4. Numerical Differentiation and Integration

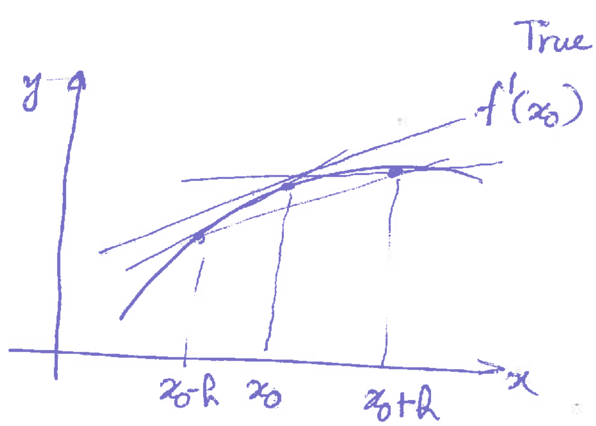
4.1. Numerical Differentiation

In this section, we numerically find $f'(x)$ evaluated at $x = x_0$.

- May be $f'(x)$ has a complicated expression, or
- $f(x)$ is not explicitly given

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0+h) - f(x_0)}{h}. \quad (\text{Small } h > 0)$$

Finite Difference formulas



(*) Two-point forward-difference formula (FDF)

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h}. \quad \text{—(1)}$$

(*) Two-point backward difference formula (BDF)

$$f'(x_0) \approx \frac{f(x_0) - f(x_0-h)}{h} \quad — (2)$$

(*) Two-point Centred difference formula (CDF)

$\frac{(1)+(2)}{2}$ $$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h}$$

ex. Let $f(x) = x^2 e^x$ Approximate $f'(1)$ using FDF, BDF, and CDF with $h = 0.2$

$x_0 = 1$.

FDF $$f'(1) \approx \frac{f(1.2) - f(1)}{0.2} = \frac{4.78 - 2.71}{0.2} = 10.35$$

BDF $$f'(1) \approx \frac{f(1) - f(0.8)}{0.2} = \frac{2.71 - 1.42}{0.2} = 6.45.$$

CDF $$f'(1) \approx \frac{f(1.2) - f(0.8)}{2(0.2)} \approx 8.4.$$

True value $f'(1) = 3e$.

absolute error $= |10.35 - 3e| = 2.19$
$|6.45 - 3e| = 1.7$
$|8.4 - 3e| = 0.24$

Errors in finite difference formulas

By the Taylor's Thm on f about x_0, we get

$$f(x) = f(x_0) + \frac{f'(x_0)}{1!}(x-x_0) + \frac{f''(\xi_1)}{2!}(x-x_0)^2$$

Set $x = x_0 + h$.

$$f(x_0+h) = f(x_0) + \frac{f'(x_0)}{1!}\cancel{(x-x_0)}\,h + \frac{f''(\xi_1)}{2!}h^2$$

for some $\xi_1 \in (x_0, x_0+h)$

Then, $$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{f''(\xi_1)}{2!}h$$

$\therefore$ The maximum error in FDF is

$$\frac{h}{2} \max_{x \in (x_0, x_0+h)} |f''(\xi_1)|$$

$$\parallel$$

$$h\, C \quad \text{where } C = \frac{\max |f''(\xi)|}{2}.$$

$\Rightarrow$ error is proportional to h^1.

$O(h^1)$ the FDF is an order 1 approximation

$\Rightarrow$ we can make the error small by making h small

$\Rightarrow$ Similarly BDF is also $O(h^1)$

Note

The fact that the formula is 1^{st}-order means that cutting h in half should cut the error approximately in half.

$\left(\frac{f''}{2}(z_1) \leftarrow \text{proportionality constant} \right)$

For central CDF, note that

$$f(x_0+h) = f(x_0) + \frac{f'(x_0)h}{1!} + \frac{f''(x_0)h^2}{2!} + \frac{f'''(z_1)h^3}{3!} \quad \text{—①}$$

$$f(x_0-h) = f(x_0) - \frac{f'(x_0)h}{1!} + \frac{f''(x_0)h^2}{2!} - \frac{f'''(z_2)h^3}{3!} \quad \text{—②}$$

for some $z_1 \in (x_0, x_0+h)$ and $z_2 \in (x_0-h, x_0)$

$$\frac{① - ②}{2h}$$

$$f(x_0+h) - f(x_0-h) = 2f'(x_0)h + \frac{[f'''(\xi_1) + f'''(\xi_2)]}{3!}h^3$$

$$\Rightarrow \quad f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} + \frac{f'''(\xi_1) + f'''(\xi_2)}{3! \quad 2} h^2$$

$\Rightarrow$ Using the IVT

$$f'''(\xi) = \frac{f'''(\xi_1) + f'''(\xi_2)}{2}$$

for some $\xi \in (\xi_2, \xi_1) \subset (x_0-h, x_0+h)$

Finally, we get

$$f'(x_0) = \frac{f(x_0+h) - f(x_0+h)}{2h} + \frac{f'''(\xi)}{6} h^2$$

The max^m error is $\dfrac{h^2}{6} \max |f'''(\xi)|$

Note

$\Rightarrow$ CDF is 2^{nd}-order accurate $\mathcal{O}(h^2)$, which is better than BDF and FDF.

ex. Consider $f(x) = x^2 e^x$.

Find the maxi^m error in approximating $f'(1)$ by the FDF, BDF, and CDF with $h = 0.2$

$$\left.\begin{aligned} f''(x) &= (x^2+4x+2)\,e^x, \text{ and} \\ f'''(x) &= (x^2+6x+6)\,e^x \end{aligned}\right\} \leftarrow \text{Increasing fun}^{ns}$$

Maxi^m error in FDF $\quad \dfrac{0.2}{2} \displaystyle\max_{x\in(1,1.2)} \underbrace{|f''(x)|}_{f''(1.2)} \approx 2.73$

BDF $\quad \dfrac{0.2}{2} \displaystyle\max_{x\in(0.8,1)} \underbrace{|f''(x)|}_{f''(1)} = 1.9$

CDF $\quad \dfrac{(0.2)^2}{6} \displaystyle\max_{x\in(0.8,1.2)} \underbrace{|f'''(x)|}_{f'''(1.2)} = 0.32$

4.1. Derivative from Lagrange Polynomial

If $f(x)$ is not explicitly given but we know $(x_i, f(x_i))$ for $i = 0, \dots, n$, then f can be approximated by the Lagrange polynomial.

Recall:

$$f(x) = \sum_{i=0}^{n} f(x_i) L_i(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

$\uparrow$ $(n+1)$ terms.

where $\xi \in (x_0, x_n)$.

and $$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}$$

Differentiating both sides and evaluating at $x = x_j$, we get

$$f'(x_j) = \sum_{i=0}^{n} f(x_i) L_i'(x_j) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{\substack{i=0 \\ i \neq j}}^{n} (x_j - x_i)$$

$(n+1)$ - Points formula to approximate $f'(x_j)$

Three-point formulas

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \qquad L_0'(x) = \frac{(x-x_1)+(x-x_2)}{(x_0-x_1)(x_0-x_2)}$$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \qquad L_1'(x) = \frac{(x-x_2)+(x-x_0)}{(x_1-x_0)(x_1-x_2)}$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \qquad L_2'(x) = \frac{(x-x_1)+(x-x_0)}{(x_2-x_0)(x_2-x_1)}$$

$$f'(x_j) = f(x_0)\left[\frac{(x-x_1)+(x-x_2)}{(x_0-x_1)(x_0-x_2)}\right] + f(x_1)\left[\frac{(x-x_2)+(x-x_0)}{(x_1-x_0)(x_1-x_2)}\right]$$

$$+ f(x_2)\left[\frac{(x-x_1)+(x-x_0)}{(x_2-x_0)(x_2-x_1)}\right]$$

$$+ \frac{f^{(3)}(\xi)}{3!} \prod_{\substack{i=0 \\ i \neq j}}^{2} (x_j - x_i)$$

* If the nodes are equally spaced and

$x_1 = x_0 + h$ and $x_2 = x_0 + 2h$,

then

$$f'(x_0) = f(x_0)\left[\frac{-h-2h}{(-h)(-2h)}\right] + f(x_1)\left[\frac{-2h+0}{(+h)(-h)}\right]$$

$$+ f(x_2)\left[\frac{-h}{(2h)(h)}\right] + \frac{f^{(3)}(\xi)}{6}(x_0-x_1)(x_0-x_2)$$

$$f'(x_0) = f(x_0)\frac{-3h}{2h^2} + f(x_1)\frac{2h}{h^2} - f(x_2)\frac{h}{2h^2}$$

$$+ \frac{f^{(3)}(\xi)}{6}(-h)(-2h)$$

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_1) - f(x_2)}{2h} + \frac{f^{(3)}(\xi)\,h^2}{3}$$

Three-Point FDF

$$f'(x_0) \approx \frac{\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right]}{2h}$$

Three - Point BDF

$$f'(x_0) \approx \frac{3f(x_0) - 4f(x_0-h) + f(x_0-2h)}{2h}$$

ex. From the following table approximate $f'(1)$ by the 3-point FDF and BDF.

x	0.6	0.8	1	1.2	1.4
$f(x)$	0.65	1.42	2.71	4.78	7.94

3-Pt FDF $\quad f'(1) \approx \dfrac{-3f(1) + 4f(1.2) - f(1.4)}{2(0.2)} = 7.62$

3-Pt BDF $\quad f'(1) = \dfrac{3f(1) - 4f(0.8) + f(0.6)}{2(0.2)} = 7.75.$

The table is given for $f(x) = x^2 e^x$. So $f'(1) = 3e$.

$\Rightarrow$ Absolute error $= |7.62 - 3e| = 0.53$

$|7.75 - 3e| = 0.4$

Note 3-Point formulas give less error than 2-Pt FDF and BDF.

4.3. Elements of Numerical Integration

The basic method involved in approximating $\int_a^b f(x)dx$ is called numerical quadrature.

Sometimes, it is hard to calculate a definite integral analytically.

ex. $\int_0^1 e^{x^2} dx$

To approximate such an integral, we break the interval $[a,b]$ into subintervals $[x_0, x_1], [x_1, x_2], \ldots [x_{n-1}, x_n]$ where

$x_i = a + ih \quad i = 0, \ldots, n$ and $h = \frac{b-a}{n}$

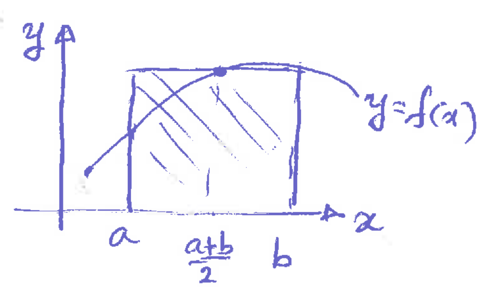
h ← step size. n ← n - number of intervals

Then, we approximate the integral by a finite sum given by

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} a_i f(x_i)$$

① Mid point Rule.

$$\int_a^b f(x)dx \approx (b-a) f\left(\frac{a+b}{2}\right)$$

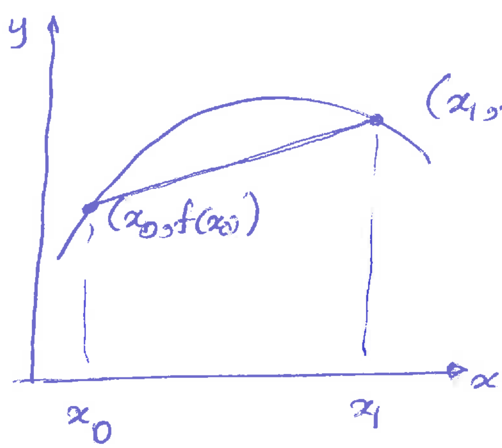


Other quadrature rules

Recall; the Lagrange interpolating polynomial

$$f(x) = \underbrace{\sum_{i=0}^{n} f(x_i) L_i(x)}_{P_1(x)} + \prod_{i=0}^{n} (x - x_i) \frac{f^{(n+1)}(\xi(x))}{(n+1)!}$$

1. The Trapezoidal rule



$$L_0(x) = \frac{(x - x_1)}{(x_0 - x_1)} \qquad L_1(x) = \frac{(x - x_0)}{(x_1 - x_0)}$$

Then,

$$f(x) = \frac{x - x_1}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1)$$

$$+ \; (x - x_0)(x - x_1) \frac{f^{(2)}(c(x))}{2!}$$

Now,

$$\int_{x_0}^{x_1} f(x)\,dx = \int_{x_0}^{x_1} \frac{(x-x_1)}{(x_0-x_1)} f(x_0)\,dx + \int_{x_0}^{x_1} \frac{(x-x_0)}{(x_1-x_0)} f(x_1)\,dx$$

$$+ \int_{x_0}^{x_1} (x-x_0)(x-x_1) \frac{f^{(2)}(c(x))}{2!}$$

$$= \frac{(x-x_1)^2}{2(x_0-x_1)} \Bigg|_{x_0}^{x_1} f(x_0) + \frac{(x-x_0)^2}{2(x_1-x_0)} \Bigg|_{x_0}^{x_1} f(x_1)$$

$$+ \int_{x_0}^{x_1} (x-x_0)(x-x_1) \frac{f^{(2)}(c(x))}{2!}$$

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{-(x_0-x_1)^{\cancel{2}}}{2\,\cancel{(x_0-x_1)}} f(x_0) + \frac{(x_1-x_0)^{\cancel{2}}}{2\,\cancel{(x_1-x_0)}} f(x_1) + \int \text{Error term}$$

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{(x_1-x_0)}{2}\left[f(x_0) + f(x_1) \right] + \int \text{Error term } dx$$

$$\frac{(b-a)}{2}\left[f(a) + f(b) \right] + \int \text{error term } dx$$

Weighted Mean Value Theorem for integrals

Suppose $f \in C[a,b]$, the Riemann integral of g exists on $[a,b]$, and $g(x)$ does not change sign on $[a,b]$

Then, there exists c in (a,b) with

$$\int_a^b f(x)g(x)\,dx = f(c)\int_a^b g(x)\,dx$$

Let's consider the integral of the error term:

$$\int_{x_0}^{x_1} \underset{\ominus}{(x-x_0)}\,\underset{\oplus}{(x-x_1)}\,\frac{f''(c(x))}{2!}\,dx.$$

$$\ominus$$

From the WMVT

$$= \frac{f''(c)}{2}\int_{x_0}^{x_1}(x-x_0)(x-x_1)\,dx$$

$$x^2-(x_0+x_1)x+x_0x_1$$

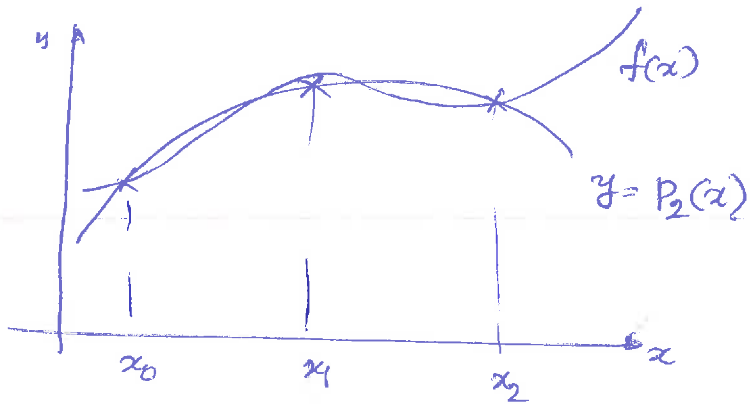
$$\cancel{(x_1-x_0)}$$

$$= \frac{f''(c)}{2}\left[\frac{x^3}{3}-(x_0+x_1)\frac{x^2}{2}+x_0x_1x\right]_{x_0}^{x_1}$$

$$= \frac{f''(c)}{2}\left[\frac{x_1^3-x_0^3}{3}-\frac{(x_0+x_1)}{2}\left[x_1^2-x_0^2\right]+x_0x_1(x_1-x_0)\right]$$

$$= -\frac{(b-a)^3}{12} f''(c)$$

Similarly for $n=2$, we have 3 points



Then,

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right] - \frac{h^5}{90} f^{(4)}(c),$$

where $h = \frac{b-a}{2} = \frac{x_2-x_0}{2}$

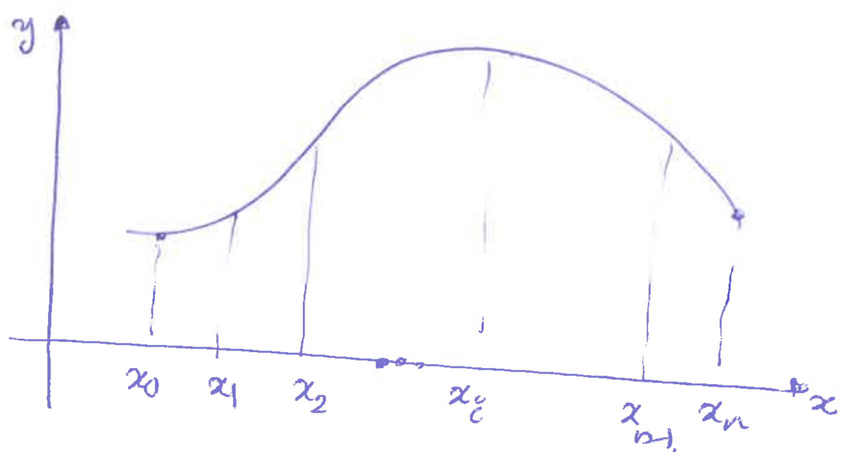
$$\int_{x_0=a}^{x_2=b} \approx \frac{(b-a)}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$$

ex. Approximate $\int_0^2 x^3\,dx$ by Midpoint, Trapezoidal, and Simpson's rule.
(ans: 2, 8, 4)

$$E_s = -\frac{h^5}{90} f^{(4)}(c) \qquad \boxed{E_S = } \quad -\frac{(b-a)^5 f^{(4)}(c)}{90 \cdot 2^5}$$

4.4. Composite Numerical Integration

The Trapezoid and Simpson's rules are limited to operating on a single interval since definite integrals are additive over subintervals, we can evaluate an integral by dividing the interval into several subintervals. Then applying the rules separately on each one, and then totaling up. This strategy is called composite numerical integration.



$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \dots + \int_{x_{n-1}}^{x_n} f(x)\,dx.$$

$x_i = a + ih$ and

$$h = \frac{b-a}{n}.$$

Composite trapezoidal rule :

Applying trapezoidal rule on each subinterval $[x_{i-1}, x_i]$, we get

$$\int_a^b f(x)\,dx = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)\,dx$$

$$\approx \sum_{i=1}^{n} \frac{h}{2}\left[f(x_{i-1}) + f(x_i)\right] \quad (\text{* each subinterval has the same length})$$

$$= \frac{h}{2}\left[f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n)\right]$$

$$= \frac{h}{2}\left[f(x_0) + f(x_n) + 2\sum_{i=1}^{n-1} f(x_i)\right]$$

Composite midpoint rule

$$\int_a^b f(x)\,dx \approx h \sum_{i=1}^{n} f\left(\frac{x_{i-1} + x_i}{2}\right)$$

Composite Simpson's rule

Consider an evenly spaced grid (n - even) (n - # of intervals)

Subintervals

$$[x_0, x_2], [x_2, x_4], \dots, [x_{n-2}, x_n]$$

$$\int_a^b f(x)\,dx = \sum_{i=1}^{n/2} \int_{x_{2i-2}}^{x_{2i}} f(x)\,dx$$

$$\approx \cancel{\frac{h}{3}} \sum_{i=1}^{n/2} \frac{h}{3}\left[f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i}) \right]$$

$$= \frac{h}{3}\Big[\left[f(x_0) + 4f(x_1) + f(x_2)\right] + \left[f(x_2) + 4f(x_3) + f(x_4)\right] +$$

$$+ \dots + \left[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right] \Big]$$

$$= \frac{h}{3}\Big[f(x_0) + f(x_n) + 4\left[f(x_1) + f(x_3) + \dots + f(x_{n-1})\right]$$

$$+ 2\left(f(x_2) + f(x_4) + \dots + f(x_{n-2}) \right) \Big]$$

$$\int_a^b f(x)dx \approx \frac{h}{3}\left[f(x_0) + f(x_n) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + 2\sum_{i=1}^{(\frac{n}{2}-1)} f(x_{2i}) \right]$$

ex. Approximate $\int_0^2 e^x dx$ using 4 subintervals in $(n=4)$

(a) Composite Trapezoidal rule

(b) " midpoint rule

(c) " Simpson's rule

(* Exact answer: $\int_0^2 e^x dx = e^2 - 1 \approx 6.389$)

(a) $n=4$ $h = \frac{2-0}{4} = 0.5$

$\Rightarrow$ 4-subintervals are $[0, 0.5], [0.5, 1], [1, 1.5], [1.5, 2]$

$x_0 \quad x_1 \quad x_2 \quad x_3 \quad x_4$

CTR $\int_0^2 e^x dx \approx \frac{h}{2}\left[e^0 + 2e^{0.5} + 2e^1 + 2e^{1.5} + e^2 \right] = 6.52$

CMR $\int_0^2 e^x dx \approx 0.5\left[e^{0.25} + e^{0.75} + e^{1.25} + e^{1.75} \right] = 6.32$

CSR $\int_0^2 e^x dx \approx \frac{0.5}{3}\left[e^0 + e^2 + 4e^{0.5} + 4e^{1.5} + 2e^1 \right] = 6.39$

HW Approximate $\int_0^2 e^{x^2}\,dx$ using CTR, and CSR

(II) Error in composite trapezoidal rule.

$$E_{T_n} = -\sum_{i=1}^{n} f''(c_i)\frac{(x_i - x_{i-1})^3}{12}$$

$$= \frac{-h^3}{12}\sum_{i=1}^{n} f''(c_i)$$

- Assume that $f''(c_i)$ is continuous. By the IVT we find $c \in [a,b]$ such that,

$$\frac{1}{n}\sum_{i=1}^{n} f''(c_i) = f''(c)$$

Then $$E_{T_n} = \frac{-h^3}{12}\, n\, f''(c)$$, where $n = \frac{b-a}{h}$.

$$E_{T_n} = -\frac{h^2}{12}(b-a)\, f''(c)$$

$$\boxed{E_{T_n} \leq \frac{+(b-a)h^2}{12} \max_{x\in[a,b]} |f''(x)|}$$

① Similarly, we get errors in the composite midpoint and Simpson's rules.

$$\boxed{E_{M_n} = \frac{(b-a)}{24} h^2 f''(c)} \qquad \boxed{E_{S_n} = -\frac{(b-a)}{180} h^4 f^{(4)}(c)}$$

Note that errors are $O(h^2)$ and $O(h^4)$

ex. Find the step size "h" and number of subintervals n - required to approximate $\int_0^2 e^x\,dx$ correct to within 10^{-2} using all 3-methods. CTR, CMR, and CSR

$f(x) = e^x \quad f'(x) = e^x \quad f''(x) = e^x \quad \dots \quad f^{(iv)}(x) = e^x$

$\max\limits_{x\in[0,2]} |f''(x)| = e^2. \qquad \max\limits_{x\in[0,2]} |f^{(iv)}(x)| = e^2.$

$(*)\ E_{T_n} \leq \frac{b-a}{12} h^2 \max\limits_{x\in[a,b]} |f''(x)|$.

$= \frac{(2-0)}{12} h^2 e^2 \leq 10^{-2}$ $\qquad n = 23$

$h = 0.087$

$$E_{M_n} \leq \frac{b-a}{24} h^2 \max_{x \in [0,2]} |f''(x)|$$

$$\frac{(2-0)}{24} h^2 e^2 \leq 10^{-2}.$$

$h = 0.125$

$n = 16.$

$$E_{S_n} \leq \frac{2}{180} h^4 e^2 \leq 10^{-2}.$$

$n = 4$

$h = 0.5.$