Chapter 4
Numerical Differentiation and Integration
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Math 128A Numerical Analysis

General Derivative Approximations

Differentiation of Lagrange Polynomials

Differentiate
\[ f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \cdots + f^{(n+1)}(ξ(x_j)) \]
with \((n+1)\)!
\(\prod_{k\neq j}(x_j - x_k)\)

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

\[
\begin{align*}
   f'(x_0) &= \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(ξ) \\
   f'(x_0) &= \frac{1}{2h}[-f(x_0 - h) + f(x_0 + h)] - \frac{h^2}{6}f^{(3)}(ξ) \\
   f'(x_0) &= \frac{1}{2h}[f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)] + \frac{h^2}{3}f^{(3)}(ξ) \\
   f''(x_0) &= \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12}f^{(4)}(ξ)
\end{align*}
\]

and the five-point formula

\[
\begin{align*}
   f'(x_0) &= \frac{1}{12h^3}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] \\
   &\quad + \frac{h^4}{30}f^{(5)}(ξ)
\end{align*}
\]

Optimal \(h\)

- Consider the three-point central difference formula:

\[
f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6}f^{(3)}(ξ_1)
\]

- Suppose that round-off errors \(\varepsilon\) are introduced when computing \(f\). Then the approximation error is

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

where \(\tilde{f}\) is the computed function and \(|f^{(3)}(x_1)| \leq M\)

- Sum of truncation error \(h^2M/6\) and round-off error \(\varepsilon/h\)

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

Richardson’s Extrapolation

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

\[
M - N(h) = K_1h + K_2h^2 + K_3h^3 + \cdots
\]

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>(N(h))</th>
<th>(O(h^2))</th>
<th>(O(h^4))</th>
<th>(O(h^6))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:</td>
<td>(N_1(h))</td>
<td>(N_2(h))</td>
<td>(N_3(h))</td>
</tr>
<tr>
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<td>(N_2(\frac{h}{2}))</td>
<td>(N_3(\frac{h}{2}))</td>
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<td>(N_2(\frac{h}{4}))</td>
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<tr>
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<td>(N_3(\frac{h}{8}))</td>
</tr>
<tr>
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<td>(N_2(\frac{h}{16}))</td>
<td>(N_3(\frac{h}{16}))</td>
</tr>
<tr>
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<td>(N_2(\frac{h}{32}))</td>
<td>(N_3(\frac{h}{32}))</td>
</tr>
<tr>
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<td>(N_2(\frac{h}{64}))</td>
<td>(N_3(\frac{h}{64}))</td>
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<tr>
<td>8:</td>
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<td>(N_2(\frac{h}{128}))</td>
<td>(N_3(\frac{h}{128}))</td>
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<tr>
<td>9:</td>
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<td>(N_2(\frac{h}{256}))</td>
<td>(N_3(\frac{h}{256}))</td>
</tr>
<tr>
<td>10:</td>
<td>(N_1(\frac{h}{512}))</td>
<td>(N_2(\frac{h}{512}))</td>
<td>(N_3(\frac{h}{512}))</td>
</tr>
</tbody>
</table>
Richardson’s Extrapolation

- If some error terms are zero, different and more efficient formulas can be derived.
- Example: If
  \[ M - N(h) = K_3 h^2 + K_4 h^4 + \cdots \]
  then an \( O(h^2) \) approximation is given for \( j = 2, 3, \ldots \) by
  \[ N_j(h) = N_{j-1}(h/2) + N_{j-1}(h) - N_{j-1}(h) \]
  \[ + 4^{j-1} - 1 \]

Trapezoidal and Simpson’s Rules

- **The Trapezoidal Rule**
  Linear Lagrange polynomial with \( x_0 = a, x_1 = b, h = b - a \), gives
  \[ \int_a^b f(x) \, dx = \frac{h}{2} [f(a) + f(b)] - \frac{h^3}{12} f'''(\xi) \]

- **Simpson’s Rule**
  Second Lagrange polynomial with \( x_0 = a, x_2 = b, x_1 = a + h, h = (b - a)/2 \) gives
  \[ \int_{x_0}^{x_2} f(x) \, dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f''''(\xi) \]

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 \( k = 0, 1, \ldots, n \).

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

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

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

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

- Let $R_{k,1}$ denote the trapezoidal approximation, then
  
  $$R_{1,1} = \frac{h}{2} [f(a) + f(b)] = \frac{(b-a)}{2} [f(a) + f(b)]$$
  
  $$R_{2,1} = \frac{1}{2} [R_{1,1} + f(a + h)]$$
  
  $$R_{3,1} = \frac{1}{2} [R_{2,1} + h_2 f(a + h_3) + f(a + 3h_3)]$$
  
  $$R_{k,1} = \frac{1}{2} \left[ R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k) \right]$$

- Apply Richardson extrapolation to these values:
  
  $$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$$

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

- The assumption $f^{(4)}(\mu) \approx f^{(4)}(\bar{\mu})$ gives the error estimate
  
  $$\left| \int_a^b f(x) \, dx - S \left( a, \frac{a+b}{2} \right) - S \left( \frac{a+b}{2}, b \right) \right| \approx \frac{1}{15} \left| S(a, b) - S \left( a, \frac{a+b}{2} \right) - S \left( \frac{a+b}{2}, b \right) \right|$$

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

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

Legendre Polynomials

- The Legendre polynomials $P_n(x)$ have the properties
  
  - For each $n$, $P_n(x)$ is a monic polynomial of degree $n$ (leading coefficient 1)
  
  - $\int_{-1}^{1} P(x) P_n(x) \, dx = 0$ 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:
    
    $$P_0(x) = 1, \quad P_1(x) = x$$
    
    $$P_2(x) = x^2 - \frac{1}{3} \quad P_3(x) = x^3 - \frac{3}{5} x$$
    
    $$P_4(x) = x^4 - \frac{6}{7} x^2 + \frac{3}{35}$$

MATLAB Implementation

```matlab
function R=romberg(f,a,b,n)
    h=b-a;
    R=zeros(n,n);
    R(1,1)=h/2*(f(a)+f(b));
    h=h/2;
    for i=2:n
        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
```
Theorem
Suppose \( x_1, \ldots, x_n \) are roots of \( P_n(x) \) and
\[
c_i = \int_{-1}^{1} \prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \, dx
\]
If \( P(x) \) is any polynomial of degree less than \( 2n \), then
\[
\int_{-1}^{1} P(x) \, dx = \sum_{i=1}^{n} c_i P(x_i)
\]

MATLAB Implementation
\[
\begin{align*}
\text{function } [x, c] &= \text{gaussquad}(n) \\
\text{P} &= \text{zeros}(n+1, n+1); \\
P([1, 2], 1) &= 1; \quad \text{for } k=1:n-1 \\
P(k+2, 1:k+2) &= ((2k+1) \cdot [P(k+1, 1:k+1) 0] - \ldots \cdot k \cdot [0 0 P(k, 1:k)]) / (k+1); \\
\text{end} \\
x &= \text{sort(roots(P(n+1, 1:n+1))}); \\
A &= \text{zeros}(n, n); \\
\text{for } i=1:n \\
A(i,:,:) &= \text{polyval}(P(i, 1:i), x)'; \\
\text{end} \\
c &= A[:, 2; 0];
\end{align*}
\]

Consider the double integral
\[
\int_{R} f(x, y) \, dA, \quad R = \{(x, y) \mid a \leq x \leq b, c \leq y \leq d\}
\]
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
\[
\int_{R} f(x, y) \, dA = \int_{a}^{b} \left( \int_{c}^{d} f(x, y) \, dy \right) \, dx
\]
and use any quadrature rule in an iterated manner.

The Composite Simpson’s rule gives
\[
\int_{a}^{b} \left( \int_{c}^{d} f(x, y) \, dy \right) \, dx = h k \sum_{i=0}^{n} \sum_{j=0}^{m} w_{i,j} f(x_i, y_j) + E
\]
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
\[
E = - \frac{(d - c)(b - a)}{180} \left[ h^3 \frac{\partial^2 f}{\partial x^2}(\bar{q}, \bar{\mu}) + k^3 \frac{\partial^2 f}{\partial y^2}(\bar{q}, \bar{\mu}) \right]
\]

The same technique can be applied to double integrals of the form
\[
\int_{a}^{b} \int_{e(x)}^{d(x)} f(x, y) \, dy \, dx
\]
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 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
$$\int_a^b \frac{1}{(x-a)^p} \, dx = \frac{(b-a)^{1-p}}{1-p} \bigg|_a^b$$

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
$$\int_b^a f(x) \, dx = \int_a^b g(x) - P_4(x) \, dx + \int_a^b P_4(x) \, dx$$

The second integral can be computed exactly:
$$\int_a^b P_4(x) \, dx = \sum_{k=0}^4 \int_a^b \frac{g^{(k)}(a)}{k!} (x-a)^{k-p} \, dx$$
$$= \sum_{k=0}^4 \frac{g^{(k)}(a)}{k!(k+1-p)} (b-a)^{k+1-p}$$

**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
  $$\int_b^a f(x) \, dx = \int_{-b}^{-a} f(-z) \, dz$$
  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 $\int_0^\infty \frac{1}{x^p} \, dx$, with $p > 1$, can be converted to an integral with left endpoint singularity at $0$ by the substitution $t = x^{-1}$, $dt = -x^{-2} \, dx$, so $dx = -x^2 \, dt = -t^{-2} \, dt$

which gives
$$\int_0^\infty \frac{1}{x^p} \, dx = \int_0^1 \frac{t^p}{t^2} \, dt = \int_0^1 \frac{1}{t^p} \, dt$$

More generally, this variable change converts $\int_0^\infty f(x) \, dx$ into
$$\int_0^\infty f(x) \, dx = \int_0^1 f\left(\frac{1}{t}\right) \, dt$$