Ch 4.6: Adaptive Integration

Helpful to have seen Richardson Extrapolation already

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See Demos/Ch4_AdaptiveIntegration.ipynb

This is ch 4.6 in $\underbrace{\text{Burden + Faires}}_{\text{Alg. 4.3 is hard to follow}}$, but we'll follow ch 5.7 in Driscoll and Braun

Idea:

Software packages (Mathematica's NIntegrate
Matlab's integral (vs "trapz")
Python's scipy.integrate.quad)

are not going to ask the user for # nodes,
instead they're going to ask for an accuracy (w/ a sensible default)

How can we do this?

Key Mathematical idea: a posteriori error estimate

"a priori" vs "a posteriori" come up a lot in other subjects too, so let's review them:

a priori = estimate before you've done work

\+ always valid

− may require knowledge you don't have Ex: $M = \max_{x \in [a,b]} |f''(x)|$

− can't exploit it when you get lucky, i.e., it's always pessimistic

Ex: Simpson's Rule

$$\int_a^b f(x)dx = \frac{h}{3}\Big(f(x_0) + 4f(x_1) + f(x_2) \Big) - \underbrace{\frac{h^5}{90} f^{(4)}(\xi)}_{\text{our "a priori" error estimate}}$$

for some $\xi \in (a,b)$, $h = \frac{b-a}{2}$

a posteriori = estimate after you've done work

\+ sometimes easier, sometimes more useful (no unknown things involved)

\+ can adapt to your specific situation, and it takes it into account if you got lucky

− not useful for prediction or planning, only useful for verifying / certifying

− in some cases (like for our usage in integration) it is a heuristic or based on unverifiable assumptions.

So, let's make an a posteriori error estimate for integration,

i.e., a practical way to evaluate the error, so we know when we have enough nodes

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Start w/ composite Simpson's rule (though you could do a similar derivation for other rules)

Write $S(n)$ to be Simpson's rule w/ n nodes, or $S(h)$

Recall non-composite Simpson has error $-\frac{h^5}{90} f^{(4)}(\xi)$ ($h = \frac{b-a}{2}$) $\xi \in (a,b)$

and composite Simpson has error $-\frac{b-a}{180} h^4 f^{(4)}(\eta)$ $\eta \in (a,b)$

So composite Simpson's Rule is $O(h^4) = O(n^{-4})$ $h = O(1/n)$

Apply Richardson extrapolation

"$S(h)$" or "$S(n)$" means approximation of integral using composite Simpson's rule w/ n nodes (or spacing h)

$$R(h/2) = S(h/2) + \frac{S(h/2) - S(h)}{15}$$

R: Richardson Extrapolation, improved estimate; $15 = 2^4 - 1$

or

$$R(2n) = S(2n) + \frac{S(2n) - S(n)}{15}$$

Richardson Extrapolation, short explanation (2025, we didn't cover this in detail earlier, so here's the short version)

$$I = S(n) + c/n^4 + O\left(\frac{1}{n^k}\right) \quad \boxed{A}$$

true integral; Composite Simpson; error terms; $k \geq 5$ is next highest error term

$$I = S(2n) + c/(2n)^4 + O\left(\frac{1}{n^k}\right) \quad \boxed{B}$$

the "c" terms cancel

Then $I = \left(-\frac{1}{15} + \frac{16}{15}\right) \cdot I = -\frac{1}{15}\boxed{A} + \frac{16}{15}\boxed{B} = \frac{16}{15} S(2n) - \frac{1}{15} S(n) + O\left(\frac{1}{n^k}\right)$ error is smaller

$$= \underbrace{S(2n) + \frac{1}{15}\left(S(2n) - S(n)\right)}_{R(2n),\ \text{the Richardson extrapolation estimate}} + O\left(\frac{1}{n^k}\right)$$

Assumption: $R(2n)$ is so much more accurate than $S(2n)$ that the error in $R(2n)$ is negligible, and so

$$E_{err} = \int_a^b f(x)dx - S(2n) \approx \underbrace{R(2n) - S(2n)}_{\text{our a posteriori error estimate}}$$

$$= \boxed{\frac{S(2n) - S(n)}{15}} = \hat{E}$$

So, basic strategy: double # of n until $|\hat{E}|$ is small.

Details:

① How small should $|\hat{E}|$ be? ie., pick a tolerance "tol" and require $|\hat{E}| < \text{tol}$?

well, it often makes sense to ask for a relative error.

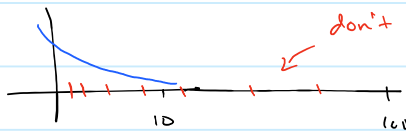
In practice, we usually do both:

Stop when $|\hat{E}| < \text{tol}_{\text{absolute}} + \text{tol}_{\text{relative}} \cdot S(n)$

② Doubling n is going to lead to a lot of nodes very quickly.

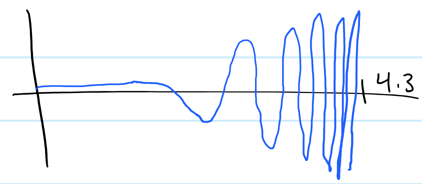
Observation: we often don't need dense nodes everywhere.

Ex: $\int_0^{100} e^{-x}\,dx$



don't need many nodes here since integrand is so small

Ex: $f(x) = (x+1)^2 \cdot \cos\left(\frac{2x+1}{x-4.3}\right)$



want a lot of nodes here

ie., we want to be ADAPTIVE

A nice, popular way to do this is Divide and Conquer (this is a general class of techniques beyond just integration)

Idea:

1) estimate $\hat{E}$ and stop if $|\hat{E}|$ is small enough

2) Split $[a,b]$ in two, $[a,c]$ and $[c,b]$ where $c = \frac{a+b}{2}$

$a \qquad c \qquad b$

note that $\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx$

Recurse, integrating on $[a,c]$ and estimating its error $\hat{E}_{left}$
and on $[c,b]$ and estimating its error $\hat{E}_{right}$

That's the basic idea.

Usually, we use composite Simpson's rule w/ $n=4$, and are careful to re-use any $f(\text{node})$ computations. See pseudocode

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Pseudocode: In 2025, we didn't write this on the board, we went through the code on the colab demo instead

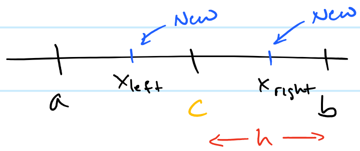
FUNCTION Adaptive Integration $(f, a, b, tol_{abs}, tol_{rel})$

$c = \frac{a+b}{2}$

return $\hat{I}$, nodes = Recursive Integral $(a, f(a), b, f(b), c, f(c))$ // and, implicitly, tol_{abs}, tol_{rel}

FUNCTION Recursive Integral $(a, f(a), b, f(b), c, f(c))$

$x_{left} = \frac{a+c}{2}$



$x_{right} = \frac{c+b}{2}$

nodes = $\{a, x_{left}, c, x_{right}, b\}$

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

$S_2 = h/3\,(f(a) + 4f(c) + f(b))$ // regular (non-composite) Simpson's rule

$S_4 = h/2 \cdot 1/3\,(f(a) + 4\cdot f(x_{left}) + 2\cdot f(c) + 4f(x_{right}) + f(b))$ // composite Simpson

$\hat{E} = 1/15\,(S_4 - S_2)$ // often use 1/10 instead of 1/15 to be more conservative

if $|\hat{E}| < tol_{abs} + tol_{rel} \cdot |S_4|$ // error is acceptable

  return S_4, nodes

else // error is too large, so bisect

  $\hat{I}_{left}$, $nodes_{left}$ = Recursive Integral $(a, f(a), c, f(c), x_{left}, f(x_{left}))$

  $\hat{I}_{right}$, $nodes_{right}$ = Recursive Integral $(c, f(c), b, f(b), x_{right}, f(x_{right}))$

  return $\hat{I}_{left} + \hat{I}_{right}$, $nodes_{left} \cup nodes_{right}$ // as lists, the first entry in $nodes_{right}$ is a duplicate of last entry in $nodes_{left}$

end

Summary

All professional integration packages are adaptive so

① they don't waste time where extra nodes aren't needed

② they automatically generate nodes until a tolerance is reached, and give a (heuristic) "guarantee" on the final error.