Romberg Integration

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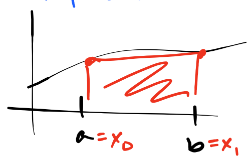
Idea: apply Richardson Extrapolation to the composite trapezoidal rule

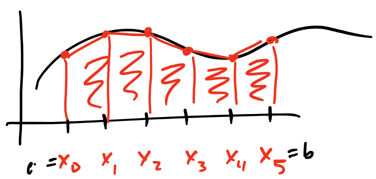
Driscoll + Braun (2017) call this the "Swiss Army knife of integration formulas"

Recall trapezoidal rule



$$\int_a^b f(x)\,dx = \underbrace{h \cdot \left(\tfrac{1}{2} f(x_0) + \tfrac{1}{2} f(x_1) \right)}_{\text{Formula}} \underbrace{- \frac{h^3}{12} f''(\eta)}_{\text{error}}$$

and composite trapezoidal rule



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

$$\underbrace{h \left(\tfrac{1}{2} f(x_0) + \sum_{j=1}^{n-1} f(x_j) + \tfrac{1}{2} f(x_n) \right)}_{\text{Formula}}$$

$$\underbrace{- \frac{b-a}{12} h^2 f''(\eta)}_{\text{error}}$$

equispaced, so $x_j = x_0 + j \cdot h$

Before we go on, let's get an alternative form for our error. We're used to writing the error term like $f^{(k)}(\eta)$ for some $\eta \in (a,b)$, but there's a variant using $f^{(k)}(b) - f^{(k)}(a)$: the Euler-Maclaurin Formula

every book calls this the "most remarkable formula in mathematics"

Euler-Maclaurin Formula

Not in Burden + Faires

Ref: "Concrete Mathematics" (Graham, Knuth, Patashnik)

Integers A, B, m:

$$\sum_{k=A}^{B-1} f(k) = \int_A^B f(x)\,dx + \sum_{k=1}^{m} \frac{B_k}{k!} \left(f^{(k-1)}(B) - f^{(k-1)}(A) \right)$$

⚠ may not always converge

$$+ R_m, \quad R_m = (-1)^{m+1} \underbrace{\int_A^B \frac{B_m(x - \lfloor x \rfloor)}{m!} f^{(m)}(x)\,dx}_{\text{Remainder, can bound usually}}$$

B_k are the Bernoulli numbers

$B_0 = 1$, $B_2 = 1/6$, $B_4 = -1/30$, $B_6 = 1/42$, $B_8 = -1/30$

$B_1 = -1/2$

$B_3 = B_5 = B_7 = B_9 = \dots = 0$ (so sometimes people don't include odd terms in the sum)

$\sum_k \binom{m}{k} B_k = B_m$

You can use the formula for all kinds of things,

ex: let $f(x) = x^{m-1}$ so $f^{(m)}(x) \equiv 0$ so $R_m = 0$ and (with some work) you can show

$$\sum_{k=0}^{n-1} k^2 = \frac{n^3}{3} - \frac{n^2}{2} + \frac{n}{6}$$ (of course you can show this other ways too, eg. telescoping series)

(you might know the version $\sum_{k=1}^{n} k^2 = \frac{n(n+1)(2n+1)}{6}$

much like $\sum_{k=1}^{n} k = \frac{n(n+1)}{2}$)

Can bound remainder $|R_m| = O\left(\frac{1}{(2\pi)^m}\right) \cdot \int_A^B |f^{(m)}(x)|\,dx$

How are we going to use the formula?

Instead of $\sum_{k=A}^{B-1}$ and $\int_A^B$, we want $\int_a^b$ like $a=0$, $b=1$

integers, like $A=1$, $B=500$

So we'll do a change-of-variables, something like $g(x) = f(hx)$

so $g'(x) = h f'(hx)$

$g''(x) = h^2 f''(hx)$

etc.

... then relabel f ...

(see a textbook! these are handwritten notes)

... and account for ½ values at endpoints ... rename "m" to "n" ...

...

$$\underbrace{h\left(\tfrac{1}{2}f(x_0) + \sum_{j=1}^{n-1} f(x_j) + \tfrac{1}{2}f(x_n)\right)}_{\text{this is composite trapezoidal rule!}} = \int_a^b f(x)\,dx + \sum_{k=1}^{\infty} h^{2k} \frac{B_{2k}}{(2k)!}\left(f^{(2k-1)}(b) - f^{(2k-1)}(a)\right)$$

only writing down even terms

Two implications:

① error for composite trapezoidal rule looks like

$$E = K_1 h^2 + K_2 h^4 + K_3 h^6 + \ldots$$

constant

So (1) we know the form of the error, hence can cancel it out using repeated Richardson extrapolation

(2) only involves even powers, so repeated Richardson extrapolation has a nice form

② if $f'(a) = f'(b)$, it's actually a $O(h^4)$ rule!

if also $f''(a) = f''(b)$, it's actually a $O(h^6)$ rule!

if f is periodic ($f(x + (b-a)) = f(x)$)

and C^∞ in the periodic sense

i.e., $f \in C^\infty[a,b]$ and $f^{(k)}(b) = f^{(k)}(a)\ \forall k$

then all errors seem to cancel, up to remainder term.

We call this spectral accuracy

(it's like applying a very high order formula to $\{x_0, x_1, \ldots, x_n\}$, then applying that same high order formula to $\{x_1, x_2, \ldots, x_n, x_0\}$, etc., then averaging, and due to periodicity ① these all approximate the same integral, and ② the weights all average to the same #, which is the same as composite trapezoidal rule)

Today, focus on implication ①:

error for composite trapezoidal rule looks like

$$E = K_1 h^2 + K_2 h^4 + K_3 h^6 + \ldots$$

constant

and let's apply Richardson Extrapolation. Fix a, b

Let $R_{k,1}$ = composite trap. rule applied to equispaced nodes $\{x_0 = a, x_1, \ldots, x_{2^{k-1}} = b\}$ w/ $n = 2^{k-1}$

So error for $R_{k,1}$ is $^{*}E_k = c_1 h^2 + c_2 h^4 + O(h^6)$, $h = \dfrac{b-a}{2^{k-1}}$

error for $R_{\tilde{k},1}$ $\quad E_{\tilde{k}} = c_1 \tilde{h}^2 + c_2 \tilde{h}^4 + O(\tilde{h}^6)$, $\tilde{h} = \dfrac{b-a}{2^{\tilde{k}-1}}$

So let $\tilde{k} = k-1$ thus $\tilde{h} = \dfrac{b-a}{2^{k-2}} = 2h$

$$^{**}E_{\tilde{k}} = c_1 (2h)^2 + c_2 (2h)^4 + O(h^6)$$

Now $E_k + \frac{1}{3}(E_k - E_{\tilde{k}}) = \frac{1}{3}(4E_k - E_{\tilde{k}})$

$$= \tfrac{1}{3}\big(\cancel{4c_1 h^2} + 4c_2 h^4 + O(h^6) - \cancel{c_1 (2h)^2} - c_2 (2h)^4 + O(h^6) \big)$$

$$= O(h^4)$$

General rule: to cancel h^k this should be $2^k - 1$ (here, $k = 2$)

$$\text{So } \int_a^b f(x)\,dx = \underbrace{R_{k,1} + \tfrac{1}{3}(R_{k,1} - R_{k-1,1})}_{\text{call this } R_{k,2}} + \underbrace{E_k + \tfrac{1}{3}(E_k - E_{k-1})}_{\text{error is } O(h^4)}$$

	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
$n=1$	$R_{1,1}$			
$n=2$	$R_{2,1}$	$R_{2,2}$		
$n=4$	$R_{3,1}$	$R_{3,2}$	$R_{3,3}$	
$n=8$	$R_{4,1}$	$R_{4,2}$	$R_{4,3}$	$R_{4,4}$

$$R_{k,2} = R_{k,1} + \frac{1}{3}\left(R_{k,1} - R_{k-1,1}\right) \quad (3 = 4^{2-1} - 1)$$

$$R_{k,3} = R_{k,2} + \frac{1}{15}\left(R_{k,2} - R_{k-1,2}\right) \quad (15 = 4^{3-1} - 1)$$

$$R_{k,4} = R_{k,3} + \frac{1}{63}\left(R_{k,3} - R_{k-1,3}\right) \quad (63 = 4^{4-1} - 1)$$

$\downarrow$ Better value of h

$\longrightarrow$ better order $O(h^j)$

Generally,

$$R_{k,j} = R_{k,j-1} + \frac{1}{4^{j-1}-1}\left(R_{k,j-1} - R_{k-1,j-1}\right)$$

Computation: compute it row-by-row
(and add a new row when you need more accuracy)

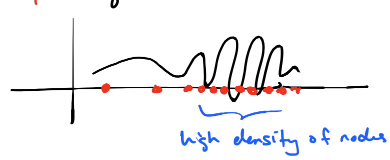
- Because $R_{k,1}$ shares half its nodes w/ $R_{k-1,1}$, we can compute a new entry in the 1st column saving ½ the function evaluations by
$$R_{k,1} = \frac{1}{2}\left(R_{k-1,1} + h_{k-1} \cdot \sum_{i=1}^{2^{k-2}} f(\underbrace{a + (2i-1)h_k}_{x_{2i-1}})\right) \qquad h_k = \frac{b-a}{2^{k-1}}$$
- so $R_{k,1}$ requires $1 + 2^{k-1}$ function evaluations
and $R_{k,j}$ for $j \geq 2$ is done via the formulas (no function evaluations)

This sounds great! We should always use it!

Didn't we say <u>Composite Simpson's Rule</u> was the default in a lot of software, though?

Yes, Romberg integration is neat, but it relies on...

(1) equispaced nodes... we'll later discuss adaptive quadrature that adds nodes where they are needed



(2) Assumes error is $c_1 h^2 + c_2 h^4 + c_3 h^6 + c_4 h^8 + \ldots$
but this relies on f'' existing and being bounded,
and $f^{(4)}$ " ______ "
$f^{(6)}$ " ______ " ...

so this can break.

$\underline{Ex}$ $f(x) = x^{3/2}$ on $[0,1]$

$f'(x) = \frac{3}{2} x^{1/2}$

$f''(x) = \frac{3}{4} \frac{1}{\sqrt{x}}$ ... on $(0,1]$ this isn't bounded!

$\underline{Ex}$ $f(x) = |x|$ on $[-1,1]$

f' does not exist at $x=0$

$\underline{Ex}$ $f(x) = \frac{1}{x^2+1}$ Runge's function

$f \in C^{\infty}(\mathbb{R})$ but $\max_x |f^{(k)}(x)|$ grows with k