Chapter 4
Numerical Differentiation and Integration

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Math 128A Numerical Analysis
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 \textit{forward-difference formula} if \( h > 0 \) and the \textit{backward-difference formula} if \( h < 0 \)
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 \(f'(x_j)\).
Using equally spaced points with $h = x_{j+1} - x_j$, we have the three-point formulas

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

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

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

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

and the five-point formula

\[
f'(x_0) = \frac{1}{12h} \left[ f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h) \right]
\]

\[
+ \frac{h^4}{30} f^{(5)}(\xi)
\]
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 \( \varepsilon \) are introduced when computing \( f \). Then the approximation error is

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

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 \( \varepsilon / h \)
- Minimize \( e(h) \) to find the optimal \( h = \sqrt[3]{3\varepsilon / M} \)
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:

<table>
<thead>
<tr>
<th></th>
<th>$O(h)$</th>
<th>$O(h^2)$</th>
<th>$O(h^3)$</th>
<th>$O(h^4)$</th>
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<tbody>
<tr>
<td>1:</td>
<td>$N_1(h)$ ≡ $N(h)$</td>
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<td>2:</td>
<td>$N_1\left(\frac{h}{2}\right)$ ≡ $N\left(\frac{h}{2}\right)$</td>
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<td>3:</td>
<td>$N_2(h)$</td>
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<td>4:</td>
<td>$N_1\left(\frac{h}{4}\right)$ ≡ $N\left(\frac{h}{4}\right)$</td>
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<td>5:</td>
<td>$N_2\left(\frac{h}{2}\right)$</td>
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<tr>
<td>6:</td>
<td>$N_3(h)$</td>
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<td>7:</td>
<td>$N_1\left(\frac{h}{8}\right)$ ≡ $N\left(\frac{h}{8}\right)$</td>
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<td>8:</td>
<td>$N_2\left(\frac{h}{4}\right)$</td>
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<td>9:</td>
<td>$N_3\left(\frac{h}{2}\right)$</td>
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<td>10:</td>
<td>$N_4(h)$</td>
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</tbody>
</table>
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 \( \{x_0, \ldots, x_n\} \) 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

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

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

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

$$
R_{1,1} = \frac{h_1}{2} [f(a) + f(b)] = \frac{(b - a)}{2} [f(a) + f(b)]
$$

$$
R_{2,1} = \frac{1}{2} [R_{1,1} + h_1 f(a + h_2)]
$$

$$
R_{3,1} = \frac{1}{2} \left\{ R_{2,1} + h_2 [f(a + h_3) + f(a + 3h_3)] \right\}
$$

$$
R_{k,1} = \frac{1}{2} \left[ R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f(a + (2i - 1)h_k) \right]
$$

- Apply Richardson extrapolation to these values:

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

\[
\left| \int_a^b f(x) \, dx - S \left( a, \frac{a + b}{2} \right) - S \left( \frac{a + b}{2}, b \right) \right| \approx \frac{1}{15} \left| S(a, b) - S \left( a, \frac{a + b}{2} \right) - S \left( \frac{a + b}{2}, b \right) \right|
\]
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
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:

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

$$\int_{-1}^{1} P(x) \, dx = \sum_{i=1}^{n} c_i P(x_i)$$
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)];
Transform integrals $\int_a^b f(x) \, dx$ into integrals over $[-1, 1]$ by a change of variables:

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

Gaussian quadrature then gives

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

\[ \int \int_{R} f(x, y) \, dA, \quad R = \{(x, y) \mid a \leq x \leq b, c \leq y \leq d\} \]

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

\[
\int \int_{R} f(x, y) \, dA = \int_{a}^{b} \left( \int_{c}^{d} f(x, y) \, dy \right) \, dx
\]

and use any quadrature rule in an iterated manner.
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

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

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

- For Gaussian 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.
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:

\[
\int_a^b \frac{P_4(x)}{(x - a)^p} \, dx = \sum_{k=0}^{4} \int_a^b \frac{g^{(k)}(a)}{k!} (x - a)^{k-p} \, dx
\]

\[
= \sum_{k=0}^{4} \frac{g^{(k)}(a)}{k!(k + 1 - p)} (b - a)^{k+1-p}
\]
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.
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

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

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

\[
\int_{a}^{\infty} f(x) \, dx = \int_{0}^{1/a} t^{-2} f\left(\frac{1}{t}\right) \, dt
\]