MA 203: Numerical Methods

Tutorial-3

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Question 1:

The Stefan-Boltzmann law can be employed to estimate the rate of radiation of energy H from a surface, as in

$$H = Ae\sigma T^4$$

where:

- H is in watts,
- A = the surface area (m^2),
- e = the emissivity (dimensionless),
- σ = Stefan-Boltzmann constant ($5.67 \times 10^{-8} \, Wm^{-2}K^{-4}$),
- T = absolute temperature (K).

Determine the error of H for a steel plate with $A = 0.15 \, m^2$, $e = 0.90$ and $T = 650 \pm 20 \, K$. Compare your results with the exact error. Repeat the computation but with $T = 650 \pm 40$. Interpret your results.

Solution:

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1. Stefan Boltzmann Law → $H = Ae\sigma T^4$

where H → rate of radiation of energy (watts)

A → surface area (m²)

e - emissivity (dimensionless)

σ - universal constant ($\sigma = 5.67 \times 10^{-8} \text{ W m}^{-2} \text{K}^{-4}$)

T - absolute temperature (K)

$A = 0.15 \text{ m}^2$

$e = 0.9$

$T = 650 \pm 20 \text{ K}$ $\Rightarrow \Delta T = 20$

If f is a func. of n independent variables; we can express error in f as follows:

$$\Delta f(x_1, \ldots, x_n) = \left|\frac{\partial f}{\partial x_1}\right| \Delta x_1 + \ldots + \left|\frac{\partial f}{\partial x_n}\right| \Delta x_n$$

here, Δx_i = error is x_i (absolute)

$= |x_i - \hat{x}_i|$

$H = Ae\sigma T^4$

$\Delta H = \left|4Ae\sigma T^3\right| \Delta T$ as $\Delta A = \Delta e = \Delta \sigma = 0$

and $\frac{\partial H}{\partial T} = 4Ae\sigma T^3$

$\Rightarrow \Delta H = (4 \times 0.15 \times 0.9 \times 5.67 \times 10^{-8} \times 650 \times 650 \times 650) \times 20$

$= 168.169$ ~~Ae\sigma T~~ W

∴ error in H = 168.169 W

H at $T = 650K \Rightarrow H = 0.15 \times 0.9 \times 5.67 \times 10^{-8} \times 650^2 \times 650^2$

$H = 1366.376$ W

∴ value of $H = 1366.376 \pm 168.169$ W

- Calculating exact error —

$$\Delta H_1 = H(T + \Delta T) - H(T)$$
$$\Delta H_2 = H(T) - H(T - \Delta T)$$

where $H(T) = A e \sigma T^4$
func. of T

$A = 0.15 m^2$
$e = 0.9$
$\sigma = 5.67 \times 10^{-8}$

Exact
~~True~~ error $= \dfrac{\Delta H_1 + \Delta H_2}{2} = \dfrac{H(T + \Delta T) - H(T)}{2} + \dfrac{H(T) - H(T - \Delta T)}{2}$

$$= \dfrac{H(650 + 20) - H(650) + H(650) - H(650 - 20)}{2}$$

$$= \dfrac{H(670) - H(630)}{2}$$

$$= \dfrac{0.15 \times 0.9 \times 5.67 \times 10^{-8} (670^4 - 630^4)}{2}$$

$$= \dfrac{1542.467 - 1205.81}{2}$$

$$= 168.328 \ W$$

exact can be defined in 2 ways, above was avg of ΔH_1 & ΔH_2
It can also be defined as $\max(\Delta H_1, \Delta H_2)$.

$\max(\Delta H_1, \Delta H_2) = \overset{max}{(1542.467 - 1366.376, \ 1366.376 - 1205.81)}$

$= \max(176.091, \ 160.566)$

$= 176.091 \ W$

∴ We can observe that exact error by avg def^n is approx. equal as the approximated error, and the exact error by max def^n differs only by a little margin.

• $T = 650 \pm 40$ K

Approximate method —

$$\Delta H = |4 A e \sigma T^3| \Delta T$$

$$= (4 \times 0.15 \times 0.9 \times 5.67 \times 10^{-8} \times 650^3) \times 40$$

$$= 336.339 \text{ W}$$

$\Rightarrow$ H will have values b/w 1366.376 ± 336.339 W

✦ exact error —

$$\Delta H_1 = H(T + \Delta T) - H(T) = H(690) - H(650)$$

$$= 0.15 \times 0.9 \times 5.67 \times 10^{-8} (690^4 - 650^4)$$

$$= 368.679 \text{ W}$$

$$\Delta H_2 = H(T) - H(T - \Delta T) = H(650) - H(610)$$

$$= 0.15 \times 0.9 \times 5.67 \times 10^{-8} (650^4 - 610^4)$$

$$= 306.546 \text{ W}$$

by avg def^n,

$$\text{exact error} = \frac{\Delta H_1 + \Delta H_2}{2}$$

$$= \frac{368.679 + 306.546}{2}$$

$$= 337.612 \text{ W}$$

by max def^n, exact error $= \max(\Delta H_1, \Delta H_2) = 368.679$ W

∴ The error calculated using approximate method is approximately equal to exact error calculated using max def avg def^n.

Question 2:

Evaluate and interpret the condition numbers for:

a. $\frac{\sin x}{1+\cos x}$ for $x = 1.0001\pi$

b. $f(x) = \sqrt{x^2 + 1} - x$ for $x = 300$

Solution:

condition number $= \dfrac{\text{Relative error in } f}{\text{Relative error in } x} \approx \dfrac{f'(\tilde{x})}{f(\tilde{x})} \dfrac{\tilde{x}}{x}$

2. a) $\dfrac{\sin x}{1 + \cos x}$ for $x = 1.0001\pi$

Condition number $= \dfrac{\text{rel. error in } f}{\text{rel. error in } x} = \dfrac{\dfrac{f(x) - f(\tilde{x})}{f(x)}}{\dfrac{x - \tilde{x}}{x}} \approx \dfrac{\dfrac{f(x) - f(\tilde{x})}{f(\tilde{x})}}{\dfrac{x - \tilde{x}}{\tilde{x}}}$

$= \dfrac{f'(\tilde{x}) \cdot \tilde{x}}{f(\tilde{x})}$

$f(x) = \dfrac{\sin x}{1 + \cos x}$

$f'(x) = \dfrac{(1 + \cos x)(\cos x) - \sin x(-\sin x)}{(1 + \cos x)^2}$

$= \dfrac{\cos x + \cos^2 x + \sin^2 x}{1 + \cos^2 x + 2\cos x}$

$= \dfrac{1 + \cos x}{(1 + \cos x)^2}$

$= \dfrac{1}{1 + \cos x}$

$f(1.0001\pi) = \dfrac{\sin(1.0001\pi)}{1 + \cos(1.0001\pi)} = -6366.1977$

$f'(1.0001\pi) = \dfrac{1}{1 + \cos(1.0001\pi)} = 20264236.895$

$\therefore$ Condition number $= \dfrac{f'(1.0001\pi)}{f(1.0001\pi)} \times 1.0001\pi$

≈ -10001 (using above values)

$|C.N| > 1 \Rightarrow$ function is ill-conditioned and unstable due to singularity at $x = \pi$.
                      undefined

2.b) $f(x) = \sqrt{x^2 + 1} - x \quad \text{for } x = 300$

$f'(x) = \dfrac{2x}{2\sqrt{x^2+1}} - 1 = \dfrac{x}{\sqrt{x^2+1}} - 1$

Condition number $= \dfrac{f'(\tilde{x})\ \tilde{x}}{f(\tilde{x})}$

$= \dfrac{\left(\dfrac{300}{\sqrt{300^2+1}} - 1\right)}{\sqrt{300^2+1} - 300} \times 300$

$= \dfrac{\dfrac{300 - \sqrt{300^2+1}}{\sqrt{300^2+1}}}{\sqrt{300^2+1}\ (\sqrt{300^2+1} - 300)} \times 300$

$= \dfrac{-1}{\sqrt{300^2+1}} \times 300$

$C.N = -0.99999$

$|C.N| < 1 \Rightarrow$ function is well conditioned and stable.

Question 3:

Real mechanical systems may involve the deflections of non-linear springs.

In Figure 1 below, a mass m is released a distance h above a non-linear spring. The resistance force F of the spring is given by

$$F = -\left(k_1 d + k_2 d^{\frac{3}{2}}\right)$$

Conservation of energy can be used to show that

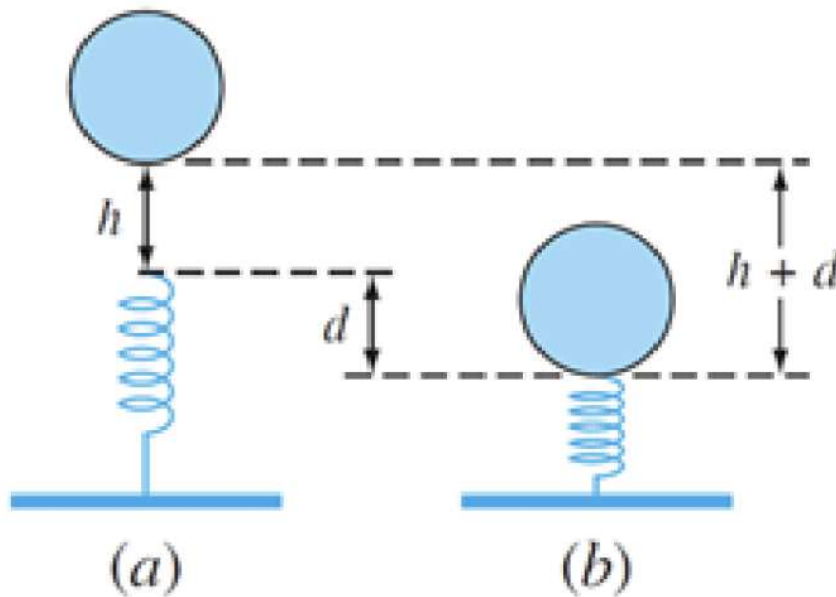$$0 = \frac{2k_2 d^{\frac{5}{2}}}{5} + \frac{1}{2} k_1 d^2 - mgd - mgh$$

Figure 1: Deflection of Spring

Solve for d using the Bisection method, given the following parameter values: $k_1 = 50{,}000\,\frac{g}{s^2}$, $k_2 = 40\,\frac{g}{s^2 m^{0.5}}$, $m = 90\,g$, $g = 9.81\,\frac{m}{s^2}$, $h = 0.45\,m$.

Solution:

The Bisection method is an iterative method that can be used to find the root of a function. The method requires an initial interval $[a, b]$ such that $f(a) \cdot f(b) < 0$. The method then iteratively halves the interval and selects the subinterval that contains the root. The process is repeated until the interval is sufficiently small.

In this case, we are looking for the value of d that satisfies the equation:

$$0 = \frac{2k_2 d^{\frac{5}{2}}}{5} + \frac{1}{2}k_1 d^2 - mgd - mgh$$

In [ ]:
```python
# Equation
def func(d, k1, k2, m, g, h):
    return (2*k2*d**(5/2))/5 + (1/2)*k1*d**2 - m*g*d - m*g*h

# Bisection method
def bisection_method(func, x_lower, x_upper, tol, k1, k2, m, g, h):
    x_mid = (x_lower+x_upper)/2
```

```
        f_lower = func(x_lower, k1, k2, m, g, h)
        f_upper = func(x_upper, k1, k2, m, g, h)
        f_mid = func(x_mid, k1, k2, m, g, h)
        n = 0

            # Ensure the initial interval is valid
        if f_lower*f_upper > 0:
            raise ValueError("The function must have opposite signs at the interval bound

        while abs(f_mid) > tol:
            if f_lower*f_mid < 0:
                x_upper = x_mid              # if the product of the function values at th
            else:
                x_lower = x_mid              # if the product of the function values at th

            x_mid = (x_lower+x_upper)/2
            f_lower = func(x_lower, k1, k2, m, g, h)
            f_upper = func(x_upper, k1, k2, m, g, h)
            f_mid = func(x_mid, k1, k2, m, g, h)
            n += 1

        return x_mid, f_mid, n
```

```
In [9]:  # Given parameters
         k1 = 50000   # (N/m)
         k2 = 40      # (N/m^(1.5))
         m = 90       # mass (kg)
         g = 9.81     # gravitational acceleration (m/s^2)
         h = 0.45     # initial height (m)
         tol = 1e-6   # tolerance for convergence

         a = 0  # Lower bound for d (m)
         b = 1  # upper bound for d (m)

         d, f, n = bisection_method(func, a, b, tol, k1, k2, m, g, h)
         print(f"The solution for d in the equation is: {d:.8f} m")
         print(f"The number of iterations is: {n}")
         print(f"The final value of the function at the root is: {f:.14f}")
```

```
The solution for d in the equation is: 0.14493285 m
The number of iterations is: 29
The final value of the function at the root is: 0.00000083563953
```

The solution for d in the equation is approximately $0.14493285\,m$. The number of iterations required for convergence is **29**, and the final value of the function at the root is approximately **0.00000083563953**.

Question 4:

The ideal gas equation of state is valid only for a limited range of pressures and temperatures. An alternative equation of state for gases is the van der Waals equation:

$$\left(p + \frac{a}{v^2}\right)(v - b) = RT$$

where v is the molar volume, and a and b are the empirical constants for a gas. A chemical engineering design project requires you to accurately estimate the molar volume of ethyl alcohol ($a = 12.02\,\text{L}^2 \cdot \text{atm} \cdot \text{mol}^{-2}$, $b = 0.08407\,\text{L} \cdot \text{mol}^{-1}$) at a temperature of $T = 400\,\text{K}$ and pressure of $p = 2.5\,\text{atm}$. Use the false position method. Compare your results with the ideal gas law prediction $v_{\text{ideal}} = \frac{RT}{p}$.

Solution:

The false position method is a numerical technique used to find the root of a function. It is an improved version of the bisection method, where instead of taking the midpoint, we use a weighted average to approximate the root more efficiently.

The van der Waals equation can be defined as a function of the molar volume v:

$$f(v) = (p + \frac{a}{v^2})(v - b) - RT = 0$$

We need to find the molar volume v that satisfies this equation.

The false position method requires two initial guesses, v_0 and v_1, such that $f(v_0)$ and $f(v_1)$ have opposite signs. The next guess, v_2, is calculated as:

$$v_2 = v_1 - f(v_1)\frac{v_1 - v_0}{f(v_1) - f(v_0)}$$

The process is repeated until the function value is within a specified tolerance.

```
In [ ]:   # Vander Waals Equation
          def f(v, p, T, R, a, b):
              return (p + (a / (v ** 2))) * (v - b) - (R * T)

          # False Position Method
          def false_position(f, x0, x1, tol=1e-6, max_iter=100):
              if f(x0) * f(x1) >= 0:
                  print("Error: No root in the initial bracket. Try different values.")
                  return None

              for i in range(max_iter):
                  x2 = x1 - (f(x1) * (x1 - x0)) / (f(x1) - f(x0)) # formula
                  print(f"Iteration {i+1}: x2 = {x2:.6f}, f(x2) = {f(x2):.6f}")
```

```python
        if abs(f(x2)) < tol:
            return x2, i+1

        if f(x0)*f(x2) < 0:
            x1 = x2
        else:
            x0 = x2

    return x2, i+1


# Constants
R = 0.08206      # L.atm/(K.mol)
a = 12.02                # L^2.atm/mol^2
b = 0.08407      # L/mol
T = 400                  # K
p = 2.5                  # atm
tol = 1e-6               # Tolerance

# Initial guesses
x0 = 10
x1 = 15

vanderwaal_v, iterations = false_position(lambda v: f(v, p, T, R, a, b), x0, x1, tol)
print(f"\nVolume according to Van der Waals equation = {vanderwaal_v:.6f} L/mol")

ideal_v = R*T / p
print(f"Volume according to ideal gas law = {ideal_v:.6f} L/mol")

print(f"Difference = {abs(ideal_v - vanderwaal_v):.6f} L/mol")
print(f"Percentage error = {(abs(ideal_v - vanderwaal_v) / ideal_v * 100):.2f}%")
print("Number of iterations:", iterations)
```

```
Iteration 1: x2 = 12.826233, f(x2) = -0.037593
Iteration 2: x2 = 12.841651, f(x2) = -0.000159
Iteration 3: x2 = 12.841716, f(x2) = -0.000001

Volume according to Van der Waals equation = 12.841716 L/mol
Volume according to ideal gas law = 13.129600 L/mol
Difference = 0.287884 L/mol
Percentage error = 2.19%
Number of iterations: 3
```

Results:

- The molar volume of ethyl alcohol at $T = 400\,\mathrm{K}$ and $p = 2.5\,\mathrm{atm}$ is approximately $12.841716\,\mathrm{L/mol}$ using the van der Waals equation of state.
- The ideal gas law prediction gives a molar volume of $13.129600\,\mathrm{L/mol}$.
- The absolute difference is $0.287884\,\mathrm{L/mol}$, which is a percentage difference of 2.19%.
- The number of iterations required was 3.