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## **Phys 331 - Numerical Techniques for the Sciences I.**

### **Midterm 1**

October 4th, 2024.

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**(1) Number representation [20pts]**

**(1a) Decimal to Binary [8pts]:** Calculate the binary representation of the decimal number 231.625.

$$\begin{array}{ccccccc} 231 \rightarrow & \frac{1}{2^7} & \frac{1}{2^6} & \frac{1}{2^5} & \frac{0}{2^4} & \frac{0}{2^3} & \frac{1}{2^2} & \frac{1}{2^1} & \frac{1}{2^0} \\ & 128 & 64 & 32 & 16 & 8 & 4 & 2 & 1 \\ & \underbrace{128+64+32} & & 16 & & & & & \\ & 192 & & 16 & & & & & \\ & \underbrace{192+32} & & & & & & & \\ & 224 & & & & & & & \end{array}$$

$$\begin{array}{cccc} .625 \rightarrow & \frac{1}{2^{-1}} & \frac{0}{2^{-2}} & \frac{1}{2^{-3}} & \frac{0}{2^{-4}} \\ & 0.5 & 0.25 & 0.125 & 0.0625 \end{array}$$

$$\Rightarrow 231.625_{10} = 11100111.1010_2$$

**(1b) Real Number Representation [12pts]:** In IEEE 754 standard, **half-precision** number representation uses 16 bits to represent real numbers: 1 bit for the sign, 5 bits for the exponent, and 11 bits for the mantissa (though only 10 are stored, because the 1st bit is always 1). The bias for the exponent is 15.

How would you express each part of the number from part (a) in 16 bit? Write your answer in Binary. If you don't have an answer from part (a), write down a random 11 digit binary number and use it:

- Sign - 0
- Exponent -  $10110_2 = 22_{10}$
- Mantissa - 1100111101

Since  $231.625 > 0$ , sign bit  $\Rightarrow 0$

For 16 bit representation the bias is 15.

Normalized binary  $\# \Rightarrow 1.1100111102_2 \times 2^7$ .

exponent = 7

exponent w/ bias  $\Rightarrow 7 + 15 = 22_{10}$

exponent in binary  $22_{10} = 10110_2$

Drop leading 1, Mantissa  $\Rightarrow 1100111101_2$

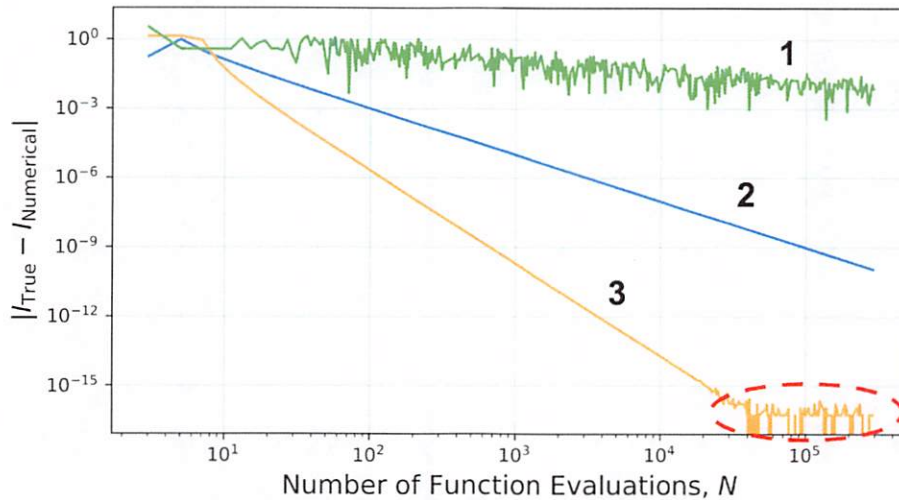
No time 😊

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## (2) Error and Numerical Integration [15pts]

Below I'm showing the accuracy of three integration methods as a function of the number of evaluations of that method. The integral is the same for each method.



(2a) Multiple Choice [5pts]: Which of the following integrators produced each of those errors? Match the number to the method:

- Trapezoid Rule - 3
- Simpson's Rule - 1
- Monte Carlo - 2

(2b) Monte Carlo Integration [5pts]: What kind of error dominates the Monte Carlo integration? Why is this distinct from the other two (grid-based) methods?

(2c) Sources of Error [5pts]: What kind of error is demonstrated in line three near  $10^5$  function evaluations (inside the dashed line)? What causes this error?

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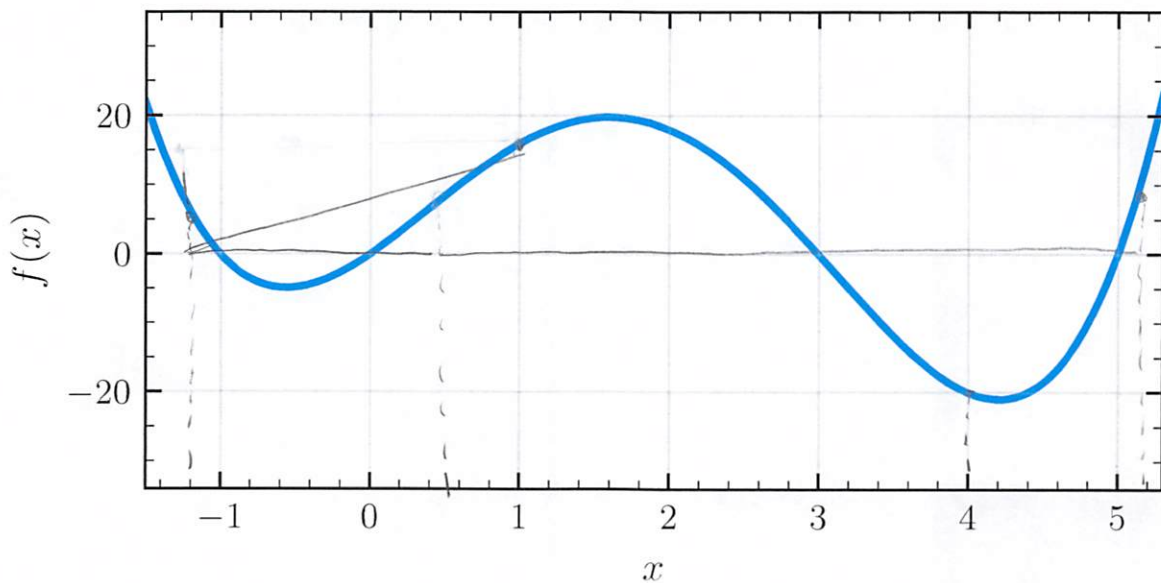
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## (2) Root finding [30pts]

For this problem we will use the quartic function

$$\begin{aligned}f(x) &= x^4 - 7x^3 + 7x^2 + 15x \\ &= x(x+1)(x-3)(x-5)\end{aligned}$$

which is shown in the plot below



**(2a) Bisection Method [10pts]** Describe how you would check whether a root is within a given interval  $[a, b]$ . If your starting interval is  $[0.5, 5.2]$  will the bisection algorithm find a root (and if so, which one)? What about  $[-1.2, 4]$ ?

We can use intermediate value thrm. The IVT states that if  $f(x)$  is continuous on  $[a, b]$  and if  $f(a)$  and  $f(b)$  have opposite signs (ie.  $f(a) \cdot f(b) < 0$ ) then there is at least one root in the interval  $[a, b]$ . If  $f(a) \cdot f(b) > 0$ , no root is guaranteed.

for the quartic function given the roots are  $x = 0, -1, 3, 5$

In the interval  $[0.5, 5.2]$ , we can evaluate the endpoints

$$f(0.5) = 0.5(0.5+1)(0.5-3)(0.5-5) = 8.4375$$

$$f(5.2) = 5.2(5.2+1)(5.2-3)(5.2-5) = 14.1856$$

Both  $f(0.5)$  and  $f(5.2)$  are positive meaning no sign change yet. We can take midpoint:  $\text{midpoint} = \frac{0.5+5.2}{2} = 2.85$

$$f(2.85) = 2.85(2.85+1)(2.85-3)(2.85-5) = 3.5488^2, \text{ still positive}$$

so continue narrowing down,  $\text{midpoint} = \frac{2.85+5.2}{2} = 4.025$

$$f(4.025) = 4.025(4.025+1)(4.025-3)(4.025-5) = -20.090^2$$

$f(4.025) < 0$  meaning there is a sign change b/w  $2.85$  and  $4.025$  so a root lies b/w these points.  $\rightarrow$  next page (attached)

2a) If we continue the bisection eventually narrowing down the interval until it converges toward  $x=3$ , which is a root of the function, ~~same~~ For the root  $x=5$ , we skip this root, even though it exists, yet we just didn't know so we take a new interval since  $f(2.85) > 0$  set  $a=2.85$  and keep  $b=5.2$ .

We will repeat the same process

$$\text{midpoint} = \frac{2.85 + 5.2}{2} = 4.025$$

~~midpoint~~  $f(4.025) = -20.09 < 0$

new interval,  $a=4.025$   $b=5.2$

$$\text{midpoint} = \frac{4.025 + 5.2}{2} = 4.6125$$

$f(4.6125) < 0$  meaning root is still b/t 4.6125 and 5.2

new interval  $a=4.6125$   $b=5.2$

$$\text{midpoint} = \frac{4.6125 + 5.2}{2} = 4.90625$$

$f(4.90625) < 0$  so now root is b/t 4.90625 and 5.2

continuing this the bisection algorithm will eventually get to a midpoint close to 5 and  $f(m)$  will approach 0, converging at  $x=5$    
  $\downarrow$   
 root

Same process applies for  $[-1.2, 4]$ .

$$f(-1.2) = -6.2544 < 0$$

$$f(4) = -20 < 0$$

Now apply bisection taking midpoint and we will see  $f(x)$  will become positive b/t  $[-1.2, 0]$  so the bisection algorithm will find the root  $x=0$  in interval  $[-1.2, 4]$ .

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(3b) **Newton-Raphson Method [14 pts]:** Unlike bisection, the Newton method needs only an initial guess,  $x_0$ , instead of a search interval. Which root do you think the Newton method will find for  $x_0 = 1$ ? Perform the first Newton-Raphson step explicitly (i.e. find  $x_1$ ), and draw a sketch of the first Newton iteration on the above figure.

$$\textcircled{1} f'(x) = 4x^3 - 14x^2 + 2x + 15$$

$$\textcircled{2} f(x_0) \text{ and } f'(x_0)$$

$$f(1) = 16$$

$$f'(1) = 7$$

$$\textcircled{3} x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 1 - \frac{16}{7} = -1.2857$$

$$x_1 \approx -1.2857$$

This means newton raphson method is now moving away from initial guess  $x_0 = 1$  toward root  $x = -1$  meaning w/  $x_0 = 1$ , method will <sup>likely</sup> converge at root  $x = -1$ .

(3c) **Fixed-point Iteration [6pts]:** Write down an auxiliary function  $g(x)$  that you could use as the basis for fixed-point iteration with the above function. Describe (but don't calculate) how you would determine if it will converge starting from  $x_0 = 2$ .

$$f(x) = 0 \text{ into form } x = g(x)$$

$$f(x) = x(x+1)(x-3)(x-5) = 0$$

take one of the factors (ex.  $x = 5$ ) and solve for  $x$

$$x = \frac{(x+1)(x-3)(x-5)}{x}$$

$$\text{or use roots directly } g(x) = \frac{x(x+1)(x-3)}{x-5}$$

To determine if the fixed point iteration will converge we must make sure  $g(x)$  is continuous on interval where we expect convergence.

Derivative test,  $g'(x)$ . if  $|g'(x)| \leq 1$  in interval of interest the  $g(x)$  is a contraction and a fixed point iteration will converge.

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#### (4) Root Finding in 2D [30pts]

For this problem we will use the complex equation

$$f(z) = z^2 - 2i$$

where  $z \in \mathbb{C}$ .

(4a) [5pts]: With  $z = x + iy$ , calculate

$$\operatorname{Re}[f] = x^2 - y^2$$

$$\operatorname{Im}[f] = 2x - 2$$

$$f(z) = (x + iy)^2 - 2i$$

$$(x + iy)^2 = x^2 + 2xiy + (iy)^2$$

$$= x^2 + 2xiy - y^2$$

$$(x + iy)^2 - (x^2 - y^2) + 2xiy$$

$$f(z) = (x^2 - y^2) + 2xiy - 2i$$

$$f(z) = (x^2 - y^2) + (2x - 2)i$$

(4b) [10pts]: Using Newton-Raphson, what would the derivative look like if I was treating the problem in 2D (i.e. if I was treating the real and imaginary parts as separate real-valued functions, not just taking the 1D derivative of  $f(z)$ )? Calculate it explicitly.

$$J = \begin{pmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{pmatrix} \quad \begin{aligned} u(x, y) &= x^2 - y^2 \\ v(x, y) &= 2x - 2 \end{aligned}$$

$$\frac{\partial u}{\partial x} = 2x$$

$$\frac{\partial v}{\partial x} = 2$$

$$\frac{\partial u}{\partial y} = -2y$$

$$\frac{\partial v}{\partial y} = 0$$

$$\Rightarrow J = \begin{pmatrix} 2x & -2y \\ 2 & 0 \end{pmatrix}$$

Newton-Raphson in 2D

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} x_n \\ y_n \end{pmatrix} - J^{-1} \cdot \begin{pmatrix} u(x_n, y_n) \\ v(x_n, y_n) \end{pmatrix}$$

$$J^{-1} = \begin{pmatrix} 0 & \frac{1}{2} \\ -\frac{1}{2y} & \frac{x}{2y} \end{pmatrix}$$

$$\text{let } (x_0, y_0) = (1, 1) \rightarrow$$

Iterations

$$0: (1, 1)$$

$$1: (1, 1)$$

$$2: (1, 1)$$

$f(1+i) = (1+i)^2 - 2i = 1 + 2i - 1 - 2i = 0$   
So 1 is a root  
and Newton Raphson  
converged quickly

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(4c) [15pts]: What is the 2D equivalent of the  $f(x)/f'(x)$  part of Newton-Raphson? I.e. what are we going to add to our first guess to look for the root? Calculate it explicitly. If you don't have an answer to part (b), describe what you should calculate here.

$$\text{Using part (b), } f(1,1) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$J = \begin{pmatrix} 2(1) & -2(1) \\ 2 & 0 \end{pmatrix} = \begin{pmatrix} 2 & -2 \\ 2 & 0 \end{pmatrix}$$

$$J^{-1} = \begin{pmatrix} 0 & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

$$\begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = J^{-1} \cdot \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

So the update does not change the initial guess since we already at a root. If we had chosen a diff initial guess, the  $\Delta x$  and  $\Delta y$  values would have provided the adjustments needed to search for root.