Taller 2 - Métodos Comp.

2.1. Simpson 3/8

En este método tenemos 4 puntos igualmente espaciados que vamos a interpolar con Lagrange para generar un polinomio de grado 3 & aproximar el área bajo su curva (integrar).

i) Polinomio de Lagrange (grado 3)

$$P_3(x) = \sum_{k=0}^{3} f(x_k) L_k(x)$$
$$= f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x) + f(x_3)L_3(x)$$

$$L_0(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}$$

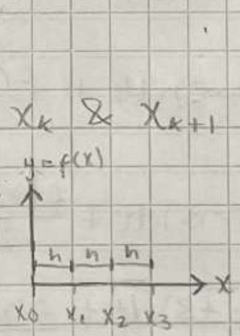
$$L_1(x) = \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}$$

$$L_3(x) = \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}$$

Sea h la distancia entre x_k & x_{k+1}, la definimos como

$h = \frac{x_3 - x_0}{3}$, y se ve así:



En los polinomios de arriba reemplazamos: $(x_0-x_1) = -h$
$(x_0-x_2) = -2h$
$(x_0-x_3) = -3h$
$\vdots$ etc.

También, x se puede definir como $x = x_0 + th$ & cada x_k como $x_0 = x_0$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$, $x_3 = x_0 + 3h$. Si reemplazo en

$(x-x_0) = th$
$(x-x_1) = x - x_0 - h = th - h$
$(x-x_2) = x - x_0 - 2h = th - 2h$
$(x-x_3) = x - x_0 - 3h = th - 3h$

Ahora reemplazo todo esto en los polinomios de arriba

$$L_0(t) = \frac{(th-h)(th-2h)(th-3h)}{(-h)(-2h)(-3h)} = \frac{h^3(t-1)(t-2)(t-3)}{-6h^3} = \frac{(t-1)(t-2)(t-3)}{-6}$$

$$L_1(t) = \frac{(th)(th-2h)(th-3h)}{h(-h)(-2h)} = \frac{h^3\, t(t-2)(t-3)}{2h^3} = \frac{t(t-2)(t-3)}{2}$$

$$L_2(t) = \frac{(th)(th-h)(th-3h)}{(2h)(h)(-h)} = \frac{h^3\, t(t-1)(t-3)}{-2h^3} = \frac{t(t-1)(t-3)}{-2}$$

$$L_3(t) = \frac{(th)(th-h)(th-2h)}{(3h)(2h)(h)} = \frac{h^3\, t(t-1)(t-2)}{6h^3} = \frac{t(t-1)(t-2)}{6}$$

ii) Integración

La integral (área bajo la curva) está dada por:

$$A \approx f(x_0)\int_{x_0}^{x_3} L_0(x) + f(x_1)\int_{x_0}^{x_3} L_1(x) + f(x_2)\int_{x_0}^{x_3} L_2(x) + f(x_3)\int_{x_0}^{x_3} L_3(x)$$

Como se hizo un cambio de variable, los límites también cambian: $x_0 = x_0 + th \to t = 0$

$x_3 = x_0 + th \to x_3 - x_0 = th \to 3h = th \to t = 3$ & $\frac{dx}{dt} = h$

$\hookrightarrow dx = h\,dt$

Se reescribe la integral como

$$A \approx \frac{f(x_0)h}{-6}\int_0^3 (t-1)(t-2)(t-3)\,dt + \frac{f(x_1)\cdot h}{2}\int_0^3 t(t-2)(t-3)\,dt$$
$$-\frac{f(x_2)h}{2}\int_0^3 t(t-1)(t-3)\,dt + \frac{f(x_3)h}{6}\int_0^3 t(t-1)(t-2)\,dt$$

$$A \approx \frac{f(x_0)h}{-6}\int_0^3 (t^2-3t+2)(t-3)\,dt + \frac{f(x_1)h}{2}\int_0^3 t(t^2-5t+6)\,dt$$
$$-\frac{f(x_2)h}{2}\int_0^3 t(t^2-4t+3)\,dt + \frac{f(x_3)h}{6}\int_0^3 t(t^2-3t+2)\,dt$$

$$A \approx \frac{f(x_0)h}{-6}\int_0^3 (t^3-6t^2+11t-6)\,dt + \frac{f(x_1)h}{2}\int_0^3 (t^3-5t^2+6t)\,dt$$
$$-\frac{f(x_2)h}{2}\int_0^3 (t^3-4t^2+3t)\,dt + \frac{f(x_3)h}{6}\int_0^3 (t^3-3t^2+2t)\,dt$$

$$A \approx \frac{f(x_0)h}{-6}\left(\frac{t^4}{4} - 2t^3 + \frac{11t^2}{2} - 6t\Big|_0^3\right) + \frac{f(x_1)h}{2}\left(\frac{t^4}{4} - \frac{5t^3}{3} + 3t^2\Big|_0^3\right)$$
$$-\frac{f(x_2)h}{2}\left(\frac{t^4}{4} - \frac{4t^3}{3} + \frac{3t^2}{2}\Big|_0^3\right) + \frac{f(x_3)h}{6}\left(\frac{t^4}{4} - t^3 + t^2\Big|_0^3\right)$$

$$A \approx -\frac{f(x_0)h}{6}\left(-\frac{9}{4}\right) + \frac{f(x_1)h}{2}\left(\frac{9}{4}\right) - \frac{f(x_2)h}{2}\left(-\frac{9}{4}\right) + \frac{f(x_3)h}{6}\left(\frac{9}{4}\right)$$

$$A \approx f(x_0)h\left(\frac{3}{8}\right) + f(x_1)h\left(\frac{9}{8}\right) + f(x_2)h\left(\frac{9}{8}\right) + f(x_3)h\left(\frac{3}{8}\right)$$

$$A \approx \frac{3}{8}h\left(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right)$$

Finalmente, dadas las siguientes equivalencias: $x_0 = x_i$
$x_1 = x_{i+1}$
$x_2 = x_{i+2}$
$x_3 = x_{i+3}$

se puede afirmar que

$$\int_{x_i}^{x_{i+3}} f(x)\,dx \approx \frac{3}{8}h\left(f(x_i) + 3f(x_{i+1}) + 3f(x_{i+2}) + f(x_{i+3})\right)$$

3:

1

$$P(v) = 4\pi \left(\frac{M}{2\pi R T}\right)^{3/2} \cdot v^2 \cdot e^{\left(-\frac{M V^2}{2RT}\right)}$$

Remplazando:

$$u = \frac{MV^2}{2RT} \qquad V=0 \rightarrow u=0 \qquad V=\infty \rightarrow u=\infty$$

$$du = \frac{\cancel{2}MV}{\cancel{2}RT}\, dV$$

$$dV = \frac{RT\, du}{MV}$$

$$V = \sqrt{\frac{2uRT}{M}}$$

$$\int_0^\infty 4\pi \left(\frac{M}{2\pi R T}\right)^{3/2} \cdot V^{\cancel{2}} \cdot e^{-u} \cdot \frac{R \cdot T}{M \cdot \cancel{V}} \cdot du$$

$$= \int_0^\infty 4\pi \sqrt{\left(\frac{M}{2\pi R T}\right)^3} \cdot \sqrt{\frac{2uRT}{M}} \cdot e^{-u} \cdot \frac{RT}{M} \cdot du$$

$$= \int_0^\infty 4\pi \cdot \sqrt{\frac{M^3}{\cancel{8}_4 \pi^3 R^3 T^3} \cdot \frac{\cancel{2}uRT}{M}} \cdot e^{-u} \cdot \frac{RT}{M} \cdot du$$

$$= \int_0^\infty 4\pi \cdot \sqrt{\frac{M^2 \cdot u}{4\pi^3 \cdot R^2 T^2}} \cdot e^{-u} \cdot \frac{RT}{M} \cdot du$$

$$= \int_0^\infty \cancel{4}^{2}\cancel{\pi} \cdot \frac{1}{\cancel{2\pi}} \cdot \sqrt{\frac{u}{\pi}} \cdot \frac{\cancel{M}}{\cancel{R \cdot T}} \cdot e^{-u} \cdot \frac{\cancel{RT}}{\cancel{M}}\, du$$

$$= \int_0^\infty 2 \cdot \sqrt{\frac{u}{\pi}} \cdot e^{-u}\, du$$ → Mediante python (código) demostramos que esta integral es igual a 1. (Cuadratura de Laguerre).

Por lo tanto:

$\int_0^\infty 2 \cdot \sqrt{\frac{u}{\pi}} \cdot e^{-u}\, du = 1$, es decir, $\int_0^\infty P(v)\, dv$ es una distribución de probabilidad.

3. 5.

$E_{int} = \frac{3}{2} nRT \rightarrow E_{int} = E_{cinética}$

$\frac{1}{2} m v^2 = \frac{3}{2} RTn \rightarrow V = V_{rms} = \sqrt{\frac{3RT}{M}}$

$\frac{1}{2} m \cdot \left(\cancel{\sqrt{\frac{3RT}{M}}}\right)^{\cancel{2}} = \frac{3}{2} RTn$

$\frac{1}{2} m \cdot \frac{3RT}{M} = \frac{3}{2} RTn$

$\frac{3}{2} \frac{m}{M} \cdot RT = \frac{3}{2} nRT \rightarrow m = n \cdot M$

$n = \frac{m}{M}$

$\frac{3}{2} n \cdot RT = \frac{3}{2} nRT.$

De esta manera se comprueba que $E_{int} = \frac{3}{2} nRT$