Chapter 4
Numerical Differentiation and Integration

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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

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

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*

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0)$$
$$f'(x_0) = \frac{1}{2h}[-f(x_0-h) + f(x_0+h)] - \frac{h^2}{6}f^{(3)}(\xi_1)$$
$$f'(x_0) = \frac{1}{2h}[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)] + \frac{h^2}{3}f^{(3)}(\xi_2)$$
$$f''(x_0) = \frac{1}{h^2}[f(x_0-h) - 2f(x_0) + f(x_0+h)] - \frac{h^2}{12}f^{(4)}(\xi)$$

and the *five-point formula*

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

Optimal h

- Consider the three-point central difference formula:

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6} f^{(3)}(\xi_1)$$

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

$$\left| f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} \right| \leq \frac{\varepsilon}{h} + \frac{h^2}{6} M = e(h)$$

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

Richardson's Extrapolation

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

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

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

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

- 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:$N_1(\frac{h}{2}) \equiv N(\frac{h}{2})$	**3:**$N_2(h)$		
4:$N_1(\frac{h}{4}) \equiv N(\frac{h}{4})$	**5:**$N_2(\frac{h}{2})$	**6:**$N_3(h)$	
7:$N_1(\frac{h}{8}) \equiv N(\frac{h}{8})$	**8:**$N_2(\frac{h}{4})$	**9:**$N_3(\frac{h}{2})$	**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

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

Numerical Quadrature

Integration of Lagrange Interpolating Polynomials

Select $\{x_0, \dots, x_n\}$ 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

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

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

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

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

Definition

The *degree of accuracy*, or *precision*, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \ldots, n$.

The Newton-Cotes Formulas

The Closed Newton-Cotes Formulas

Use nodes $x_i = x_0 + ih$, $x_0 = a$, $x_n = b$, $h = (b-a)/n$:

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

$$a_i = \int_{x_0}^{x_n} L_i(x)\,dx = \int_{x_0}^{x_n} \prod_{j \neq i} \frac{(x - x_j)}{(x_i - x_j)}\,dx$$

$n = 1$ gives the Trapezoidal rule, $n = 2$ gives Simpson's rule.

The Open Newton-Cotes Formulas

Use nodes $x_i = x_0 + ih$, $x_0 = a + h$, $x_n = b - h$,
$h = (b-a)/(n+2)$. Setting $n = 0$ gives the Midpoint rule:

$$\int_{x_{-1}}^{x_1} f(x)\,dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi)$$

Composite Rules

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

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

Theorem

Let $f \in C^4[a,b]$, n even, $h = (b-a)/n$, $x_j = a + jh$, $\mu \in (a,b)$. The *Composite Simpson's rule* for n subintervals is

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right] - \frac{b-a}{180} h^4 f^{(4)}(\mu)$$

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

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

Romberg Integration

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

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

- 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

MATLAB Implementation

```
function R = romberg(f, a, b, n)
% Compute integral of f(x) from a to b using Romberg integration.

h = b-a;
R = zeros(n,n);
R(1,1) = h/2 * (f(a) + f(b));
for i = 2:n
    R(i,1) = 1/2 * (R(i-1,1) + h*sum(f(a + ((1:2^(i-2))-0.5)*h)));
    for j = 2:i
        R(i,j) = R(i,j-1) + (R(i,j-1)-R(i-1,j-1)) / (4^(j-1)-1);
    end
    h = h/2;
end
```

Error Estimation

- The error term in Simpson's rule requires knowledge of $f^{(4)}$:

$$\int_a^b f(x)\,dx = S(a,b) - \frac{h^5}{90} f^{(4)}(\mu)$$

- Instead, apply it again with step size $h/2$:

$$\int_a^b f(x)\,dx = S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16}\left(\frac{h^5}{90}\right) f^{(4)}(\tilde{\mu})$$

- The assumption $f^{(4)}(\mu) \approx f^{(4)}(\tilde{\mu})$ gives the error estimate

$$\begin{aligned} &\left|\int_a^b f(x)\,dx - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \\ &\approx \frac{1}{15}\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| \end{aligned}$$

Adaptive Quadrature

- To compute $\int_a^b f(x)\,dx$ within a tolerance $\varepsilon > 0$, first apply Simpson's rule with $h = (b-a)/2$ and with $h/2$
- If
$$\left|S(a,b) - S\left(a, \frac{a+b}{2}\right) - S\left(\frac{a+b}{2}, b\right)\right| < 15\varepsilon$$
then the integral is sufficiently accurate
- If not, apply the technique to $[a,(a+b)/2]$ and $[(a+b)/2, b]$, and compute the integral within a tolerance of $\varepsilon/2$
- Repeat until each portion is within the required tolerance

Gaussian Quadrature

- Basic idea: Calculate both nodes $x_1, \ldots, x_n$ and coefficients $c_1, \ldots, c_n$ such that

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} c_i f(x_i)$$

- Since there are $2n$ parameters, we might expect a degree of precision of $2n - 1$
- Example: $n = 2$ gives the rule

$$\int_{-1}^{1} f(x)\,dx \approx f\left(\frac{-\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

with degree of precision 3

Legendre Polynomials

- The *Legendre polynomials* $P_n(x)$ have the properties
  1. For each n, $P_n(x)$ is a monic polynomial of degree n (leading coefficient 1)
  2. $\int_{-1}^{1} P(x)P_n(x)\,dx = 0$ when $P(x)$ is a polynomial of degree less than n
- The roots of $P_n(x)$ are distinct, in the interval $(-1,1)$, and symmetric with respect to the origin.
- Examples:

$$
\begin{aligned}
P_0(x) &= 1, & P_1(x) &= x \\
P_2(x) &= x^2 - \frac{1}{3} & P_3(x) &= x^3 - \frac{3}{5}x \\
P_4(x) &= x^4 - \frac{6}{7}x^2 + \frac{3}{35}
\end{aligned}
$$

Gaussian Quadrature

Theorem

Suppose $x_1, \ldots, x_n$ are roots of $P_n(x)$ and

$$c_i = \int_{-1}^{1} \prod_{j \neq i}^{n} \frac{x - x_j}{x_i - x_j}\, dx$$

If $P(x)$ is any polynomial of degree less than $2n$, then

$$\int_{-1}^{1} P(x)\, dx = \sum_{i=1}^{n} c_i P(x_i)$$

Computing Gaussian Quadrature Coefficients

MATLAB Implementation

```
function [x, c] = gaussquad(n)
% Compute Gaussian quadrature points and coefficients.

P = zeros(n+1,n+1);
P([1,2],1) = 1;
for k = 1:n-1
    P(k+2,1:k+2) = ((2*k+1)*[P(k+1,1:k+1) 0] - ...
                    k*[0 0 P(k,1:k)]) / (k+1);
end
x = sort(roots(P(n+1,1:n+1)));

A = zeros(n,n);
for i = 1:n
    A(i,:) = polyval(P(i,1:i),x)';
end
c = A \ [2; zeros(n-1,1)];
```

Arbitrary Intervals

Transform integrals $\int_a^b f(x)\,dx$ into integrals over $[-1,1]$ by a change of variables:

$$t = \frac{2x-a-b}{b-a} \Leftrightarrow x = \frac{1}{2}[(b-a)t+a+b]$$

Gaussian quadrature then gives

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{(b-a)t+(b+a)}{2}\right)\frac{(b-a)}{2}\,dt$$

Double Integrals

- Consider the double integral

$$\iint_R f(x,y)\,dA, \qquad R = \{(x,y)\,|\,a \le x \le b, c \le y \le d\}$$

- Partition $[a,b]$ and $[c,d]$ into even number of subintervals n, m
- Step sizes $h = (b-a)/n$ and $k = (d-c)/m$
- Write the integral as an iterated integral

$$\iint_R f(x,y)\,dA = \int_a^b \left(\int_c^d f(x,y)\,dy \right)\,dx$$

and use any quadrature rule in an iterated manner.

Composite Simpson's Rule Double Integration

The Composite Simpson's rule gives

$$\int_a^b \left(\int_c^d f(x,y)\,dy \right)\,dx = \frac{hk}{9}\sum_{i=0}^{n}\sum_{j=0}^{m} w_{i,j} f(x_i, y_j) + E$$

where $x_i = a + ih$, $y_j = c + jk$, $w_{i,j}$ are the products of the nested Composite Simpson's rule coefficients (see below), and the error is

$$E = -\frac{(d-c)(b-a)}{180}\left[h^4 \frac{\partial^4 f}{\partial x^4}(\bar{\eta}, \bar{\mu}) + k^4 \frac{\partial^4 f}{\partial y^4}(\hat{\eta}, \hat{\mu}) \right]$$

$$\begin{array}{cccccc}
d & \bullet 1 & \bullet 4 & \bullet 2 & \bullet 4 & \bullet 1 \\
 & \bullet 4 & \bullet 16 & \bullet 8 & \bullet 16 & \bullet 4 \\
c & \bullet 1 & \bullet 4 & \bullet 2 & \bullet 4 & \bullet 1 \\
 & a & & & & b
\end{array}$$

Non-Rectangular Regions

The same technique can be applied to double integrals of the form

$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dy\,dx$$

The step size for x is still $h = (b-a)/n$, but for y it varies with x:

$$k(x) = \frac{d(x) - c(x)}{m}$$

Gaussian Double Integration

- For Guassian integration, first transform the roots $r_{n,j}$ from $[-1, 1]$ to $[a, b]$ and $[c, d]$, respectively
- The integral is then

$$\int_a^b \int_c^d f(x, y)\, dy\, dx \approx \frac{(b-a)(d-c)}{4} \sum_{i=1}^{n} \sum_{j=1}^{n} c_{n,i} c_{n,j} f(x_i, y_j)$$

- Similar techniques can be used for non-rectangular regions

Improper Integrals with a Singularity

The improper integral below, with a singularity at the left endpoint, converges if and only if $0 < p < 1$ and then

$$\int_a^b \frac{1}{(x-a)^p} dx = \left. \frac{(x-a)^{1-p}}{1-p} \right|_a^b = \frac{(b-a)^{1-p}}{1-p}$$

More generally, if

$$f(x) = \frac{g(x)}{(x-a)^p}, \quad 0 < p < 1, \quad g \text{ continuous on } [a, b],$$

construct the fourth Taylor polynomial $P_4(x)$ for g about a:

$$P_4(x) = g(a) + g'(a)(x-a) + \frac{g''(a)}{2!}(x-a)^2 + \frac{g'''(a)}{3!}(x-a)^3 + \frac{g^{(4)}(a)}{4!}(x-a)^4$$

and write

$$\int_a^b f(x)\,dx = \int_a^b \frac{g(x) - P_4(x)}{(x-a)^p} dx + \int_a^b \frac{P_4(x)}{(x-a)^p} dx$$

The second integral can be computed exactly:

$$\begin{aligned}\int_a^b \frac{P_4(x)}{(x-a)^p} dx &= \sum_{k=0}^{4} \int_a^b \frac{g^{(k)}(a)}{k!} (x-a)^{k-p}\,dx \\ &= \sum_{k=0}^{4} \frac{g^{(k)}(a)}{k!(k+1-p)} (b-a)^{k+1-p}\end{aligned}$$

Improper Integrals with a Singularity

For the first integral, use the Composite Simpson's rule to compute the integral of G on $[a, b]$, where

$$G(x) = \begin{cases} \frac{g(x) - P_4(x)}{(x-a)^p}, & \text{if } a < x \leq b \\ 0, & \text{if } x = a \end{cases}$$

Note that $0 < p < 1$ and $P_4^{(k)}(a)$ agrees with $g^{(k)}(a)$ for each $k = 0, 1, 2, 3, 4$, so $G \in C^4[a, b]$ and Simpson's rule can be applied.

Singularity at the Right Endpoint

- For an improper integral with a singularity at the right endpoint b, make the substitution $z = -x$, $dz = -dx$ to obtain

$$\int_a^b f(x)\,dx = \int_{-b}^{-a} f(-z)\,dz$$

  which has its singularity at the left endpoint
- For an improper integral with a singularity at c, where $a < c < b$, split into two improper integrals

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

Infinite Limits of Integration

An integral of the form $\int_a^\infty \frac{1}{x^p} dx$, with $p > 1$, can be converted to an integral with left endpoint singularity at 0 by the substitution

$$t = x^{-1}, \quad dt = -x^{-2}\, dx, \text{ so } dx = -x^2 dt = -t^{-2} dt$$

which gives

$$\int_a^\infty \frac{1}{x^p} dx = \int_{1/a}^0 -\frac{t^p}{t^2} dt = \int_0^{1/a} \frac{1}{t^{2-p}} dt$$

More generally, this variable change converts $\int_a^\infty f(x)\, dx$ into

$$\int_a^\infty f(x)\, dx = \int_0^{1/a} t^{-2} f\left(\frac{1}{t}\right)\, dt$$