Elements of Numerical Integration (Quadrature)

Sunday, October 4, 2020 4:31 PM

What? Why?

We saw that numerical differentiation via finite differences is unstable (BAD)

but analytical differentiation is easy (GOOD): just use

chain rule, product rule, sum rule

In contrast, analytical integration is not easy! "Most" integrals do not have a closed form. Fortunately, numerical integration is stable.

Main idea

In Calc I you saw the "trapezoid", "midpoint" formulas.

These are examples of "quadrature" rules, ie., numerical integration.

They are Riemann sums and converge to the integral as $h \to 0$.

We'll use $h > 0$

For nodes $\{x_0, x_1, \ldots, x_n\}$, often equispaced ($x_{i+1} - x_i = h$),

our strategy is to fit an interpolant to these nodes, then

integrate the interpolant "by hand" (since it's usually a polynomial)

This lecture:

interpolate w/ a polynomial (n is small)

Next lecture:

interpolate w/ a piecewise polynomial (n is large),

"composite" formulas

(You could interpolate w/ a spline, but historically this wasn't done since finding splines by hand is hard)

(non-Composite) interpolatory quadrature

Goal: Find $I = \int_a^b f(x)\,dx$, we can evaluate f but don't know its antiderivative

We'll evaluate f on the $n+1$ nodes $\{x_0, x_1, \ldots, x_n\}$ and interpolate, forming the polynomial $p_n(x) := \sum_{i=0}^{n} f(x_i) L_{n,i}(x)$

$\uparrow$ degree $\le n$

where

$$L_{n,i}(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}$$ is the Lagrange polynomial

Then (key conceptual idea!)

$$I_n := \int_a^b p_n(x) = \int_a^b \sum_{i=0}^{n} f(x_i) L_{n,i}(x)\, dx$$

$$= \sum_{i=0}^{n} f(x_i) \underbrace{\int_a^b L_{n,i}(x)\, dx}_{w_i}$$

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

is our estimate of I.

The weights do not depend on $f(x_i)$, only on x_i.

In the common case of equispaced nodes, they really only depend on n (or h), so we can precompute them!

Key Fact!

Any estimate of I in the form $\sum_{i=0}^{n} w_i f(x_i)$ is a quadrature rule

Aside: an alternative approach, which is a bad idea in 1D but can be a good idea in high dimensions, is to estimate $I \approx \sum_{i=0}^{n} \frac{1}{n+1} f(x_i)$, $x_i \in [a,b]$ chosen randomly

↳ ie. equi-weights

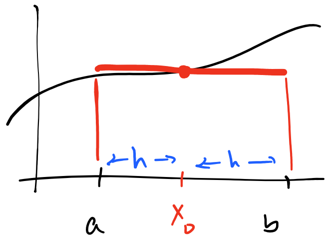
This is Monte Carlo (and quasi-Monte Carlo) integration.

First formula: $n=0$ "midpoint" aka "rectangle" formula

⚠ we always have $n+1$ nodes

$n=0$? $\int_a^a f(x)dx$? The professor's gone crazy!

No, we still want $\int_a^b f(x)dx$ $b>a$ but we're not going to have $a = x_0, \dots$ Instead, pick $x_0 = \frac{b-a}{2}$

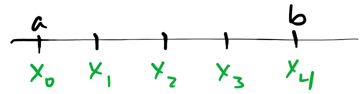


both
$x_{i+1} = x_i + h$
but closed: $x_0 = a$
open: $x_0 = a + h$

In general, we have 2 types of equispaced nodes:

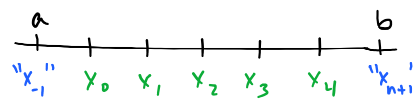
① Closed, meaning $\{x_0 = a,\ x_1, \dots, x_{n-1},\ x_n = b\}$

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



and

② Open, meaning $\{x_0 > a,\ x_1, \dots, x_{n-1},\ x_n < b\}$



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

So, back to $n=0$: nodes $\{x_0\}$, must do "open", $h = \frac{b-a}{n+2} = \frac{b-a}{2}$

The unique interpolant to $f(x_0)$ of degree 0 is the constant function,
$p(x) = f(x_0)$, and $\int_a^b p(x)\,dx = f(x_0)\cdot(b-a)$

So $w_0 = (b-a)$, $I_0 = \sum_{i=0}^{0} w_i f(x_i) = f(x_0)(b-a)$.

Simple enough... what about analyzing the error though?

letting $h = \frac{b-a}{2}$, $x_0 = \frac{a+b}{2}$, Taylor expand around x_0 (assume f'' exists)

$$f(x) = f(x_0) + f'(x_0)(x-x_0) + f''(\xi)(x-x_0)^2/2! \quad \text{for some } \xi \in (a,b)$$

So

$$I = \int_a^b f(x)dx = \underbrace{f(x_0)(b-a)}_{I_0} + \underbrace{f'(x_0)\int_a^b (x-x_0)dx + \int_a^b f''(\xi)\frac{(x-x_0)^2}{2!}dx}_{\text{error}}$$

$\frac{1}{2}(x-x_0)^2\Big|_a^b = \frac{1}{2}h^2 - \frac{1}{2}h^2 = 0$

since $(b-x_0) = (x_0 - a) = h$

NOT quite as simple as

$$f''(\xi)\int_a^b \frac{(x-x_0)^2}{2!}dx = f''(\xi)\frac{(x-x_0)^3}{3!}\Big|_a^b$$

$$= f''(\xi)h^3/3$$

Why not? we can't pull this out of the integral since $\xi = \xi(x)$ (depends on x)

2 ways to fix:

① $f \in C^2[a,b] \Rightarrow f'' \in C[a,b] \overset{EVT}{\Rightarrow} \exists M$ st. $\forall \xi \in [a,b]$, $|f''(\xi)| \le M$

and our error is

$$E = \left|\int_a^b f''(\xi(x))\frac{(x-x_0)^2}{2}dx\right| \le \int_a^b |f''(\xi(x))| \cdot \frac{(x-x_0)^2}{2}dx$$

$$\le M \cdot \int_a^b \frac{(x-x_0)^2}{2}dx$$

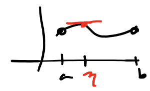
$$= M/3\ h^3$$

② Recall MVT etc:

Aside:

MVT: $F \in C^1[a,b]$ then $\exists\, \eta \in (a,b)$ s.t. $F'(\eta) = \dfrac{F(b)-F(a)}{b-a}$

eg. $F(a)=F(b)$



MVT, integral form, let $F(x) = \int_0^x f(t)\,dt$, $F' = f$

so via MVT $\exists\, \eta$ s.t. $f(\eta) = \dfrac{1}{b-a} \overbrace{\int_a^b f(t)\,dt}^{F(b)-F(a)}$

MVT, weighted version (Thm 1.13)

let $g(x)$ not change sign over $[a,b]$, $f \in C[a,b]$,

then $\exists\, \eta$ s.t. $f(\xi) = \dfrac{\int_a^b f(t)\,g(t)\,dt}{\int_a^b g(t)\,dt}$ $\Big\}= b-a$ if $g = 1$

... so, $\displaystyle\int_a^b \underbrace{f''(\xi(x))}_{\text{"}f\text{"}}\underbrace{\frac{(x-x_0)^2}{2}}_{\text{"}g(x)\text{"}}\,dx$, apply wtd. MVT

$$\exists\, \eta \text{ s.t. } \underbrace{f''(\xi(\eta))}_{\text{some } \xi \in (a,b)} = \frac{\left.\int_a^b f''(\xi(x))\,(x-x_0)^2/2\,dx\right\} E}{\int_a^b (x-x_0)^2/2\,dx = \frac{1}{3}h^3}$$

so $$E = f''(\xi)\cdot \frac{1}{3} h^3$$

so, conclusion, error due to midpoint rule is at most

$$E = \boxed{M/3\; h^3} \quad \text{where} \quad M = \max_{x \in [a,b]} |f''(x)|$$

Right now, a, b, n are given,
So we can't choose h
We can either increase n, or use a composite rule.

Implication Suppose f is a constant function (degree 0 polynomial)

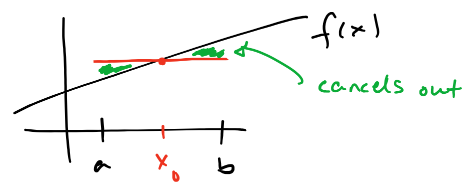
then by looking at picture, clearly error in midpt. rule is 0. Or, via our derivation,

$$M = \max_x |f''(x)| = 0,$$ so another way to see it

And actually, let f be linear (degree 1 polynomial)

then $M = 0$ also! So we make no error!

(what's happening? Our positive and negative errors exactly cancel)



If f is quadratic, then $M \neq 0$, so we do make an error.

Definition The "degree of accuracy" or "degree of precision"] our book

or "degree of exactness"] other books

of a quadrature rule is the largest integer k such that polynomials of degree k have 0 integration error.

Ex. Our midpt. rule has degree of exactness <u>1</u>

<u>Next</u>, more rules (different values of n, <u>closed</u> nodes)