Mathematical Methods

Lecture 2

Numerical Solution of ODEs:

Forward-Euler: $\dot{x} = f(t,x)$, $x = x(t)$

$\Delta t = t_{n+1} - t_n$

$x_{n+1} = x_n + f(x_n, t_n)\,\Delta t$

- explicit, often unstable
- first-order
- Fast

Backward-Euler: $x_n = x_{n+1} - f(x_{n+1}, t_{n+1})\,\Delta t$

- implicit, often good stability
- First-order
- more expensive

Midpoint-Method: "estimate" slope first at midpoint

$$K = f(t_n, x_n)$$

$$x_{n+1} = x_n + \Delta t\, f\Big(\underbrace{t_n + \tfrac{1}{2}\Delta t,\ x_n + \tfrac{1}{2}\Delta t \cdot k}_{\text{midpoint}}\Big)$$

- explicit
- 2nd-order
- easy to implement.

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Runge-Kutta

Widely used: 4-th order Runge-Kutta

$$x_{n+1} = x_n + \frac{1}{6}\Delta t\,(k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = f(t_n, x_n)$$
$$k_2 = f(t_n + \tfrac{1}{2}\Delta t,\ x_n + \tfrac{1}{2}\Delta t\, k_1)$$
$$k_3 = f(t_n + \tfrac{1}{2}\Delta t,\ x_n + \tfrac{1}{2}\Delta t\, k_2)$$
$$k_4 = f(t_n + \Delta t,\ x_n + \Delta t \cdot k_3)$$

Note: This generalizes also to systems of ODEs (hence, even to PDEs).

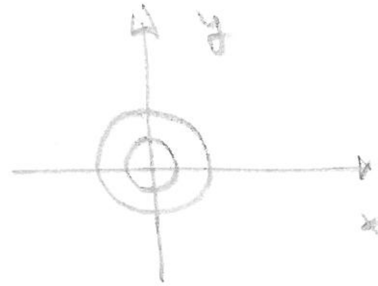
Other methods:
- variable step-size
- multi-step methods (Adams-Bashforth)
- exponential time differencing

Example: Harmonic oscillator: $\ddot{x} + x = 0$

write $\dot{x} = y \Rightarrow \dot{x} = y$
$\dot{y} = -x$

Note $E = \frac{1}{2}(x^2 + y^2)$ is conserved

$\Rightarrow$



phase space: circles
(test for numerics)

Operator and matrices:

Remember $L = \frac{d^2}{dt^2} + 1$ with periodic boundary conditions.
Then $L \cos t = \left(\frac{d^2}{dt^2} + 1\right) \cos t = 0$. So $L f = 0$ is solved by $f(t) = \cos t$ if we prescribe $f(0) = 1$.

The problem $L f = 0$, $f(0) = 1$ can be discretized and written as a linear system of equations.
(and Matlab can solve this system)

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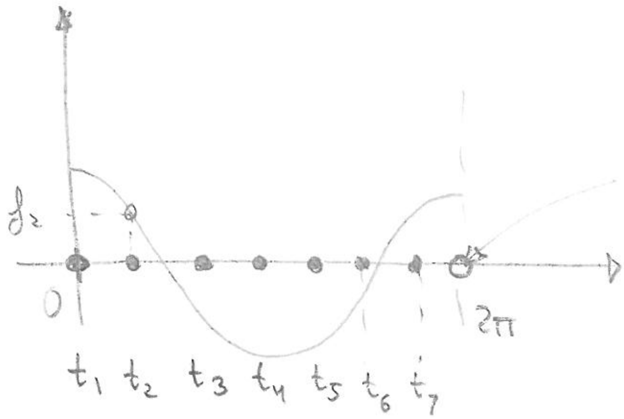

The discrete approximation of f'' at t_2, for example, is

$$\frac{\frac{f_3 - f_2}{\Delta t} - \frac{f_2 - f_1}{\Delta t}}{\Delta t} = \frac{f_3 - 2f_2 + f_1}{(\Delta t)^2}$$

At t_1, it is $\dfrac{f_2 - 2f_1 + f_7}{(\Delta t)^2}$ (periodicity)

at t_7 it is $\dfrac{f_1 - 2f_7 + f_6}{(\Delta t)^2}$.

Now we can try to write $\frac{d^2}{dt^2} f \approx A f$ in a discretized way.

$$
\begin{pmatrix}
-\frac{2}{(\Delta t)^2} & \frac{1}{(\Delta t)^2} & 0 & 0 & 0 & 0 & \frac{1}{(\Delta t)^2} \\
\frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2} & \frac{1}{(\Delta t)^2} & 0 & 0 & 0 & 0 \\
0 & \frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2} & \frac{1}{(\Delta t)^2} & 0 & 0 & 0 \\
0 & 0 & \frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2} & \frac{1}{(\Delta t)^2} & 0 & 0 \\
0 & 0 & 0 & \frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2} & \frac{1}{(\Delta t)^2} & 0 \\
0 & 0 & 0 & 0 & \frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2} & \frac{1}{(\Delta t)^2} \\
\frac{1}{(\Delta t)^2} & 0 & 0 & 0 & 0 & \frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2}
\end{pmatrix}
\begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \end{pmatrix}
$$

Short, we write this as

$$
\begin{pmatrix}
-\frac{2}{(\Delta t)^2} & \frac{1}{(\Delta t)^2} & 0 & \cdots & \frac{1}{(\Delta t)^2} \\
\frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2} & \frac{1}{(\Delta t)^2} & \cdots & 0 \\
0 & \ddots & \ddots & \ddots & \vdots \\
\vdots & & \ddots & \ddots & 0 \\
\frac{1}{(\Delta t)^2} & 0 & \cdots & \frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2}
\end{pmatrix}
\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ \vdots \\ f_n \end{pmatrix}
$$

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The condition $f(0) = f_1 = 1$ can be added as a row in the matrix

$$\begin{pmatrix} 1 & 0 & \cdots & 0 \\ & & \vdots & \\ & & \vdots & \end{pmatrix} \begin{pmatrix} f_1 \\ \vdots \\ f_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix}$$

Hence $\left\{ \begin{array}{l} f(0) = 1 \\ Lf = 0 \end{array} \right\}$ can be written ($-\frac{2}{(\Delta t)^2} + 1$ on the diagonal)

$$\begin{pmatrix} 1 & 0 & 0 & \cdots & \cdots & 0 \\ -\frac{2}{(\Delta t)^2}+1 & \frac{1}{(\Delta t)^2} & 0 & \cdots & \cdots & \frac{1}{(\Delta t)^2} \\ \frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2}+1 & \frac{1}{(\Delta t)^2} & \cdots & \cdots & 0 \\ 0 & \frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2}+1 & \frac{1}{(\Delta t)^2} & \cdots & 0 \\ \vdots & & & & & \vdots \\ \frac{1}{(\Delta t)^2} & 0 & \cdots & \cdots & \frac{1}{(\Delta t)^2} & -\frac{2}{(\Delta t)^2}+1 \end{pmatrix} \begin{pmatrix} f_1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ f_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ \vdots \\ \vdots \\ 0 \end{pmatrix}$$

Note : To solve linear systems in Matlab: $Ax = b$

$x = A \backslash b$

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Review of linear algebra:

scalar product in $\mathbb{R}^n$: $\langle a,b\rangle = \sum_{k=1}^{n} a_k b_k$

Scalar product in $\mathbb{C}^n$: $\langle a,b\rangle = \sum_{k=1}^{n} \overline{a_k}\, b_k$

complex conjugate

$A=(a_{ij})$ transpose: $A^T=(a_{ji})$

$$A=\begin{pmatrix}1&3\\2&4\end{pmatrix},\quad A^T=\begin{pmatrix}1&2\\3&4\end{pmatrix}$$

Remember, for matrices: AB is usually not BA.

If $AB=BA$ we say that A and B commute.

(or $[A,B]=AB-BA=0$)

Note: Even two symmetric matrices do not necessarily commute (only if they have the same eigenspaces)

$$\begin{pmatrix}1&0\\0&0\end{pmatrix}\begin{pmatrix}1&2\\2&1\end{pmatrix}=\begin{pmatrix}1&2\\0&0\end{pmatrix}$$

$$\begin{pmatrix}1&2\\2&1\end{pmatrix}\begin{pmatrix}1&0\\0&0\end{pmatrix}=\begin{pmatrix}1&0\\2&0\end{pmatrix}$$

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A vector v is an eigenvector of A if $\exists \lambda$ such that $Av = \lambda v$, λ is called eigenvalue. ($v \neq 0$, A a square matrix)

We can compute the eigenvalues by solving $f(x) = 0$ for $f(x) = \det(xI - A)$ (which is called characteristic polynomial)

Example:

$$A = \begin{pmatrix} 1 & 2 & -1 \\ 1 & 0 & 1 \\ 4 & -4 & 5 \end{pmatrix}$$

$$f(x) = x^3 - 6x^2 + 11x - 6 = (x-1)(x-2)(x-3)$$

$$v_1 = \begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix}, \quad v_2 = \begin{pmatrix} -2 \\ 1 \\ 4 \end{pmatrix}, \quad v_3 = \begin{pmatrix} -1 \\ 1 \\ 4 \end{pmatrix}$$

Note: $[V, D] = eig(A)$ in matlab