Trapezoidal and Simpson's quadrature rules

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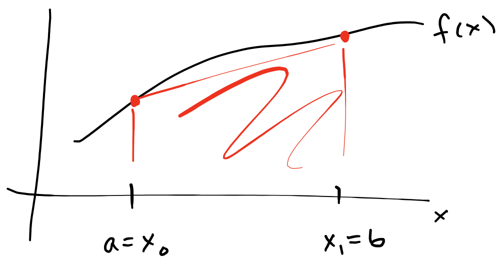
last time we derived the midpoint rule ($n=0$, open nodes, error $\frac{h^3}{3} f''(\xi)$)
$h = \frac{b-a}{2}$ degree of exactness 1

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

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



$h = b-a$

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

Lagrange polynomials

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

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

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

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

$$\underset{(n=1)}{I_n} = \int_a^b P_n(x)dx = \underbrace{\frac{f(x_0)}{x_0-x_1}}_{-h} \cdot \underbrace{\int_a^b (x-x_1)dx}_{\frac{1}{2}(x-x_1)^2\big|_a^b = -\frac{1}{2}h^2} + \underbrace{\frac{f(x_1)}{x_1-x_0}}_{h} \underbrace{\int_a^b (x-x_0)dx}_{\frac{1}{2}(x-x_0)^2\big|_a^b = \frac{1}{2}h^2}$$

(recall $x_0 = a$, $x_1 = b$, $h = b-a = x_1 - x_0$)

$$= \frac{1}{2} h f(x_0) + \frac{1}{2} h f(x_1)$$

$$= \frac{h}{2}\left(f(x_0) + f(x_1) \right), \quad \text{so} \quad w_0 = w_1 = \frac{h}{2}$$

$$I_1 = \sum_{i=0}^{1} w_i f(x_i)$$

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.

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

so, $n=1$, error $e(x) = f(x) - P_n(x)$

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

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

so $$\left| \int_a^b \frac{f''(\xi(x))}{2}(x-x_0)(x-x_1)\,dx \right| \le \frac{M}{2}\int_a^b \left(x^2 - (x_0+x_1)x + x_0x_1\right)dx$$

$$= \frac{M}{2}\left(\frac{1}{3}x^3 - \frac{1}{2}(\underbrace{x_0}_{=a}+\underbrace{x_1}_{=b})x^2 + \underbrace{x_0x_1}_{=a\cdot b}\,x \right)\Bigg|_{a=x_0}^{b=x_1}$$

$$= \frac{M}{2}\Big(\frac{1}{3}b^3 - \frac{1}{2}(a+b)b^2 + a\cdot b\cdot b$$
$$- \frac{1}{3}a^3 + \frac{1}{2}(a+b)a^2 - a\cdot b\cdot a \Big)$$

$$= \frac{M}{2}\left(-\frac{1}{6}b^3 + \frac{1}{2}ab^2 - \frac{1}{2}a^2b + \frac{1}{6}a^3 \right)$$

note $$(b-a)^3 = (b-a)(b^2 - 2ab + a^2)$$
$$= b^3 - 2ab^2 + a^2b - a^3 + 2a^2b - ab^2$$
$$= b^3 - 3ab^2 + 3a^2b - a^3$$

$$= -\frac{M}{12}(b-a)^3$$

$$= \frac{-M}{12}h^3$$

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

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

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

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

It has a smaller constant, but same order of h

$(\tfrac{1}{12} < 8/3)$

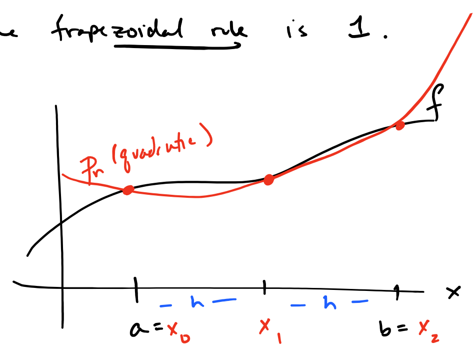
By similar reasoning as before, since $M = \max_{x\in[a,b]} |f''(x)|$,

the degree of exactness of the trapezoidal rule is 1.

Simpson's Rule

(aka Cavalieri-Simpson) $\quad n=2$ closed

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



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

symmetry makes sense

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

to approximate $I = \int_a^b f(x)\,dx$

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

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

⚠ 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 $f'(x) = 3a_3 x^2 + \ldots$

$f''(x) = 6a_3 x + \ldots$

$f'''(x) = 6a_3$

$f^{(4)}(x) = 0 \Rightarrow M = 0$ 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 Formula

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

odd ☹ $n=1$, 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 ☺ $n=2$, 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 ☹ $n=3$, Simpson's "3/8" Rule, weights $\frac{3}{8}h(1,3,3,1)$

$E = -3\frac{h^5}{80} f^{(4)}(\xi)$,

degree of exactness 3

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

$$E = -\frac{8}{945} h^7 f^{(6)}(\xi)$$

degree of exactness 5

general formula for Closed Newton-Cotes

n even, $E = \dfrac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \displaystyle\int_0^n t^2 (t-1)\cdot \ldots \cdot (t-n)\, dt$

and degree of exactness $n+1$

n odd, $E = \dfrac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \displaystyle\int_0^n t(t-1)\cdot \ldots \cdot (t-n)\, dt$

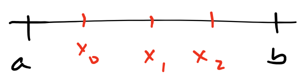
and degree of exactness n

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

... so n = even is a bit nicer!

Open Newton-Cotes Formulas

$\{x_0, x_1, \ldots, x_n\}$ with "x_{-1}" $= a$, "x_{n+1}" $= b$, $h = \dfrac{b-a}{n+2}$



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

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

degree of exactness 1

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

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

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

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

general formula

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

Open Newton Cotes, $n+1$ pts,

n even, error $E \approx h^{n+3} f^{(n+2)}(\xi)$

degree of exactness $n+1$

n odd, $E \approx h^{n+2} f^{(n+1)}(\xi)$

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)