Composite Quadrature

Tuesday, October 6, 2020 1:15 PM

Recap

Goal: estimate $\int_a^b f(x)\,dx = I$, usually via $\int_a^b p_n(x)\,dx = I_n$ where p_n is n degree polynomial interpolating f on the nodes $\{x_0, x_1, \dots, x_n\}$. We discussed the case of equispaced nodes and the corresponding open/closed Newton Cotes formulae.

($h = \frac{b-a}{n+2}$ open, $h = \frac{b-a}{n}$ closed)

Our metrics for accuracy:

1) show error $E = |I - I_n| = O(h^k)$

$$k = \begin{cases} n+2 & n \text{ odd} \\ n+3 & n \text{ even} \end{cases}$$

2) order of exactness (aka degree of accuracy)

highest degree polynomial that has no error via the scheme

$$= \begin{cases} n & n \text{ odd} \\ n+1 & n \text{ even} \end{cases}$$

So to improve accuracy, we want to decrease h, i.e., increase n

but w/ large n:

1) need to lookup or derive formula every time we change n

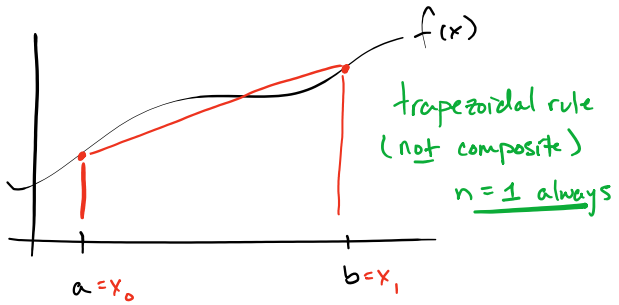
(also might get negative weights $\Rightarrow$ less stable)

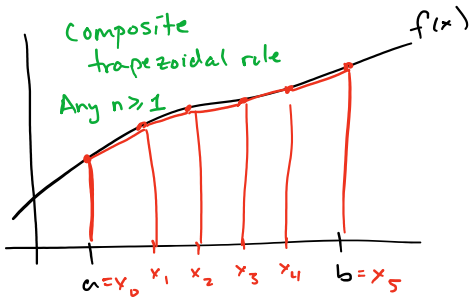
2) interpolating polynomial p_n has Runge phenomenon

3) we decrease h (i.e. increase n) to reduce the error bound, but this bound only holds if $f \in C^{n+1}$ or C^{n+2}

... thus simple alternative is **composite** integration

i.e., break $[a,b]$ into pieces, apply our old quadrature rules to each piece, then sum.





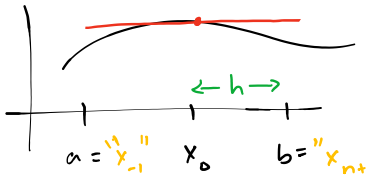
That's the idea. Now, details and analysis.

For notation, there are several ways you could do it. We'll follow Burden + Faires

Composite midpoint rule

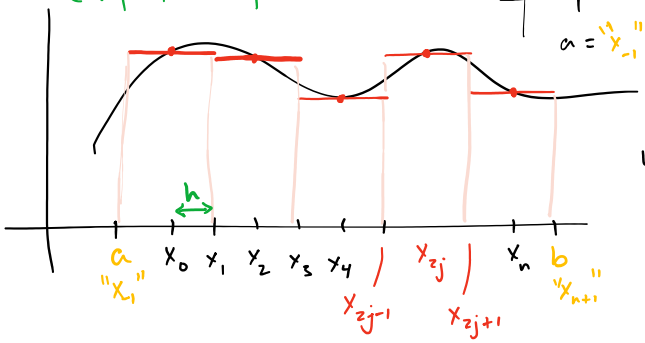
$n=0$, open

Recall (non-composite) midpoint rule



weight is $2h$

Composite midpoint



with our book's convention, we don't actually evaluate f at all the "nodes", only even nodes (somewhat confusing, but we can still keep our definition $h = \frac{b-a}{n+2}$)

$\Rightarrow n$ must be even

Formula:

$$\int_{x_{-1}}^{x_{n+1}} f(x)\,dx = \underbrace{\int_{x_{-1}}^{x_1} f(x)\,dx}_{2h f(x_0) + \frac{h^3}{3} f''(\xi)} + \underbrace{\int_{x_1}^{x_3} f(x)\,dx}_{2h f(x_2) + \frac{h^3}{3} f''(\tilde{\xi})} + \cdots + \underbrace{\int_{x_{n-1}}^{x_{n+1}} f(x)\,dx}_{2h f(x_n) + \frac{h^3}{3} f''(\tilde{\tilde{\xi}})}$$

non-composite midpoint; error

$h := \frac{b-a}{n+2}$

assume $|f''(\xi)| \le M$

$$= 2h \sum_{j=0}^{n/2} f(x_{2j}) + \frac{n}{2}\left(\frac{h^3}{3} M\right)$$

a bit loose

note $n = O(\frac{1}{h})$

$O(h^2)$ error

Formula: Composite midpoint

a more precise characterization: Thm. 4.6

$$\frac{b-a}{6} h^2 f''(\eta) \quad \text{for some } \eta \in (a,b)$$

In implementation, it might be simpler to relabel nodes, counting just the even ones.

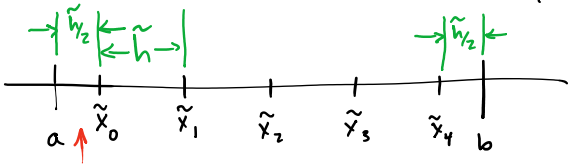
book's notation

Old notation $\{x_0, x_1, x_2, \ldots, x_n\}$ (n even)

New notation $\{\tilde{x}_0, \tilde{x}_1, \ldots, \tilde{x}_m\}$ ← simpler notation

$m = n/2$

$\tilde{x}_j = x_{2j}$



⚠ In this new notation, while node spacing is $\tilde{h}$, the first node is offset by $\tilde{h}/2$

Old formula: $I \approx 2h \sum_{j=0}^{n/2} f(x_{2j})$

$h = \frac{b-a}{n+2}$

($m = n/2$ i.e. $n = 2m$)

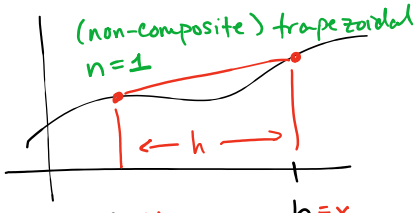
New formula:

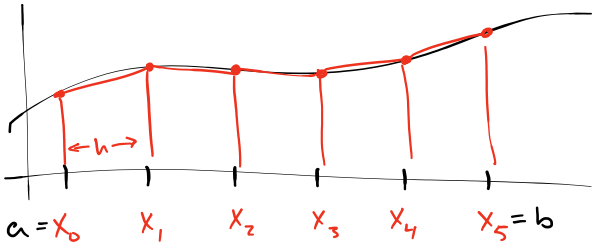
$$\tilde{h} = \frac{b-a}{m+1} = \frac{2\cdot(b-a)}{2(m+1)} = 2h$$

Simplest quadrature formula ever! → so $\boxed{I \approx \tilde{h} \sum_{j=0}^{m} f(\tilde{x}_j)}$

Composite Trapezoidal Rule

In this case, notation is simpler, no need for "$\tilde{x}$" version, and no restriction that n is even





↑ closed rule

(non-composite) formula (assuming $f \in C^2[a,b]$)

$$I = \int_a^b f(x)dx = \frac{h}{2}\left(f(x_0)+f(x_1)\right) - \frac{h^3}{12}f''(\xi)$$

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

so composite:

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

"h" = "b" − "a" ("n" = 1) = $x_1 - x_0 = h$

$$= \frac{h}{2}\left(f(x_0)+f(x_1)\right) - \frac{h^3}{12}f''(\xi) + \frac{h}{2}\left(f(x_1)+f(x_2)\right) - \frac{h^3}{12}f''(\tilde{\xi}) + \dots + \frac{h}{2}\left(f(x_{n-1})+f(x_n)\right) - \frac{h^3}{12}f''(\tilde{\tilde{\xi}})$$

once; appears twice; twice…; twice…; once

$$= \frac{h}{2}\left(f(x_0) + 2\cdot\sum_{j=1}^{n-1} f(x_j) + f(x_n)\right) - \frac{b-a}{12}h^2 f''(\eta) \qquad \eta \in (a,b)$$

(*) FORMULA

interior nodes treated differently

this is Thm. 4.5

Very similar to composite midpoint rule, except

1) nodes are closed, not open (for midpoint, $x_0 = a + h/2$; trapezoid, $x_0 = a$)

2) adjust weights on 1st and last node

Note: if $f(a) = f(b)$, the formula simplifies to $h\sum_{j=0}^{n-1} f(x_j)$

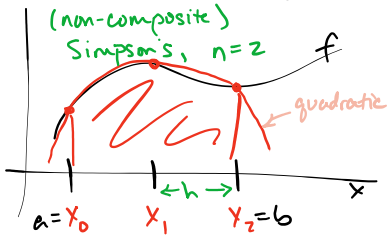
If also $f'(a) = f'(b)$, $f''(a) = f''(b)$, etc. then we'll see the error decays very quickly!

"periodic"

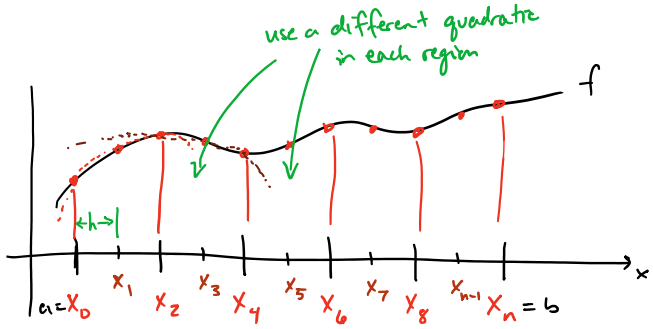
Composite Simpson's Rule

The "industry standard", ie., your goto method for all but very tricky (highly oscillatory) functions

We'll use book's notation



(closed, $h = \frac{b-a}{n} = \frac{b-a}{2}$)



⚠ Need n even like midpt. rule

$$I = \int_a^b f(x)\,dx = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx$$

$$= \frac{h}{3}\left(f(x_0)+4f(x_1)+f(x_2)\right) + \frac{h}{3}\left(f(x_2)+4f(x_3)+f(x_4)\right) + \cdots + \frac{h}{3}\left(f(x_{n-2})+4f(x_{n-1})+f(x_n)\right)$$

$$- \frac{h^5}{90} f^{(4)}(\xi) \qquad - \frac{h^5}{90} f^{(4)}(\tilde{\xi}) \qquad - \frac{h^5}{90} f^{(4)}(\tilde{\tilde{\xi}})$$

appears twice

$$= \frac{h}{3}\left(f(x_0) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)\right) - \frac{b-a}{180} h^4 f^{(4)}(\eta)$$

(★) FORMULA Composite Simpson's

$h = \frac{b-a}{n}$, n even

for some $\eta \in (a,b)$ — Thm 4.4

Stability

We saw that for differentiation, finite difference schemes were unstable algorithms

i.e., total error was like

$$\frac{e}{h} + h^k$$

error: $f(x) - \tilde{f}(x)$ (floating pt.)

$\frac{e}{h}$: roundoff (computer)

h^k: approximation (math)

k = order of method (1, 2, 3, etc)

So we couldn't take $h \to 0$ because roundoff error $\to \infty$ then.

For integration, things are better: it is stable in general.

Ex: let each computation have error e_i, $\tilde{f}(x_i) = f(x_i) + e_i$ with each $|e_i| \le \varepsilon$ for some small ε

Consider Composite Simpson's Rule

$$\frac{h}{3}\left(f(x_0)+e_0 + 2\cdot\sum_{j=1}^{n/2-1} f(x_{2j})+e_{2j} + 4\sum_{j=1}^{n/2} f(x_{2j-1})+e_{2j-1} + f(x_n)+e_n\right)$$

So error is $\frac{h}{3}\left(e_0 + 2\sum_{j=1}^{n/2-1} e_{2j} + 4\sum_{j=1}^{n/2} e_{2j-1} + e_n\right)$

Use triangle inequality, $|a+b| \le |a| + |b|$, and $|\sum a_i| \le \sum |a_i|$

So $|\text{error}| \le \frac{h}{3}\left(\varepsilon + 2\left(\frac{n}{2}-1\right)\varepsilon + 4\left(\frac{n}{2}\right)\varepsilon + \varepsilon \right)$ (cancel)

$= \frac{h}{3}(3n\varepsilon) = nh\varepsilon$ and $h = \frac{b-a}{n}$

$= (b-a)\varepsilon$

So we make roundoff error, but it's not too large (if f is well-conditioned and x, $f(x)$ near 1, then $\varepsilon \approx \varepsilon_{\text{machine}} \approx 10^{-16}$)

and most importantly, roundoff error does not increase as $h \to 0$ or $n \to \infty$.

So we can just pick h very small (n very large) to make the "mathematical" error as small as we like.