

CE 311K - McKinney

HW-13 Numerical Integration

1. Integrate the following function

$$I = \int_0^3 x e^{2x} dx$$

- (a) analytically
- (b) Trapezoid Rule using $n = 4$, and
- (c) Simpson's Rule using $n = 4$.

Compute the percent error for both numerical integrations using the analytical value as the true value.

(a) analytically

$$I = \int_0^3 x e^{2x} dx$$

$$\text{Let } u = x, \text{ then } du = dx; dv = e^{2x} dx, \text{ and } v = \frac{1}{2} e^{2x}$$

$$\int u dv = uv - \int v du$$

$$\int x e^{2x} dx = x \left(\frac{1}{2} e^{2x} \right) - \int \frac{1}{2} e^{2x} dx$$

$$I = \int_0^3 x e^{2x} dx = \frac{e^{2x}}{4} (2x - 1) \Big|_0^3 = 504.536$$

Using $n = 4$

$x_0 = 0$	$f(x_0) = 0$
$x_1 = 0.75$	$f(x_1) = 3.36$
$x_2 = 1.5$	$f(x_2) = 30.13$
$x_3 = 2.25$	$f(x_3) = 202.54$
$x_4 = 3$	$f(x_4) = 1210.29$

(b) Trapezoid Rule

$$\int_a^b f(x)dx \approx \frac{(b-a)}{2} [f(a) + f(b)] = \frac{(3-0)}{2} [0 + 1210.29] = 630.8784$$

error = -25.04%

(c) Simpson's Rule.

$$\int_a^b f(x)dx \approx \frac{(b-a)}{3} [f(a) + 4f(\frac{a+b}{2}) + f(b)] = \frac{(3-0)}{3} [0 + 4(3.36 + 202.29) + 1210.29] = 523.5356$$

error = -3.77%

2. Integration provides a means to compute how much mass enters or leaves a reactor over a specified time period, as in

$$M = \int_{t_1}^{t_2} Qc dt$$

where t_1 and t_2 are the initial and final times. This formula makes intuitive sense if you recall the analogy between integration and summation. Thus the integral represents the summation of the product of flow times concentration to give the total mass entering or leaving from t_1 to t_2 . If the flow rate is constant, Q can be moved outside the integral. The outflow chemical concentration from a completely mixed reactor is measured as:

$t, \text{ min}$	0	5	10	15	20	30	40	50	60
$c, \text{ mg/m}^3$	10	20	30	40	60	80	70	50	60

For an outflow of $Q = 10 \text{ m}^3/\text{min}$, use Simpson's 1/3 rule to estimate the mass of chemical that exits the reactor from $t = 0$ to 60 min. Solve the integral using Simpson's rule for the mass entering the reactor.

$$\int_a^b f(x)dx \approx \frac{\Delta x}{3} (f_0 + 4f_1 + 2f_2 + 4f_3 + \dots + 2f_{n-2} + 4f_{n-1} + f_n)$$

$$\begin{aligned} \int_0^{60} c(t)dt &\approx Q \frac{\Delta t}{3} (c_0 + 4c_1 + 2c_2 + 4c_3 + c_4) + Q \frac{\Delta t}{3} (c_4 + 4c_5 + 2c_6 + 4c_7 + c_8) \\ &= 10 * \frac{5}{3} (10 + 4 * 20 + 2 * 30 + 4 * 40 + 60) + 10 * \frac{10}{3} (60 + 4 * 80 + 2 * 70 + 4 * 50 + 60) \\ &= 10 * (616.67 + 2600) \\ &= 321667.0 \text{ mg } (0.321667 \text{ kg}) \end{aligned}$$

3. Integrate the function tabulated in the following table using the Trapezoid Rule.

x	$f(x)$	x	$f(x)$
1.6	4.953	2.8	16.445
1.8	6.050	3.0	20.086
2.0	7.389	3.2	24.533
2.2	9.025	3.4	29.964
2.4	11.023	3.6	36.598
2.6	13.464	3.8	44.701

If the values in the table are from the exponential function $f(x) = e^x$, find the true value of the integral and compute the percent error in your integration.

$$\int_a^b f(x)dx \approx \frac{\Delta x}{2}(f_0 + 2f_1 + 2f_2 + \dots + 2f_{n-2} + 2f_{n-1} + f_n) = \frac{\Delta x}{2}(f_0 + 2\sum_{i=1}^{n-1} f_i + f_n)$$

$$\int_{1.6}^{3.8} f(x)dx \approx \frac{0.2}{2}(4.953 + 2 * 349.154 + 44.701) = 39.88$$

$$\begin{aligned} \int_{1.6}^{3.8} e^x dx &= e^x \Big|_{1.6}^{3.8} \\ &= e^{3.8} - e^{1.6} \\ &= 44.701 - 4.953 \\ &= 39.748 \end{aligned}$$

Error

$$Error = \left| \frac{39.748 - 39.88}{39.748} \right| * 100 = 0.33\%$$