Chapter 3
Numerical Differentiation and Integration

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MATH 561 Numerical Analysis

Numerical Differentiation

Problem

For a given differentiable function f, approximate the derivative $f'(x_0)$ in terms of the values of f at x_0 and at nearby points $x_1, x_2, \ldots, x_n$ (not necessarily equally spaced or in natural order). Estimate the error of the approximation obtained.

?Using Polynomial approximation or Polynomial interpolation.?

Examples: inspired by definition of derivatives

forward difference

backward difference

Numerical Differentiation

Forward and Backward Differences

Inspired by the definition of derivative:

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h},$$

choose a small h and approximate

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}.$$

The error term for the linear Lagrange polynomial gives:

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi).$$

Also known as the forward-difference formula if $h > 0$ and the backward-difference formula if $h < 0$.

General Derivative Approximations

Differentiation of Lagrange Polynomials

Differentiate

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x))$$

to get for $j = 0, \ldots, n$,

$$f'(x_j) = \sum_{k=0}^{n} f(x_k){L_k}'(x_j) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{k \neq j} (x_j - x_k)$$

This is the $(n+1)$-point formula for approximating $f'(x_j)$.

Commonly Used Formulas

Using equally spaced points with $h = x_{j+1} - x_j$, we have the three-point formulas

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3} f'''(\xi_0)$$

$$f'(x_0) = \frac{1}{2h}[-f(x_0-h) + f(x_0+h)] - \frac{h^2}{6} f'''(\xi_1)$$

$$f'(x_0) = \frac{1}{2h}[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)] + \frac{h^2}{3} f'''(\xi_2)$$

$$f''(x_0) = \frac{1}{h^2}[f(x_0-h) - 2f(x_0) + f(x_0+h)] - \frac{h^2}{12} f^{(4)}(\xi)$$

and the five-point formula

$$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30} f^{(5)}(\xi)$$

General Derivative Approximations; Newton's Formula

We know

$$f(x) = p_n(f;x) + r_n(x)$$

with the interpolation polynomial in Newton' form

$$p_n(f;x) = f_0 + \sum_{k=1}^{n} [x_0, \ldots, x_k]f \prod_{i=0}^{k-1} (x - x_i)$$

and the error term

$$r_n(x) = \prod_{i=0}^{n} (x - x_i) \frac{f^{(n+1)}(\xi(x))}{(n+1)!}$$

Differentiating and evaluated at x_0:

$$p'_n(f;x_0) = [x_0, x_1]f + \sum_{k=2}^{n} [x_0, \ldots, x_k]f \prod_{i=1}^{k-1} (x_0 - x_i)$$

$$r'_n(x_0) = \frac{f^{(n+1)}(\xi(x_0))}{(n+1)!} \prod_{k=1}^{n} (x_0 - x_k)$$

General Derivative Approximations; Newton's Formula

Therefore,

$$f'(x_0) = p_n'(f; x_0) + e_n, \text{ with } e_n = r_n'(x_0)$$

The error

$$e_n = O(H^n), \text{ as } H \to 0, \text{ with } H = \max_i |x_0 - x_i|$$

See Examples.

Optimal h

- Consider the three-point central difference formula:

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f'''(\xi_1)$$

- Suppose that round-off errors ϵ are introduced when computing f. Then the approximation error is

$$|f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h}| \leqslant \epsilon/h + \frac{h^2}{6}M = e(h)$$

  where $\tilde{f}$ is the computed function and $|f'''(x)| \leqslant M$.
- Sum of truncation error $h^2M/6$ and round-off error ϵ/h
- Minimize $e(h)$ to find the optimal $h = \sqrt[3]{3\epsilon/M}$.

So the error is at least $O(\epsilon^{2/3})$, not $O(\epsilon)$. Significant loss of accuracy! Even worse for high-order formulae.

Richardson's Extrapolation

Richardson's extrapolation is used to generate high-accuracy results while using loworder formulas.

- Suppose $N(h)$ approximates an unknown M with error

$$M - N(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$

the an $O(h^j$ approximation is given for $j = 2, 3, \ldots$ by

$$N_j(h) = N_{j-1}(\frac{h}{2}) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1}$$

- The results can be written in a table:

$O(h)$	$O(h^2)$	$O(h^3)$	$O(h^4)$
1: $N_1(h) \equiv N(h)$			
2: $N_1(h/2) \equiv N(h/2)$	3: $N_2(h)$		
4: $N_1(h/4) \equiv N(h/4)$	5: $N_2(h/2)$	6: $N_3(h)$	
7: $N_1(h/8) \equiv N(h/8)$	8: $N_2(h/4)$	9: $N_3(h/2)$	10: $N_4(h)$

Richardson's Extrapolation

- If some error terms are zero, different and more efficient formulas can be derived
- Example: if

$$M - N(h) = K_2 h^2 + K_4 h^4 + \cdots$$

then an $O(h^{2j})$ approximation is given for $j = 2, 3 \ldots$ by

$$N_j(h) = N_{j-1}(h/2) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}$$

Numerical Integration

Problem

The basic problem is to calculate the definite integral of a given function f, extended over a finite interval $[a, b]$.

- f is well-behaved
- f has integrable singularity; improper integrals

Numerical Integration; Numerical Quadrature

Integration of Lagrange Interpolating Polynomials

Select $\{x_0, \ldots, x_n\}$ in $[a, b]$ and integrate the Lagrange polynomial $P_n(x) = \sum_{i=0}^{n} f(x_i)L_i(x)$ and its truncation error term over $[a, b]$ to obtain

$$\int_a^b f(x)dx = \sum_{i=0}^{n} a_i f(x_i) + E(f)$$

with

$$a_i = \int_a^b L_i(x)dx$$

and

$$E(f) = \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^{n} f^{(n+1)}(\xi(x))dx$$

Trapezoidal and Simpson's Rules

The Trapezoidal Rule

Linear Lagrange polynomial with $x_0 = a, x_1 = b, h = b - a$, gives

$$\int_a^b f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi)$$

Simpson's Rule

Linear Lagrange polynomial with

$x_0 = a, x_1 = a + h, x_2 = b, h = (b - a)/2$, gives

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi)$$

The Composite Trapezoidal Rules

Assume partition of the interval $[a, b]$:

$$a = x_0 < x_1 < \cdots < x_n = b, x_k = a + kh, h = (b - a)/n.$$

On $[x_k, x_{k+1}]$, the trapezoidal rule:

$$\int_{x_k}^{x_{k+1}} f(x)dx = \int_{x_k}^{x_{k+1}} p_1(f; x)dx + \int_{x_k}^{x_{k+1}} R_1(x)dx$$

with

$$p_1(f; x) = f_k + (x - x_k)[x_k, x_{k+1}]f,$$
$$R_1(x) = (x - x_k)(x - x_{k+1})\frac{f''(\xi(x))}{2}.$$

So

$$\int_{x_k}^{x_{k+1}} f(x)dx = \frac{h}{2}(f_k + f_{k+1}) - \frac{1}{2}h^3 f''(\xi_k),\ x_k < \xi_k < x_{k+1}$$

The Composite Trapezoidal Rule

One $[a, b]$,

$$\int_a^b f(x)dx = h(\frac{1}{2}f_0 + f_1 + \cdots + f_{n-1} + \frac{1}{2}f_n) + E_n^T(f),$$

with

$$E_n^T(f) = -\frac{1}{12}h^3 \sum_{k=0}^{n-1} f''(\xi_k) = -\frac{1}{12}h^2(b-a)[\frac{1}{n}\sum_{k=0}^{n-1} f''(\xi_k)]$$

Theorem

Let $f \in C^2[a, b], h = (b-a)/n, x_j = a + jh, \mu \in (a, b)$. The Composite Trapezoidal rule for n subintervals is

$$\int_a^b f(x)dx = \frac{h}{2}[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)] - \frac{b-a}{12}h^2 f''(\mu)$$

The Composite Simpson's Rules

Using quadratic interpolation at x_k, x_{k+1}, x_{k+2}, the Simpson's rule:

$$\int_{x_k}^{x_{k+2}} f(x)dx = \frac{h}{3}(f_k + 4f_{k+1} + f_{k+2}) - \frac{1}{90}h^5 f^{(4)}(\xi_k), x_k < \xi_k < x_{k+2},$$

On $[a, b]$, the composite Simpson's rule (n even),

$$\int_a^b f(x)dx = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 4f_{n-1} + f_n) + E_n{}^s(f),$$

with $E_n^s = -\frac{1}{180}(b-a)h^4 f^{(4)}(\xi), a < \xi < b.$

Proof by Exercise 9!

The Composite Trapezoidal Rules for Trigonometric Polynomials

Trigonometric polynomial of degree m on $[0, 2\pi]$:

$$\mathbf{T}_m[0, 2\pi] = \{t(x) : t(x) = a_0 + \sum_{k=1}^{m} a_k \cos(kx) + \sum_{k=1}^{m} b_k \sin(kx).\}$$

For the composite Trapezoidal rule, we have

$$E_n^T(f) = 0 \text{ for all } f \in \mathbf{T}_{n-1}[0, 2\pi]$$

Proof with complex exponential functions

The Composite Trapezoidal Rules for Complex Exponential Functions

For complex exponential $e_v(x) = e^{ivx}$, we have

$$\begin{aligned} E_n^T(e_v) &= \int_0^{2\pi} e_v(x)dx - \frac{2\pi}{n}[\frac{1}{2}e_v(0) + \sum_{k=1}^{n-1} e_v(\frac{k2\pi}{n}) + \frac{1}{2}e_v(2\pi) \\ &= \int_0^{2\pi} e^{ivx}dx - \frac{2\pi}{n}\sum_{k=0}^{n-1} e^{ivk2\pi/n}. \end{aligned}$$

If $v = 0,\ E_n^T(e_0) = 0$, otherwise,

$$E_n^T(e_v) = \begin{cases} -2\pi, \text{ if } v = 0(mod\ n), v > 0 \\ -\frac{2\pi}{n}\frac{1 - e^{ivn2\pi/n}}{1 - e^{iv2\pi/n}} = 0, \text{ if } v \neq 0(mod\ n). \end{cases}$$

In Particular, $E_n^T(e_v) = 0,\ v = 0, 1, \ldots, n-1$.

The Composite Trapezoidal Rules for Trigonometric Polynomials

We see

$$E_n^T(\cos v\cdot) = \left\{ \begin{array}{c} -2\pi,\ v = 0(mod\ n), v \neq 0 \\ 0,\ otherwise \end{array} \right\}, \quad E_n^T(\sin v\cdot) = 0.$$

If f is 2π-periodic with uniformly convergent Fourier expansion:

$$f(x) = \sum_{v=0}^{\infty} [a_v(f)\cos vx + b_v(f)\sin vx]$$

then

$$E_n^T(f) = \sum_{v=0}^{\infty} [a_v(f)E_n^T(\cos v\cdot) + b_v(f)E_n^T(\sin v\cdot)] = -2\pi \sum_{l=1}^{\infty} a_{ln}(f).$$

So

$$E_n^T(f) = O(n^{-r}) \text{ as } n \to \infty \ (f \in C^r[\mathbf{R}],\ 2\pi\text{-periodic}).$$

Romberg Integration

- Compute a sequence of n integrals using the Composite Trapezoidal rule, where $m_1 = 1, m_2 = 2, m_3 = 4, \ldots$ and $m_n = 2^{n-1}$.
- The step sizes are then $h_k = (b-a)/m_k = (b-a)/2^{k-1}$
- The Trapezoidal rule becomes

$$\int_a^b f(x)dx = \frac{h_k}{2}[f(a) + f(b) + 2(\sum_{i=1}^{2^{k-1}-1} f(a + ih_k))] - \frac{b-a}{12}h_k^2 f''(x_k)$$

Romberg Integration

- Let $R_{k,1}$ denote the trapezoidal approximation, then

$$
\begin{aligned}
R_{1,1} &= \frac{h_1}{2}[f(a) + f(b)] = \frac{b-a}{2}[f(a) + f(b)] \\
R_{2,1} &= \frac{1}{2}[R_{1,1} + h_1 f(a + h_2)] \\
R_{3,1} &= \frac{1}{2}\{R_{2,1} + h_2[f(a + h_3) + f(a + 3h_3)]\} \\
R_{k,1} &= \frac{1}{2}[R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k)]
\end{aligned}
$$

- Apply Richardson extrapolation to these values:

$$
R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}
$$

Romberg Integration–Implementation

MATLAB Code

function R = romberg(f,a,b,n)

$h = b - a;$

$R = zeros(n, n);$

$R(1, 1) = h/2 * (f(a) + f(b));$

for $i = 2 : n$

$\quad R(i, 1) = 1/2 * (R(i-1, 1) + h * sum(f(a + ((1 : 2^{(i-2)}) - 0.5) * h)));$

$\quad$ for $j = 2 : i$

$\quad\quad R(i, j) = R(i, j-1) + (R(i, j-1) - R(i-1, j-1))/(4^{(j-1)} - 1);$

$\quad$ end

$\quad h = h/2;$

end