I. Simpson's rule

a. Show Simpson's rule on $[-1, 1]$ by given equation

Assume $p_3(x) = a_3x^3 + a_2x^2 + a_1x + a_0$, then follow the interpolation conditions

$$\begin{cases} a_3 + a_2 + a_1 + a_0 = y(1) \\ a_0 = y(0) \\ a_1 = y'(0) \\ -a_3 + a_2 - a_1 + a_0 = y(-1) \end{cases}$$

We can get the four coefficients

$$\begin{cases} a_3 = \dfrac{y(1) - y(-1) - 2y'(0)}{2} \\ a_2 = \dfrac{y(1) + y(-1) - 2y(0)}{2} \\ a_1 = y'(0) \\ a_0 = y(0) \end{cases}$$

namely, $p_3(x) = \frac{y(1)-y(-1)-2y'(0)}{2}x^3 + \frac{y(1)+y(-1)-2y(0)}{2}x^2 + y'(0)x + y(0)$

$$I^S(y) = \int_{-1}^{1} p_3(x)\mathrm{d}x = \frac{y(1) + y(-1) + 4y(0)}{3} \tag{1}$$

b. Derive $E^S(y)$

According to theorem 3.27, we get

$$y(x) - p_3(x) = \frac{y^{(4)}(\xi(x))}{24}x^2(x + 1)(x - 1) \tag{2}$$

Apply integral on $[-1, 1]$ to each side,

$$E^S(y) = I(y) - I^S(y) = \int_{-1}^{1} y(x) - p_3(x)\mathrm{d}x \tag{3}$$

$$= \int_{-1}^{1} \frac{y^{(4)}(\xi(x))}{24}x^2(x + 1)(x - 1)\mathrm{d}x \tag{4}$$

$$\tag{5}$$

We can find $\zeta \in [-1, 1]$ such that

$$E^S(y) = \frac{y^{(4)}(\zeta)}{24}\int_{-1}^{1} x^2(x + 1)(x - 1)\mathrm{d}x = -\frac{y^{(4)}(\zeta)}{90} \tag{6}$$

by theorem 0.56

c. Using (a), (b) and a change of variable

Define $h = \frac{b-a}{n}$ where n is even and $x_k = a + kh$ where $h = 0, 1, \cdots, n$. Firstly, We can consider the first subinterval $[x_0, x_2]$ with (a) conclusion

$$I_1^S(y) = \frac{h}{3}(y(x_0) + 4y(x_1) + y(x_2)) = \int_{x_0}^{x_2} f_1(x)\mathrm{d}x \tag{7}$$

where f_1 is obtained by conditions $f_1(x_0) = y(x_0)$ and $f_1(x_1) = y(x_1)$ and $f_1'(x_1) = y'(x_1)$ and $f_1(x_2) = y(x_2)$, besides, the index 1 stands for the x_1. Similar with (b), we can get

$$E_1^S(y) = \frac{y^{(4)}(\zeta)}{24}\int_{x_0}^{x_2} (x - x_1)^2(x - x_0)(x - x_2)\mathrm{d}x = -\frac{h^5}{90}y^{(4)}(\zeta_1) \tag{8}$$

Secondly, sum up all the subintervals

$$I_n^S(y) = \sum_{i=0}^{n/2-1} I_{2i+1}^S(y) = \sum_{i=0}^{n/2-1} \frac{h}{3}[y(x_{2i}) + 4y(x_{2i+1}) + y(x_{2i+2}))] \tag{9}$$

Accodingly, the remainder is

$$E_n^S(y) = \sum_{i=0}^{n/2-1} E_{2i+1}^S(y) = -\frac{h^5}{90}\sum_{i=0}^{n/2-1} y^{(4)}(\zeta_{2i+1}) = -\frac{h^5}{90}\cdot\frac{n}{2}y^{(4)}(\zeta) \tag{10}$$

by using theorem 0.42. Notice that $b-a=nh$, therefore,

$$E_n^S(y) = -\frac{(b-a)}{180}h^4 y^{(4)}(\zeta) \tag{11}$$

II. Estimate the number of subintervals required

a. by the composite trapezoidal rule

Define $f(x) = e^{-x^2}$, then $f''(x) = 2(2x^2-1)e^{-x^2} \in (-2, \frac{2}{e})$ for $x \in (0,1)$. According to theorem 7.14, there $\exists \xi \in (0,1)$ such that

$$E_n^T(f) = -\frac{h^2}{12}f''(\xi) \tag{12}$$

where $h = \frac{b-a}{n} = \frac{1}{n}$, so that $|E_n^T(f)| = |\frac{f''(\xi)}{12n^2}| < \frac{1}{6n^2}$. When the absolute error $|E_n^T(f)| \le 0.5\times 10^{-6}$, we can get n must be greater than 578.

b. by the composite Simpson' rule

We can deduce that $f^{(4)}(x) = 4e^{-x^2}(4x^4-12x^2+3)$ which reaches the minimum on $x = \frac{5-\sqrt{10}}{2}$ and hits the top on $x=0$. In other word, $f^{(4)}(x) \in [f^{(4)}(\frac{5-\sqrt{10}}{2}), f^{(4)}(0)] = [-7.36, 12]$ so that $|f^{(4)}(x)| \le 12$. As a result, the absolute error is

$$|E_n^S(f)| = \frac{1}{180n^4}f^{(4)}(\xi) \le \frac{1}{15n^4} \tag{13}$$

When the absolute error $|E_n^S(f)| \le 0.5\times 10^{-6}$, we can get n must be greater than 20.

III. Guass-Laguerre quadrature formula

a. Construct a polynomial orthogonal to $\mathbb{P}_1$

Define $p(x) = kx+m$, then we can get

$$\int_0^\infty p(t)\pi_2(t)\rho(t)\mathrm{d}t = k(2a+b+6) + m(a+b+2) \tag{14}$$

by using formula $\int_0^\infty t^m e^{-t} = m!$. The condition requires $\int_0^\infty p(t)\pi_2(t)\rho(t)\mathrm{d}t = 0$ for $\forall k, m \in \mathbb{R}$ so that

$$\begin{cases} 2a+b+6=0 \\ a+b+2=0 \end{cases}$$

Consequently, we obtain the coefficients

$$\begin{cases} a=-4 \\ b=2 \end{cases}$$

Namely, the polynomial $\pi_2(x) = x^2-4x+2$ orthogonal to $\mathbb{P}_1$.

b. Derive two-point Guass-Laguerre quadrature formula and express $E_2(f)$

According to corollary 7.22, we can get

$$\omega_1 = \int_0^\infty \frac{v_n(t)}{(t-t_1)v_n'(t_1)} e^{-t}\mathrm{d}t = \int_0^\infty \frac{t-t_2}{t_1-t_2} e^{-t}\mathrm{d}t = \frac{1-t_2}{t_1-t_2} \tag{15}$$

$$\omega_2 = \int_0^\infty \frac{v_n(t)}{(t-t_2)v_n'(t_2)} e^{-t}\mathrm{d}t = \int_0^\infty \frac{t-t_1}{t_2-t_1} e^{-t}\mathrm{d}t = \frac{1-t_1}{t_2-t_1} \tag{16}$$

$$\tag{17}$$

Since the function $\pi_2(t)$ has zeros at $t_1 = 2-\sqrt{2}$ and $t_2 = 2+\sqrt{2}$. Consequently, the two-point Gruass-Laguerre quadrature formula is

$$I^G(f) = \frac{2+\sqrt{2}}{4} f(2-\sqrt{2}) + \frac{2-\sqrt{2}}{4} f(2+\sqrt{2}) \tag{18}$$

As for the reminder, we can utilize theorem 7.28

$$E_2^G(f) = \frac{f^{(4)}(\tau)}{24} \int_0^\infty e^{-t} v_n^2(t)\mathrm{d}t = \frac{f^{(4)}(\tau)}{6} \tag{19}$$

where $\tau \in (0, \infty)$.

c. Apply formula in (b) to approximate I and estimate error

When $f(t) = \frac{1}{1+t}$, we can get

$$\begin{cases} f(2-\sqrt{2}) = \dfrac{3+\sqrt{2}}{7} \\ f(2+\sqrt{2}) = \dfrac{3-\sqrt{2}}{7} \\ f^{(4)}(\tau) = \dfrac{24}{(1+\tau)^5} \end{cases}$$

Next, take them into formula (18) and (19)

$$I = \frac{4}{7} + \frac{4}{(1+\tau)^5} \tag{20}$$

Using the exact value $I = 0.596347361\cdots$, we know that $\tau \approx 1.76$.