arccos}\left(1 - \frac{(kh)^2}{2}\right) = kh + \frac{(kh)^3}{24} + \cdots$$

$$\text{so} \quad k = k + \underbrace{\frac{k^3h^2}{24}}_{O(h^2)}$$

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General solution for $kh < 2$

$$f_n = A e^{jkx_n} + B e^{-jkx_n}$$

Compare with general solution for continuous problem

$$f(x) = A e^{ikx} + B e^{-ikx}$$

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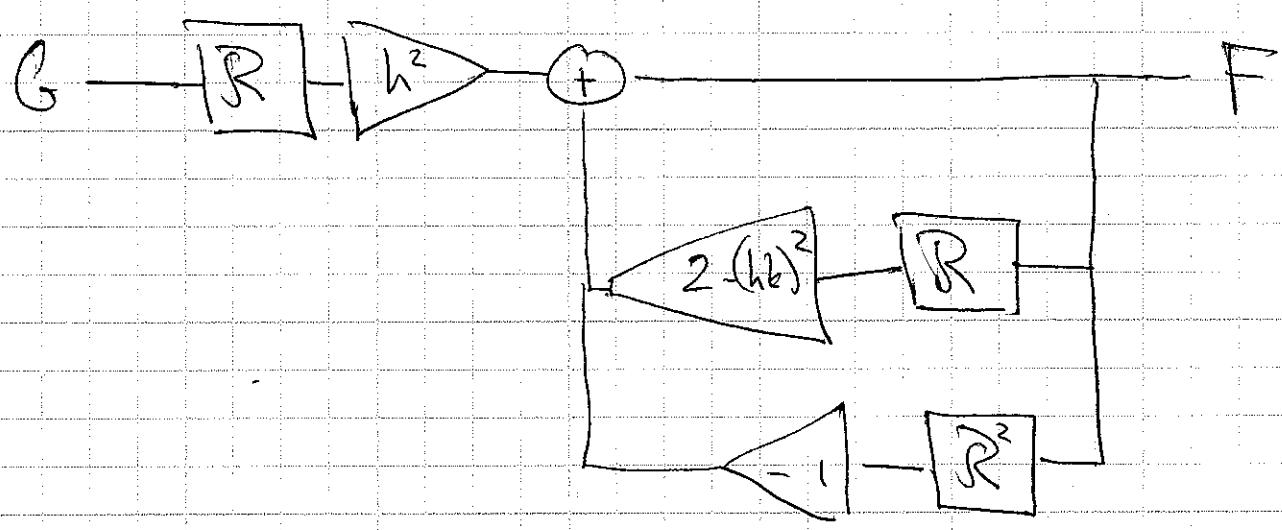
Think about it from 6.003 viewpoint

$$\frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} + k^2 f_n = g_n$$

$$\frac{f[n+1] - 2f[n] + f[n-1]}{h^2} + k^2 f[n] = g[n]$$

$$f[n+1] = 2f[n] - f[n-1] - (hk)^2 f[n] + h^2 g[n]$$

$$f[n] = 2f[n-1] - f[n-2] - (hk)^2 f[n-1] + h^2 g[n-1]$$



$$F = 2\mathcal{R}F - \mathcal{R}^2 F - (hk)^2 \mathcal{R}F + h^2 \mathcal{R}G$$

$$\left(1 - [2-(hk)^2]\mathcal{R} + \mathcal{R}^2\right) F = h^2 \mathcal{R} G$$

$$F = \frac{h^2 z}{1 - [2-(hk)^2] z + z^2} G$$

To find poles:

$$z^2 - [2-(hk)^2] z + 1 = 0$$

if hk is small, system is stable

$$z = \frac{[2-(hk)^2] \pm \sqrt{[2-(hk)^2]^2 - 4}}{2}$$

$$= \frac{2-(hk)^2 \pm \sqrt{-4(hk)^2 + (hk)^4}}{2}$$

$$= 1 - \frac{(hk)^2}{2} \pm j(hk)\sqrt{1 - \frac{(hk)^2}{4}} \quad \text{small } hk$$

$$\text{or} = 1 - \frac{(hk)^2}{2} \pm \frac{(hk)^2}{2}\sqrt{1 - \frac{4}{(hk)^2}} \quad \text{large } hk$$

Numerov differencing

$$\frac{d^2f}{dx^2} + k^2 f = q$$

$$\frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} \underbrace{- \frac{h^2}{12} f_n^{IV}}_{\substack{\text{lowest-order} \\ \text{discretization error}}} + k^2 f_n = q_n$$

$$f_n^{IV} \approx \frac{f''_{n+1} - 2f''_n + f''_{n-1}}{h^2}$$

$$= \frac{(q-k^2f)_{n+1} - 2(q-k^2f)_n + (q-k^2f)_{n-1}}{h^2}$$

Plug in to get

$$\frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} - \frac{h^2}{12}\left[\frac{(q-k^2f)_{n+1} - 2(q-k^2f)_n + (q-k^2f)_{n-1}}{h^2}\right]$$

$$+ k^2 f_n = q_n$$

$$\frac{f_{n+1} - 2f_n + f_{n-1}}{h^2} + k^2\left(\frac{f_{n+1} + 10f_n + f_{n-1}}{12}\right) = \frac{q_{n+1} + 10q_n + q_{n-1}}{12}$$

$$+ O(h^4)$$

Solutions are

$$f_n = A e^{jKx_n} + B e^{-jKx_n}$$

Plug in, and eventually get

~~Kh Arc~~

$$\cos Kh = \frac{12 - 5(kh)^2}{12 + 5(kh)^2}$$

$$Kh \cong kh + \frac{(kh)^5}{480} + \cdots$$

$$K = k + O(h^4)$$

$\Rightarrow$ Much more accurate!