Physics 371: Final

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Problem 1: Centered derivative approximation (20 pts.)

Show that the centered derivative formula for the second derivative is exact for the function $f(x) = a + b\,x + c\,x^2$. Why is that?

Centered derivative formula

$$f''(x) \sim \frac{f(x+\Delta x) + f(x-\Delta x) - 2f(x)}{\Delta x^2}$$

$$f''(x) \sim \frac{1}{\Delta x^2}\Big[\cancel{a} + \cancel{bx} + \cancel{b\Delta x} + c(x+\Delta x)^2 + \cancel{a} + \cancel{b}(x - \cancel{\Delta x}) + c(x-\Delta x)^2 - \cancel{2a} - \cancel{2bx} - 2cx^2\Big]$$

$$\sim \frac{1}{\Delta x^2}\big[2\cancel{cx^2} + 2c\Delta x^2 - 2\cancel{cx^2}\big]$$

$$\sim 2c$$

$$f(x) = a + bx + cx^2$$

$$f'(x) = b + 2cx$$

$$f''(x) = 2c$$

true because centered derivative formula is exact up to 2nd order in Δx

Problem 2: Gaussian elimination (20 pts.)

Given a linear system of equations $\sum_n A_{mn} x_n = b_m$, where A_{mn} is an element of a known N dimensional matrix, b_m is an element of a known N dimensional vector, and x_m is an element of the vector of unknowns, describe how you would construct an algorithm to find the unknowns. Use nested for loops. Indicate clearly the operations and the indices which are looped over.

to make $\bar{A}$ upper triangular / also calculate modified $\vec{b}$

for (k = 1 ; k <= N-1 ; k++)
{
for (j = k+1 ; j <= N ; j++)
{
for (i = k ; i <= N ; i++)
{
$A_{ji} = A_{ji} - \frac{A_{jk} A_{ki}}{A_{kk}}$
}
$b_j = b_j - \frac{A_{jk} b_k}{A_{kk}}$
}
}

for (i = N, ..., 1) determines x's
{
sum = $\frac{b_i}{A_{ii}}$

for (j = N-1, ..., i)
{
sum = sum $- \frac{A_{ij} x_j}{A_{ii}}$
}
x_i = sum
}

Problem 3: Advection equation (20 pts.)

The advection equation is given by $\frac{\partial A}{\partial t} = -c\frac{\partial A}{\partial x}$. The Lax scheme to solve this equation is given by $A_i^{n+1} = \frac{A_{i+1}^n + A_{i-1}^n}{2} - c\frac{\Delta t}{2\Delta x}(A_{i+1}^n - A_{i-1}^n)$. Derive the implicit analog of this scheme and calculate its stability.

implicit scheme:

$\cancel{\vec{A}^{n+1} = \bar{\bar{M}}\vec{A}^n}$

$$\frac{\partial A}{\partial t} = -c\frac{\partial A}{\partial x}$$

$$\frac{\vec{A}^{n+1} - \vec{A}^n}{\Delta t} = -c\ \bar{\bar{M}}\vec{A}^n \rightarrow \text{implicit}$$

$$\bar{\bar{M}} = -\frac{c}{2\Delta x}\begin{pmatrix} & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & \end{pmatrix}$$

can also write

$$\frac{\vec{A}^{n+1} - \vec{A}^n}{\Delta t} = \bar{\bar{M}}\left(\frac{\vec{A}^{n+1} + \vec{A}^n}{2}\right)$$

$$\vec{A}^{n+1} = \vec{A}^n + \Delta t\,\bar{\bar{M}}\left(\frac{\vec{A}^{n+1} + \vec{A}^n}{2}\right) \qquad \bar{\bar{N}} = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

Lax

$$= \bar{\bar{N}}\vec{A}^n + \Delta t\,\bar{\bar{M}}\left(\frac{\vec{A}^{n+1} + \vec{A}^n}{2}\right)$$

$$\left(\bar{\bar{I}} - \frac{\Delta t\,\bar{\bar{M}}}{2}\right)\vec{A}^{n+1} = \left(\bar{\bar{N}} + \frac{\Delta t\,\bar{\bar{M}}}{2}\right)\vec{A}^n$$

apply Lax again

$$\boxed{\vec{A}^{n+1} = \left(\bar{\bar{N}} - \frac{\bar{\bar{M}}}{2\Delta t}\right)^{-1}\left(\bar{\bar{N}} + \frac{\bar{\bar{M}}}{2\Delta t}\right)\vec{A}^n}$$

implicit Lax !!!

stability: $A_j^n = \tilde{A}^n e^{ik\Delta x j}$

$$A^{n+1} = \left|\left[\frac{\cos k\Delta x - ic\frac{(\sin k\Delta x)\Delta t}{4\Delta x}}{\cos k\Delta x + ic\frac{(\sin k\Delta x)\Delta t}{4\Delta x}}\right]\right| A^n$$

unconditionally stable

Problem 4: Eigenvalues of matrices (20 pts.)

Given a matrix **A** describe how you would find its *largest* and *second largest* eigenvalue and eigenvector.

largest eigenvalue:

→ take vector $\vec{v}$ (any vector, randomly chosen)

→ act on it with $\bar{\bar{A}}$ many times

$$[\bar{\bar{A}}]^N \vec{v} \Rightarrow \vec{v}' = \vec{v}_{max} \; (N \text{ large})$$

$\vec{v}'$ → eigenvector with largest eigenvalue

eigenvalue determined from $\bar{\bar{A}}\vec{v}' = \lambda \vec{v}'_{max}$

Proof: $\vec{v} = \sum_n a_n \vec{f}_n$

$\vec{f}_n$ → eigenvectors of $\bar{\bar{A}}\vec{f}_n = \lambda_n \vec{f}_n$

$$\Rightarrow \bar{\bar{A}}^N \vec{v} = \sum_n a_n \bar{\bar{A}}^N \vec{f}_n = \sum_n a_n \lambda^N \vec{f}_n$$

for largest eigenvalue contribution will increase exponentially compared to the others → after many iterations only λ largest will remain (others → negligible)

2nd largest eigenvalue

- after finding λ_{max} and $\vec{v}_{max}$
- choose vector randomly $\vec{v}$
- ~~orthogonal~~ subtract component of $\vec{v}$ parallel to $\vec{v}_{max}$ (Gram-Schmidt) $\Rightarrow \vec{v} = \vec{v} - (\vec{v} \cdot \vec{v}_{max}) \cdot \vec{v}_{max}$
- multiply by $\bar{\bar{A}}$

→ repeat these two steps many times

Problem 5: Integration by quadrature (20 pts.)

Given the function $f(x) = ax^2 + bx^5$ on the interval $[0,1]$, propose a two-point quadrature integration scheme to evaluate the integral exactly. Show that the scheme is indeed exact by performing the integration by the scheme proposed and by analytical integration.

2-pt. quadrature:

choose two pts on interval

$\rightarrow x_1 = 1/2 \qquad x_2 = 1$ (for example)

choose functions $q_1(x) = x^2 \qquad q_2(x) = x^5$

quadrature formula: $I \approx w_1 f(x_1) + w_2 f(x_2)$

for $q_1(x)$: $\frac{w_1}{4} + w_2 = \int_0^1 x^2 dx = \frac{1}{3}$

for $q_2(x)$: $\frac{w_1}{32} + w_2 = \int_0^1 x^5 dx = \frac{1}{6}$

$\frac{7w_1}{32} = \frac{1}{6} \rightarrow \boxed{w_1 = \frac{32}{42} = \frac{16}{21} \\ w_2 = \frac{7}{21} - \frac{4}{21} = \frac{3}{21} = \frac{1}{7}}$

does it work?

$I = \int_0^1 (ax^2 + bx^5) dx = \frac{a}{3} + \frac{b}{6}$

$\sim w_1 \left(\frac{a}{4} + \frac{b}{32}\right) + w_2 (a + b)$

$= \frac{4}{21}a + \frac{b}{42} + \frac{1}{7}a + \frac{1}{7}b = \frac{a}{3} + \frac{b}{6}$