CS321-002

Introduction to Numerical Methods

Lecture 4

Numerical Integration

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October 17, 2000

Definite Integral

a definite integral has an interval for integration. For a fixed integration interval, the result is a number

$$\int_0^{\frac{\pi}{2}} \sin x \, dx = 1$$

an indefinite integral does not have an integration interval. The result of an indefinite integral (antiderivative) is a class of functions

$$\int \sin x \, dx = -\cos x + C$$

numerical integration is for computing definite integrals

Fundamental Theorem of Calculus:

$$\int_a^b F'(x) \, dx = F(b) - F(a)$$

$$\int_a^x F'(t) \, dt = F(x) - F(a)$$

Partition

the definite integral of a function can be viewed as the area under a curve. This point of view lends us means to compute definite integral

let P be a partition of the interval of $[a, b]$ as

$$P = \{a = x_0 < x_1 < x_2 < \cdots < x_{n-1} < x_n = b\}$$

we have n subintervals as $[x_i, x_{i+1}]$. Let m_i be the greatest lower bound of (a nonnegative function) $f(x)$ on $[x_i, x_{i+1}]$ as

$$m_i = \inf\{f(x) : x_i \leq x \leq x_{i+1}\}$$

and M_i as the least upper bound on the same subinterval

$$M_i = \sup\{f(x) : x_i \leq x \leq x_{i+1}\}$$

Lower and Upper Sums

the lower sums and upper sums of f corresponding to the given partition P is

$$L(f;P) = \sum_{i=0}^{n-1} m_i\,(x_{i+1} - x_i)$$

$$U(f;P) = \sum_{i=0}^{n-1} M_i\,(x_{i+1} - x_i)$$

if we consider the definite integral of a nonnegative f as the area under the curve, we have

$$L(f;P) \leq \int_a^b f(x)\,dx \leq U(f;P)$$

for all partitions P

if f is continuous on $[a,b]$, then the above inequality defines the definite integral. The integral also exists if f is monotone (either increasing or decreasing) on $[a,b]$

Riemann-Integrable Functions

if the greatest lower bound equals the least upper bound for all partitions of $[a, b]$, i.e.,

$$\inf_P U(f; P) = \sup_P L(f, P)$$

then f is said to be Riemann-integrable

every continuous function defined on a closed and bounded interval of the real line is Riemann-integrable

we have

$$\lim_{n \to \infty} L(f; P_n) = \int_a^b f(x)\, dx = \lim_{n \to \infty} U(f; P_n)$$

where $P_0, P_1, \ldots, P_n, \ldots$ are a sequence of partitions such that the length of the largest subinterval in P_n converges to 0 as $n - \infty$

we can construct nested (refined) partitions

Computation

1.) need a procedure to evaluate $f(x)$

2.) determine a partition (how many subintervals) of the interval $[a, b]$

3.) compute m_i and M_i on each subinterval

4.) compute the sums $L(f; P)$ and $U(f; P)$

5.) an approximate value is obtained

$$\int_a^b f(x)\,dx \approx \frac{1}{2}[U(f;P) + L(f;P)]$$

6.) the error of this approximation is bounded by

$$\frac{1}{2}[U(f;P) - L(f;P)]$$

Trapezoid Rule

a strategy that is better than estimating both the upper and the lower bounds of the area beneath a curve is to use trapezoids

the interval $[a, b]$ is first divided into subintervals $[x_i, x_{i+1}], 0 \leq i \leq n - 1$. A typical trapezoid has the subinterval $[x_i, x_{i+1}]$ as its base, and the two vertical sides are $f(x_i)$ and $f(x_{i+1})$. The area is given by the base times the average height. the basic trapezoid rule for the subinterval $[x_i, x_{i+1}]$ is

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \frac{1}{2}[f(x_i) + f(x_{i+1})]$$

the total area under the curve is

$$\int_a^b f(x)\,dx \approx T(f; P) = \sum_{i=0}^{n-1} A_i$$

$$= \frac{1}{2} \sum_{i=0}^{n-1} (x_{i+1} - x_i)[f(x_i) + f(x_{i+1})]$$

Uniform Spacing

the lengths of the subintervals in a partition can be different. For fast computation, a uniform partition of the interval may be advantageous

let n be the number of subintervals, then $h = (b-a)/n$ is the uniform interval spacing. The nodal points are $x_i = a + i\,h, i = 0, 1, \ldots, n$. Hence the composite trapezoid rule is

$$T(f;P) = \frac{h}{2} \sum_{i=0}^{n-1} [f(x_i) + f(x_{i+1})]$$

note that the end point of an interval is the starting point of the next interval. This fact can save almost half of the computation,

$$\int_a^b f(x)\,dx \approx h \left\{ \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2}[f(x_0) + f(x_n)] \right\}$$

Error Analysis

if $f''(x)$ exists and is continuous on $[a, b]$, the error of the composite trapezoid rule T is

$$\int_a^b f(x)\,dx - T = -\frac{b-a}{12}\,h^2\,f''(\xi) = O(h^2)$$

for some ξ in (a, b)

Proof. using polynomial interpolation, (p. 198)

Example. show that

$$\int_a^{a+h} f(x)\,dx =$$
$$\frac{h}{2}[f(a) + f(a+h)] - \frac{h^3}{12}f''(a) + \cdots$$

need to define

$$F(t) = \int_a^t f(x)\,dx$$

then by the Fundamental Theorem of Calculus, we have $F'(t) = f(t)$. Note that $F(a) = 0$

Estimate Grid Spacing

Example. if the composite trapezoid rule is used to compute

$$\int_0^1 e^{-x^2}\,dx$$

with an error of at most 0.5×10^{-4}, what is the uniform grid spacing h?

from the graph of the second derivative

$$f''(x) = (4x^2 - 2)e^{-x^2}$$

we find that

$$|f''(x)| \leq |f''(0)| = 2$$

we need

$$\left| -\frac{b-a}{12} h^2 f''(\xi) \right| \leq \frac{1}{6} h^2 < 0.5 \times 10^{-4}$$

it follows that $h \leq 0.01732$. The number of subintervals is $n \geq [1/h] = 58$

Recursive Trapezoid Formula

given a parameter n, dividing $[a, b]$ into 2^n equally spaced subintervals, we have

$$\begin{aligned} T(f;P) &= h\sum_{i=1}^{n-1} f(x_i) + \frac{h}{2}[f(x_0) + f(x_n)] \\ &= h\sum_{i=1}^{n-1} f(a + i\,h) + \frac{h}{2}[f(a) + f(b)] \end{aligned}$$

note that $n = 2^n$ and $h = (b - a)/2^n$

$$R(n, 0) = h\sum_{i=1}^{2^n-1} f(a + i\,h) + \frac{h}{2}[f(a) + f(b)]$$

notice that $R(n, 0)$ can be viewed as dividing each subinterval of $R(n - 1, 0)$ into two equal sub-subintervals. If we already computed $R(n-1, 0)$, how can we compute $R(n, 0)$ cheaply?

Recursive Formula

if $R(n-1,0)$ is available, $R(n,0)$ can be computed as

$$R(n,0) = \frac{1}{2}R(n-1,0)+h\sum_{k=1}^{2^n-1} f[a+(2k-1)h]$$

for $n \geq 1$ using $h = (b-a)/2^n$. Initial starting value is

$$R(0,0) = \frac{1}{2}(b-a)[f(a)-f(b)]$$

the trick is to only sum the function values at every other grid points.

Proof. note that

$$R(n,0) = h\sum_{i=1}^{2^n-1} f(a+i\,h) + C$$

with $C = h[f(a)+f(b)]/2$ and

$$R(n-1,0) = 2h\sum_{j=1}^{2^{n-1}-1} f(a+2j\,h) + 2C$$

Two Dimensional Integration

for one dimensional numerical integration on $[0, 1]$, using uniform space $h = 1/n$

$$\int_0^1 f(x)\,dx \approx \frac{1}{2h}[f(0) + 2\sum_{i=1}^{n-1} f\left(\frac{i}{n}\right) + f(1)]$$
$$= \sum_{i=0}^{n} A_i\, f\left(\frac{i}{n}\right)$$

for two dimensional integration on a unit square

$$\int_0^1 \int_0^1 f(x,y)\,dx\,dy \approx \int_0^1 \sum_{i=0}^{n} A_i\, f\left(\frac{i}{n}, y\right)\,dy$$
$$= \sum_{i=0}^{n} A_i \int_0^1 f\left(\frac{i}{n}, y\right)\,dy$$
$$\approx \sum_{i=0}^{n} A_i \sum_{j=0}^{n} A_j\, f\left(\frac{i}{n}, \frac{j}{n}\right)$$
$$= \sum_{i=0}^{n}\sum_{j=0}^{n} A_i\, A_j\, f\left(\frac{i}{n}, \frac{j}{n}\right)$$

Romberg Algorithm

recursive composite trapezoid method

$$R(0,0) = \frac{1}{2}(b-a)[f(a)+f(b)]$$

for $h = 1/2^n$ and $n \geq 1$

$$R(n,0) = \frac{1}{2}R(n-1,0) + h\sum_{k=1}^{2^n-1} f[a+(2k-1)h]$$

using Richardson extrapolation, we can have

$$R(i,j) = R(i,j-1) + \frac{1}{4^j-1}[R(i,j-1) - R(i-1,j-1)]$$

for $i \geq j$ and $j \geq 1$. This is the Romberg algorithm, which may yield better approximate values for larger j

$$\begin{array}{llll} R(0,0) & & & \\ R(1,0) & R(1,1) & & \\ R(2,0) & R(2,1) & R(2,2) & \\ R(3,0) & R(3,1) & R(3,2) & R(3,3) \end{array}$$