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 \( h = \frac{3\sqrt{3\varepsilon / M}}{1} \)
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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</thead>
<tbody>
<tr>
<td>1:</td>
<td>$N_1(h) \equiv N(h)$</td>
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<tr>
<td>2:</td>
<td>$N_1(h/2) \equiv N(h/2)$</td>
<td>3:</td>
<td>$N_2(h)$</td>
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<td>4:</td>
<td>$N_1(h/4) \equiv N(h/4)$</td>
<td>5:</td>
<td>$N_2(h/2)$</td>
<td>6:</td>
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<tr>
<td>7:</td>
<td>$N_1(h/8) \equiv N(h/8)$</td>
<td>8:</td>
<td>$N_2(h/4)$</td>
<td>9:</td>
</tr>
</tbody>
</table>
Richardson’s Extrapolation

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

\[ M - N(h) = K_2h^2 + K_4h^4 + \cdots \]

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

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

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

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

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

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

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

- 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
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:**

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

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

Gaussian quadrature then gives

\[
\int_{a}^{b} f(x) \, dx = \int_{-1}^{1} f \left( \frac{(b - a)t + (b + a)}{2} \right) \frac{(b - a)}{2} \, dt
\]
Consider the double integral
\[ \int_{\mathcal{R}} \int f(x, y) \, dA, \quad \mathcal{R} = \{(x, y) \mid a \leq x \leq b, c \leq y \leq d\} \]

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

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 $h = (b - a)/n$, but for $y$ it varies with $x$:

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

$$
\int_a^b \frac{1}{(x - a)^p} \, dx = \frac{(x - a)^{1-p}}{1 - p} \bigg|_a^b = \frac{(b - a)^{1-p}}{1 - p}
$$

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 $a$:

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

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

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

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