UCLA Math151A
Fall 2021
Lecture 19
2021/11/08

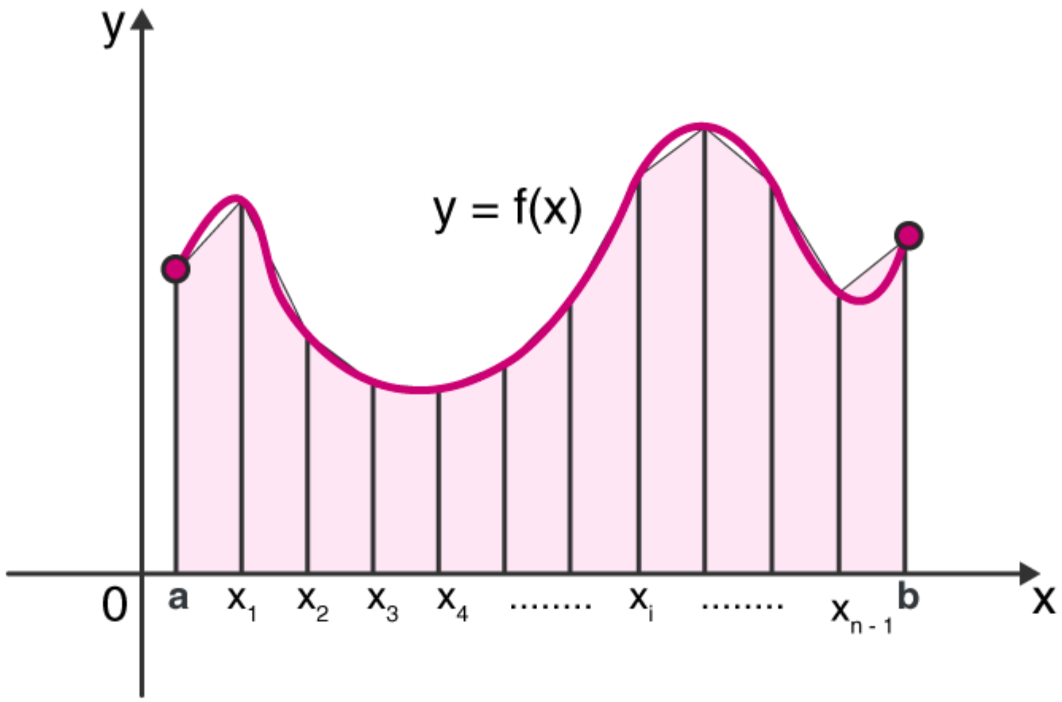
Composite Quadrature (continued),

Numerical Stability of Differentiation and Integration

Today

- composite quadrature rule
- computational cost
- stability

Recall C.T.R.:



given $(n+1)$ equispaced points, $h = \frac{b-a}{n}$,

Let $f \in C^2([a,b])$, $\displaystyle\int_a^b f(x)dx = \sum_{j=0}^{n-1} \int_{x_j}^{x_{j+1}} f(x)dx$

$$= \sum_{j=0}^{n-1} \left(\frac{h}{2} \left(f(x_j) + f(x_{j+1})\right) - \frac{h^3}{12} f''(\xi_j) \right), \qquad \xi_j \in (x_j, x_{j+1})$$

$$C.T.R. = \sum_{j=0}^{n-1} \frac{h}{2} \left(f(x_j) + f(x_{j+1})\right) = \frac{h}{2} \left(f(x_0) + 2 \sum_{j=1}^{n-1} f(x_j) + f(x_n) \right)$$

$f \in C^2([a,b])$,

$$\int_a^b f(x)dx = \frac{h}{2}\left(f(x_0) + 2\sum_{j=1}^{n-1} f(x_j) + f(x_n)\right) + ERROR$$

$$Error = \frac{-h^3}{12}\sum_{j=0}^{n-1} f''(\xi_j) = \frac{-h^3}{12} n \frac{\sum_{j=0}^{n-1} f''(\xi_j)}{n}, \qquad \xi_j \in (x_j, x_{j+1}).$$

$$MIN \leq f''(\xi_j) \leq MAX$$

$$\Rightarrow \quad MIN \leq \frac{\sum_{j=0}^{n-1} f''(\xi_j)}{n} \leq MAX$$

$$\Rightarrow \quad Error = -\frac{h^3}{12} n f''(\mu) \; = -\frac{h^2}{12}\frac{b-a}{n} n f''(\mu) \; = -\frac{h^2}{12}(b-a) f''(\mu).$$

Final C.T.R. formula:

$$\boxed{\int_a^b f(x)dx = \frac{h}{2}\left(f(x_0) + 2\sum_{j=1}^{n-1} f(x_j) + f(x_n)\right) - \frac{h^2}{12}(b-a)f''(\mu)}$$

Example 19.1. $f(x) = e^x$.

$$I := \int_0^1 e^x dx \; = e^1 - e^0 = e - 1 \approx 1.7183\ldots$$

n=1 picking $x_0 = 0, x_1 = 1, h = 1,\; I \approx \frac{1}{2}(e^0 + e^1) = 1.8591\ldots.$

n=2 $I \approx \frac{1}{4}(e^0 + 2e^{1/2} + e^1) = 1.7539\ldots.$

n=4 $I \approx \frac{1}{8}(e^0 + 2e^{1/4} + 2e^{1/2} + 2e^{3/4} + e^1) = 1.7272\ldots.$

n=8 $I \approx 1.7205\ldots.$

Composite Simpson's Rule (C.S.R.)

Recall, for 3 points x0, x1, x2 (equispaced), in HW6 Q3 you showed

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) + ERROR.$$

And for $f \in C^5([x_0, x_2])$ then

$$Error = -\frac{h^5}{12}(\frac{1}{3}f^{(4)}(\xi_1) + \frac{1}{5}f^{(4)}(\xi_2))$$

It can be shown $\exists \xi \in (x_0, x_2)$

$$Error = -\frac{h^5}{90}f^{(4)}(\xi)$$

See lec19-extra-reading.pdf

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) + ERROR.$$

$$Error = -\frac{h^5}{90} f^{(4)}(\xi) \qquad f \in C^4([a,b]).$$

The Composite Simpson's Rule (C.S.R.) assumes that **n is even.**

Example:

$$\{a = x_0, x_2, x_4, x_6, x_8 = b\} \text{ with } n = 8.$$

We then use Simpson's rule on each interval

$$[x_0, x_2], [x_2, x_4], [x_4, x_6], [x_6, x_8].$$

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2)) + ERROR.$$

$$Error = -\frac{h^5}{90} f^{(4)}(\xi) \qquad f \in C^4([a,b]).$$

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

$$= \sum_{j=1}^{n/2} \frac{h}{3}(f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})) - \underline{\sum_{j=1}^{n/2} \frac{h^5}{90} f^{(4)}(\xi_j)}$$

Error analysis similar to C.T.R.

$$= \underline{\frac{h^5}{90}\frac{n}{2}\sum_{j=1}^{n/2}\frac{f^{(4)}(\xi_j)}{n/2}} \qquad = \frac{h^5}{90}\frac{n}{2} \qquad f^{(4)}(\zeta) \quad \text{by IVT, for some } \zeta \in (a,b).$$

$$|\text{C.S.R error}| = \frac{h^4}{180}(b-a)|f^{(4)}(\zeta)|$$

Final C.T.R. formula:

$$\int_a^b f(x)dx = \frac{h}{2}\left(f(x_0) + 2\sum_{j=1}^{n-1} f(x_j) + f(x_n)\right) - \frac{h^2}{12}(b-a)f''(\mu)$$

Final C.S.R. formula:

$$\int_a^b f(x)dx = \sum_{j=1}^{n/2} \frac{h}{3}(f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})) - \frac{h^4}{180}(b-a)f^{(4)}(\zeta)$$

CTR had error $O(h^2)$, here we have $O(h^4)$

Note that however CSR requires higher order continuity of f(x) (C2 v.s. C4). If you don't have it, there is no guarantees on the error, it is usually better to use the lower order formula CTR.

Computational Cost Estimate

Suppose we fix an error tolerance τ.

For a given numerical quadrature formula and a given $f(x)$, how many points n are required to guarantee that $|Error| < \tau$?

Example 19.2. $f(x) = \frac{1}{x+4}$, $I = \int_0^2 \frac{1}{4+x} dx$.

Use Composite Traperzoidal Rule with $\tau = 10^{-5}$.

$$|Error| = \frac{h^2}{12}(b-a)|f''(\mu)| = \frac{h^2}{12} 2 \left| \frac{2}{(4+\mu)^3} \right|$$

$$\leq \frac{h^2}{6} \frac{2}{64} < \tau = 10^{-5}$$

$$\Rightarrow \qquad h < 0.04389 \qquad \Rightarrow \qquad n \geq 46.$$

A similar analysis for the C.S.R. gives $n \geq 6$.

Numerical Stability of Numerical Differentiation and Numerical Integration

Theorem 19.1. Composite traperzoidal/simpson's rule (and other composite quadrature rules) are stable with respect to numerical roundoff errors. Integration is stable.

Theorem 19.2. In contrast, in general numerical differentiation formulas are not stable w.r.t. roundoff errors. Differentiation is unstable.

We need to study **Numerical Roundoff Error** in the Context of Differentiation and Integration

First, for differentiation.

Recall: $x \approx fl(x)$

Recall centered difference

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

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

In exact arithmetic, we know (assuming $f \in C^3$)

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

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

$$M = \max_{x \in [a,b]} |f'''(x)|. \qquad \leq \frac{h^2}{6} M$$

We'll use this error bound in our analysis below.

Since we are using floating point, let

$$\tilde{f}(x_0 + h) := fl(f(x_0 + h)) \quad \Big| \quad f(x_0 + h) = \tilde{f}(x_0 + h) + \epsilon_1$$

$$\tilde{f}(x_0 - h) := fl(f(x_0 - h)) \quad \Big| \quad f(x_0 - h) = \tilde{f}(x_0 - h) + \epsilon_2.$$

Assume h can be represented exactly.

Then the floating point approximation to the true $f'(x_0)$ is

$$\frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} = \frac{f(x_0 + h) - f(x_0 - h)}{2h} + \frac{\epsilon_1 - \epsilon_2}{2h}$$

$$\frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h}=\frac{f(x_0+h)-f(x_0-h)}{2h}+\frac{\epsilon_1-\epsilon_2}{2h}$$

Error is: $$|f'(x_0)-\frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h}|$$

$$=|f'(x_0)-\frac{f(x_0+h)-f(x_0-h)}{2h}+\frac{\epsilon_2-\epsilon_1}{2h}|$$

$$\leq|f'(x_0)-\frac{f(x_0+h)-f(x_0-h)}{2h}|+|\frac{\epsilon_2-\epsilon_1}{2h}|$$

$$\leq\underline{\frac{M}{6}h^2}+|\underline{\frac{\epsilon_2-\epsilon_1}{2h}}|$$

the truncation error vanishes.

the second part increases.

$$\text{Error} \leq \frac{M}{6}h^2 + \left|\frac{\epsilon_2 - \epsilon_1}{2h}\right|$$

To minimize the error, we let

$$\epsilon := \left|\frac{\epsilon_2 - \epsilon_1}{2}\right| \qquad\qquad g(h) := \frac{M}{6}h^2 + \frac{\epsilon}{h}$$

Then $g'(h) = \frac{M}{3}h - \frac{\epsilon}{h^2} = 0$ results in

$$h = \left(\frac{3\epsilon}{M}\right)^{1/3}$$

This is the optimal choice of h which minimized the error.

$$\text{Error} \leq \frac{M}{6}h^2 + \left|\frac{\epsilon_2 - \epsilon_1}{2h}\right| \qquad \text{optimal}\, h = \left(\frac{3\epsilon}{M}\right)^{1/3}$$

Consider HW6 Q6,

$$f(x) = e^x, f'''(x) = e^x, x_0 = 1,$$

$$x \in [x_0 - h, x_0 + h]$$

$$M = \max|f'''(x)| \approx e^1 = 2.71828...$$

Suppose $\epsilon = 10^{-k}$ for some integer k, then

$$k = 15 \Rightarrow h = 1.0334 \times 10^{-5}$$

$$k = 14 \Rightarrow h = 2.2264 \times 10^{-5}$$

$$k = 16 \Rightarrow h = 4.7967 \times 10^{-6}$$

the optimal h is actually only $O(10^{-5})$ to $O(10^{-6})$ in this example!