Physics 371: Midterm 1

Name:
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SOLUTIONS

Problem 1: Centered derivative approximation (25 pts.)

Derive the centered derivative approximation for the third derivative of a function $f'''(x)$, when the function is represented on a grid with $x_i, i = 0, \ldots N-1$, with $x_i = i\Delta x$ at the point j, where $j > 2$.

Two solutions:

1.)
$$f'''(x) = \frac{f''(x+\Delta x) - f''(x-\Delta x)}{2\Delta x}$$
$$= \frac{f(x+2\Delta x) + f(x) - 2f(x+\Delta x) - f(x) - f(x-2\Delta x) + 2f(x-\Delta x)}{2\Delta x^3}$$
$$= \frac{f(x+2\Delta x) - 2f(x+\Delta x) + 2f(x-\Delta x) - f(x-2\Delta x)}{2\Delta x^3}$$

2.)
$$\left.\begin{array}{l} f(x+2\Delta x) = f + 2\Delta x f' + 2\Delta x^2 f'' + \frac{4\Delta x^3 f'''}{3} \\ f(x+\Delta x) = f + \Delta x f' + \frac{\Delta x^2 f''}{2} + \frac{\Delta x^3 f'''}{6} \\ f(x-\Delta x) = f - \Delta x f' + \frac{\Delta x^2 f''}{2} - \frac{\Delta x^3 f'''}{6} \\ f(x-2\Delta x) = f - 2\Delta x f' + 2\Delta x^2 f'' - \frac{\cancel{4}\,\Delta x^3 f'''}{3} \end{array}\right]\begin{array}{l} \times 1 \\ \times -2 \\ \times 2 \\ \times -1 \end{array}$$

$$\frac{f(x+2\Delta x) - 2f(x+\Delta x) + 2f(x-\Delta x) - f(x-2\Delta x)}{2\Delta x^3}$$

Problem 2: Initial value problem (25 pts.)

Consider the initial value problem $y'' = y$, for $t \geq 0$, with initial conditions $y(0) = 1$, and $y'(0) = 2$.

1.) Express this second order equation as a system of first order equations. (5 pts.)

2.) Perform a two-step propagation using a time step of $\Delta t = 0.5$, according to the Euler algorithm. (5 pts.)

3.) Perform two-step propagation using a time step of $\Delta t = .5$, according to the Verlet algorithm. (5 pts.)

4.) Using the analytic solution of the differential equation calculate the order of the error for the Verlet algorithm. (10 pts.)

1.) $y'' = y \Rightarrow y, v = y' \Rightarrow v = y'$
$v' = y$

2.) $y(0) = 1$
$y'(0) = 2 = v(0)$

$v(\Delta t) = v(0) + (\Delta t)\, y(0)$
$= 2 + (0.5)\cdot 1 = 2.5$
$y(\Delta t) = y(0) + \Delta t\, y'(0)$
$= 1 + (0.5)\cdot 2 = 2$
$v(2\Delta t) = 2.5 + (0.5)\cdot 2 = 3.5$
$y(2\Delta t) = 2 + (0.5)\cdot 2.5 = 3.25$

3.) Verlet not self-starting
start $\Rightarrow$ using an Euler step of Δt

$y(0) = 1 \quad y(\Delta t) = 2$

Verlet: $\dfrac{y(t+2\Delta t) + y(t) - 2y(t+\Delta t)}{\Delta t^2} = y'' = y(t+\Delta t)$

$y(t+2\Delta t) = 2y(t+\Delta t) - y(t) + \Delta t^2\, y(t+\Delta t)$

$y(2\Delta t) = 4 - 1 + (0.5)^2 \cdot 2 = 3.5$

$\left(y(2\Delta t) = 2y(\Delta t) - y(0) + \Delta t^2\, y(\Delta t) \right)$

4 $\rightarrow$ see on worksheet

Problem 3: Newton's method for matrix inversion (25 pts.)

Consider the function $\mathbf{F}(\mathbf{X}) = \mathbf{A} - \mathbf{X}^{-1}$, where $\mathbf{F}$, $\mathbf{A}$, and $\mathbf{X}$ are matrices. The root of $\mathbf{F}(\mathbf{X})$ is $\mathbf{X}^* = \mathbf{A}^{-1}$. Show that Newton's method gives us the iterative scheme $\mathbf{X}_{n+1} = 2\mathbf{X}_n - \mathbf{X}_n\mathbf{A}\mathbf{X}_n$, where $\mathbf{X}_1$ is an initial guess for $\mathbf{A}^{-1}$.

(3rd sol'n on worksheet 8)

1) in diagonal representation

$$F_i(x) = A_i - (x^{-1})_i = A_i - \frac{1}{x_i}$$

$$F_i(x^*) = F_i(x) + (x_i^* - x_i)\frac{\partial F_i(x)}{\partial x_i}$$

$$= A_i - \frac{1}{x_i} + (x_i^* - x_i)\left(-\frac{1}{x_i^2}\right) = 0$$

$$\Downarrow$$

$$x_i^* = 2x_i - x_i A_i x_i$$

in other basis: $\bar{\bar{X}}_n^* = 2\bar{\bar{X}}_n - \bar{\bar{X}}_n \bar{\bar{A}} \bar{\bar{X}}_n$

$$\Downarrow$$

$$\bar{\bar{X}}_{n+1} = 2\bar{\bar{X}}_n - \bar{\bar{X}}_n \bar{\bar{A}} \bar{\bar{X}}_n$$

2) also: from

$$\bar{\bar{X}}_{n+1} = 2\bar{\bar{X}}_n - \bar{\bar{X}}_n \bar{\bar{A}} \bar{\bar{X}}_n$$

$$\Rightarrow \Delta\bar{\bar{X}}_n = \bar{\bar{X}}_n - \bar{\bar{X}}_n \bar{\bar{A}} \bar{\bar{X}}_n \qquad (\Delta\bar{\bar{X}}_n = \bar{\bar{X}}_{n+1} - \bar{\bar{X}}_n)$$

$$\Delta\bar{\bar{X}}_n = \bar{\bar{X}}_n(\bar{\bar{I}} - \bar{\bar{A}}\bar{\bar{X}}_n) = \bar{\bar{X}}_n(\bar{\bar{X}}_n^{-1} - \bar{\bar{A}})\bar{\bar{X}}_n$$

$$= -\bar{\bar{X}}_n \bar{\bar{F}}(\bar{\bar{X}}_n)\bar{\bar{X}}_n$$

in diagonal basis $\Delta x_n^{(i)} = -x_n^i F_i x_n^i$

$$= -\frac{F_i(\bar{\bar{X}}_n)}{F_i'(\bar{\bar{X}}_n)}$$

also on worksheet 2

recall Newton's method: $\delta x = -\dfrac{f(x)}{f'(x)}$

Problem 4: Random number generation (25 pts.)

Given an unnormalized probability density $P(x) = \sin^2(x)$ with $0 \le x \le 2\pi$.

1.) Normalize $P(x)$. (5 pts.)

2.) Using a uniform random number generator, propose an algorithm which produces a sequence of random numbers distributed according to $P(x)$. (20 pts.)

1.) $P(x) \to \int_0^{2\pi} \tilde{P}(x)\,dx = 1 \qquad \int_0^{2\pi} \sin^2(x)\,dx = \pi$

$$\tilde{p}(x) = \frac{\sin^2 x}{\pi}$$

2.) sequence of random numbers:

cumulative distribution:

$$C(x) = \int_0^x dx' \frac{\sin^2(x')}{\pi}$$

$$= \int_0^x dx' \left[\frac{1}{2} - \frac{\cos 2x'}{2}\right] \frac{1}{\pi}$$

$$= \frac{x}{2\pi} - \frac{\sin 2x}{4\pi}$$

algorithm:

- sample uniform random number ξ
- find $x \Rightarrow \frac{x}{2\pi} - \frac{\sin 2x}{4\pi} = \xi$
- inversion can be done by Newton's method or bisection

Worksheet 1:

Problem 2:

part 4

exact solution: $y = Ae^{t} + Be^{-t}$

$$y_0 = A + B$$

$$y_1 = Ae^{\Delta t} + Be^{-\Delta t}$$

Verlet

$$y_2 = 2y_1 - y_0 + \Delta t^2 y_1$$

$$y_2 = 2A\left(1 + \Delta t + \frac{\Delta t^2}{2} + \frac{\Delta t^3}{6} + \frac{\Delta t^4}{24}\right)$$

$$+ 2B\left(1 - \Delta t + \frac{\Delta t^2}{2} - \frac{\Delta t^3}{6} + \frac{\Delta t^4}{24}\right)$$

$$- A - B$$

$$+ \Delta t^2 A\left(1 + \Delta t + \frac{\Delta t^2}{2}\right)$$

$$+ \Delta t^2 B\left(1 - \Delta t + \frac{\Delta t^2}{2}\right)$$

Verlet y_2 up to 4^{th} order

$$y_2 = A\left(1 + 2\Delta t + 2\Delta t^2 + \frac{8\Delta t^3}{6} + \frac{7\Delta t^4}{12}\right)$$

$$+ B\left(1 - 2\Delta t + 2\Delta t^2 - \frac{8\Delta t^3}{6} + \frac{7\Delta t^4}{12}\right)$$

exact

$$y_2 = A\left(1 + 2\Delta t + 2\Delta t^2 + \frac{8\Delta t^3}{6} + \frac{16\Delta t^4}{24}\right)$$

$$+ B\left(1 - 2\Delta t + 2\Delta t^2 - \frac{8\Delta t^3}{6} + \frac{16\Delta t^4}{24}\right)$$

$\Rightarrow$ error $O(\Delta t^4)$

Worksheet 2:

Problem 3:

3rd Sol'n

$$F(\vec{x}) = \bar{\bar{A}} - \bar{\bar{x}}^{-1}$$

$(\vec{x}_{n+1} - \vec{x}_n)\bar{\bar{F}}(\vec{x})$ should tend to zero as we iterate

$$(\bar{\bar{x}}_{n+1} - \bar{\bar{x}}_n)(\bar{\bar{A}} - \bar{\bar{x}}_n^{-1}) \to 0$$

$$\bar{\bar{x}}_{n+1}\bar{\bar{A}} - \bar{\bar{x}}_n\bar{\bar{A}} - \bar{\bar{x}}_{n+1}\bar{\bar{x}}_n^{-1} + \bar{\bar{I}} = 0$$

using $\bar{\bar{x}}_{n+1} = \bar{\bar{A}}^{-1}$

$$\Rightarrow \bar{\bar{x}}_{n+1} = 2\bar{\bar{x}}_n - \bar{\bar{x}}_n\bar{\bar{A}}\bar{\bar{x}}_n$$