

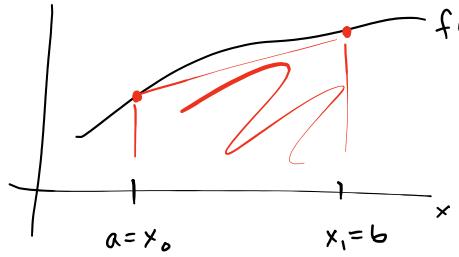
Trapezoidal and Simpson's quadrature rules

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Last time we derived the midpoint rule ($n=0$, open nodes, error $\frac{h^3}{3} f''(\xi)$)
 $h = \frac{b-a}{2}$ degree of exactness 1

Now, add two new rules, trapezoidal and Simpson's

Trapezoidal Rule ($n=1$, closed nodes)



$\{x_0 = a, x_1 = b\}$ nodes

Lagrange polynomials

$$L_{1,0} = \frac{x - x_1}{x_0 - x_1}$$

$$L_{1,1} = \frac{x - x_0}{x_1 - x_0}$$

$$\text{so } P_n(x) = \sum_{i=0}^{n-1} f(x_i) L_{n,i}(x) = f(x_0) \cdot \frac{x - x_1}{x_0 - x_1} + f(x_1) \cdot \frac{x - x_0}{x_1 - x_0}$$

so our approximation of $I = \int_a^b f(x) dx$ is

$$\begin{aligned} I_n &= \int_a^b P_n(x) dx = \underbrace{\frac{f(x_0)}{x_0 - x_1} \cdot \int_a^b (x - x_1) dx}_{-\frac{1}{2} h^2 (x-x_1)^2 \Big|_a^b} + \underbrace{\frac{-f(x_1)}{x_1 - x_0} \int_a^b (x - x_0) dx}_{\frac{1}{2} h^2 (x-x_0)^2 \Big|_a^b} \\ &\quad (\text{recall } x_0 = a, x_1 = b, h = b-a) \\ &= -\frac{1}{2} h^2 \\ &= \frac{1}{2} h [f(x_0) + f(x_1)] \\ &= \frac{h}{2} (f(x_0) + f(x_1)), \quad \text{so } w_0 = w_1 = \frac{h}{2} \\ &I_2 = \sum_{i=0}^1 w_i f(x_i) \end{aligned}$$

What about the approximation error?

Recall Thm 3.3: $\{x_0, x_1, \dots, x_n\} \subseteq [a, b]$ are distinct nodes, $f \in C^{n+1}[a, b]$, then $\forall x \in [a, b], \exists \xi \in (a, b)$ s.t.

$$f(x) = \underbrace{P_n(x)}_{\text{interpolating polynomial}} + \underbrace{\frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^n (x - x_i)}_{\text{error } e}$$

$$\text{so, } n=1, \text{ error } e(x) = f(x) - P_1(x)$$

$$= \frac{f''(\xi)}{2!} (x - x_0)(x - x_1)$$

thus the error in our approximation of the integral is

$$E = \int_a^b f(x) dx - \int_a^b p_n(x) dx = \int_a^b e(x) dx$$

$$= \int_a^b \frac{f''(\xi)}{2} (x-x_0)(x-x_1) dx$$

recall $\xi = g(x)$ so can't pull out

now either use weighted MVT

(since $g(x) = (x-x_0)(x-x_1)$ doesn't change sign on $[a,b]$)

or bound

$$M := \max_{x \in [a,b]} |f''(x)| \quad (\text{assuming } f \in C^2[a,b])$$

$$\begin{aligned} \text{so } \left| \int_a^b f''\left(\frac{g(x)}{2}\right) (x-x_0)(x-x_1) dx \right| &\leq \frac{M}{2} \int_a^b (x^2 - (x_0+x_1)x + x_0 x_1) dx \\ &= \frac{M}{2} \left(\frac{1}{3} x^3 - \frac{1}{2} (x_0+x_1) x^2 + x_0 x_1 x \right) \Big|_{a=x_0}^{b=x_1} \\ &= \frac{M}{2} \left(\frac{1}{3} b^3 - \frac{1}{2} (a+b) b^2 + a \cdot b \cdot b \right. \\ &\quad \left. - \frac{1}{3} a^3 + \frac{1}{2} (a+b) a^2 - a \cdot b \cdot a \right) \\ &= \frac{M}{2} \left(-\frac{1}{6} b^3 + \frac{1}{2} ab^2 - \frac{1}{2} a^2 b + \frac{1}{6} a^3 \right) \\ &= -\frac{M}{12} (b-a)^3 \\ &= -\frac{M}{12} h^3 \end{aligned}$$

Trapezoidal Rule

$$\text{So... error } |E| \leq \frac{M}{12} h^3 \quad h = b-a$$

$$\dots \text{similar to midpt. rule } |E| \leq \frac{M}{3} \tilde{h}^3 \quad \tilde{h} = \frac{b-a}{2} = \frac{h}{2}$$

$$= 8/3 M h^3$$

We expect trapezoidal to be more accurate than midpoint, right?

It has a smaller constant, but same order of h

$$(1/12 < 8/3)$$

By similar reasoning as before, since $M = \max_{x \in [a,b]} |f''(x)|$,

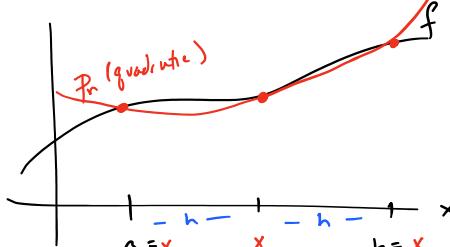
The degree of exactness of the trapezoidal rule is 1.

Simpson's Rule

(aka Cavalieri-Simpson)

$$\{x_0 = a, x_1, x_2 = b\}$$

$n=2$
Closed



Same thing as before: construct interpolating polynomial of degree $n=2$ and integrate that.

$$\text{Skipping details, } I_2 = \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2))$$

$$\text{to approximate } I = \int_a^b f(x) dx$$

symmetry makes sense

and error is bounded by $\frac{M}{90} h^5$ where $M = \max_{x \in [a, b]} |f^{(4)}(x)|$
 $h = \frac{b-a}{2}$ that's new

As before, our weights don't depend on f or even a, b
just on h (assuming equispaced closed nodes)

What's the degree of exactness of Simpson's rule?

3, since if $f(x) = a_3 x^3 + a_2 x^2 + a_1 x + a_0$
then $f'(x) = 3a_3 x^2 + \dots$
 $f''(x) = 6a_3 x + \dots$
 $f'''(x) = 6a_3$
 $f^{(4)}(x) = 0 \Rightarrow M=0$ so no error.

More generally, any interpolating quadrature formula
with $(n+1)$ distinct nodes has degree of
exactness at least n , since it interpolates degree n
polynomials
... but it can be higher (ex. midpoint rule is
exact for 1-degree polynomials)

What's the max? Up to a degree of exactness $2n+1$
(but not using equispaced nodes) via Gaussian quadrature (ch 4.7)

Generalizing

Integrating the interpolating polynomial, for equispaced grids,
leads to the family of Newton-Cotes Formulas

Closed Newton-Cotes Formula $\{x_0=a, x_1, x_2, \dots, x_{n-1}, x_n=b\}$ $h = \frac{b-a}{n}$

odd n : $n=1$, Trapezoidal Rule, weights $\frac{h}{2}(1, 1)$ ← i.e. $\frac{h}{2}(f(x_0) + f(x_1))$
error $E = -\frac{h^3}{12} f''(\xi)$ for some $\xi \in (a, b)$
degree of exactness 1

even n : $n=2$, Simpson's Rule, weights $\frac{h}{3}(1, 4, 1)$ ← i.e. $\frac{h}{3}(f(x_0) + 4f(x_1) + f(x_2))$
error $E = -\frac{h^5}{90} f^{(4)}(\xi)$,
degree of exactness 3

odd n : $n=3$, Simpson's "3/8" Rule, weights $\frac{3}{8}h(1, 3, 3, 1)$
error $E = -\frac{3h^5}{80} f^{(4)}(\xi)$,
degree of exactness 3

even \circ $n=4$, weights $\frac{2}{45}h$ ($7, 32, 12, 32, 7$)

$$E = -\frac{8}{45}h^7 f^{(6)}(\xi)$$

degree of exactness 5

general formula for Closed Newton-Cotes

$$n \text{ even}, E = h \frac{f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n) dt \quad \text{and degree of exactness } n+1$$

$$n \text{ odd}, E = h \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n) dt \quad \text{and degree of exactness } n$$

$$\sum_{i=0}^n w_i f(x_i), \quad w_i = \int_a^b L_{n,i}(x) dx, \quad L_{n,i}(x) = \prod_{\substack{j \neq i \\ j=0}} \frac{(x-x_j)}{(x_i-x_j)}$$

... so n even is a bit nicer!

Open Newton-Cotes Formulas

$$\{x_0, x_1, \dots, x_n\} \text{ with } x_0 = a, x_n = b, h = \frac{b-a}{n+1}$$

$$\begin{array}{c} + + + + + \\ a \quad x_0 \quad x_1 \quad x_2 \quad b \end{array}$$

$n=0$, Midpoint Rule, weights $2h$

$$\text{error } E = \frac{h^3}{3} f''(\xi) \text{ for some } \xi \in (a, b)$$

degree of exactness 1

$n=1$, weights $\frac{3}{2}h$ ($1, 1$)

$$E = \frac{3}{4}h^3 f''(\xi), \text{ degree of exactness 1}$$

$n=2$, weights $\frac{4}{3}h$ ($2, -1, 2$) in general, we dislike this (negative), more issues w/ roundoff

$$E = \frac{14}{45}h^5 f^{(4)}(\xi), \text{ degree of exactness 3}$$

general formula

(paraphrased - see Thm. 4.3 in book for full details)

Open Newton-Cotes, $n+1$ pts,

$$n \text{ even}, \text{ error } E \approx h \frac{f^{(n+2)}(\xi)}{(n+2)!} \quad \text{degree of exactness } n+1$$

$$n \text{ odd}, \quad E \approx h \frac{f^{(n+1)}(\xi)}{(n+1)!} \quad \text{degree of exactness } n$$

Summary

Closed or Open Newton-Cotes formulas for various " n " (so $n+1$ nodes)

Sometimes you might not be able to evaluate f at the end points, but otherwise closed formulas probably make

more sense.

Even n gives more bang-for-the-buck than odd n

* Simpson's rule ($n=2$, closed) is the most common choice

Not yet addressed

- composite rules (ie., piecewise polynomials)
make more sense when n is large
(ie., if we want high accuracy) Fundamental
- Romberg integration: apply Richardson extrapolation
- Beyond equispaced nodes: Gaussian quadrature
- 2D and higher-dimensional integrals
- Improper integrals ($a = -\infty$ or $b = \infty$, for example)
- Adaptive methods (automatically determine n to reach given tolerance), aka "automatic integration"
(professional quality software)