Numerical Differentiation and Integration

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Numerical Differentiation and Integration

- Many engineering applications require numerical estimates of derivatives of functions
- Especially true, when analytical solutions are not possible
- **Differentiation**: Use finite differences
- **Integration (definite integrals)**: Weighted sum of function values at specified points (area under the curve).
Application: Integral of a Normal Distribution

- Represented as a Gaussian, a scaled form of \( f(x) = e^{-x^2} \), very important function in statistics.
- Not easy to determine indefinite integral - use numerical techniques.

\[
A = \int_{a}^{b} e^{-x^2} dx
\]
Application: Integral of a Sinc

$$f(x) = \frac{\sin(x)}{x}$$
Numerical Differentiation: Approach

⇒ Evaluate the function at two consecutive points, separated by \( \Delta x \), of the independent variable, and taking their difference:

\[
\frac{df(x)}{dx} \approx \frac{f(x + \Delta x) - f(x)}{\Delta x}
\]

⇒ Fit a function to a set of points that define the relationship between the independent and dependent variables, such as an nth order polynomial; then differentiate the polynomial
Finite Differences

Forward Difference

\[
\frac{df(x)}{dx} = \frac{f(x + \Delta x) - f(x)}{\Delta x}
\]

Backward Difference

\[
\frac{df(x)}{dx} = \frac{f(x) - f(x - \Delta x)}{\Delta x}
\]

Two Step Method, Central Difference

\[
\frac{df(x)}{dx} = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta x}
\]
Finite Differences: Example

Example 11.1 Forward, Backward, and Central Differences

To illustrate the three kinds of difference formula, consider the data points $(x_0, y_0) = (1, 2), (x_1, y_1) = (2, 4), (x_2, y_2) = (3, 8), (x_3, y_3) = (4, 16),$ and $(x_4, y_4) = (5, 32).$ Using the forward difference formula, we estimate $f'(x_2) = f'(3),$ with $h = x_3 - x_2 = 1,$ as

$$f'(x_2) \approx \frac{f(x_3) - f(x_2)}{x_3 - x_2} = \frac{y_3 - y_2}{1} = 16 - 8 = 8.$$  

Using the backward difference formula, we find that

$$f'(x_2) \approx \frac{f(x_2) - f(x_1)}{x_2 - x_1} = \frac{y_2 - y_1}{1} = 8 - 4 = 4.$$  

With the central difference formula, the estimate for $f''(x_2),$ with $h = 1,$ is

$$f'(x_2) \approx \frac{f(x_3) - f(x_1)}{x_3 - x_1} = \frac{y_3 - y_1}{2} = \frac{16 - 4}{2} = 6.$$
Forward Differences: Derivation

Finite difference formulas can be derived from the Taylor series.

\[ f(x + h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\eta), \]

For \( h = x_{i+1} - x_i \),

\[ f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{h}{2} f''(\eta), \]

where \( x_i < \eta < x_{i+1} \).
Backward Differences: Derivation

\[ f(x + h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\eta), \]

For \( h = x_{i-1} - x_i \),

\[ f(x_i + h) = f(x_i + x_{i-1} - x_i) = f(x_{i-1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2}f''(\eta) \]

\[ f'(x_i) = \frac{f(x_{i-1}) - f(x_i)}{h} - \frac{h}{2}f''(\eta) \]

where \( x_{i-1} < \eta < x_i \).
Central Differences: Derivation

Use the next higher order Taylor polynomial,

\[ f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2} f''(x_i) + \frac{h^3}{6} f'''(\eta_1), \]

\[ f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2} f''(x_i) - \frac{h^3}{6} f'''(\eta_2) \]

with \( x < \eta_1 < x + h, x - h < \eta_2 < x \)

Thus,

\[ f(x_{i+1}) - f(x_{i-1}) = 2hf'(x_i) + \frac{h^3}{6} [f'''(\eta_1) + f'''(\eta_2)] \]

or,

\[ f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{h^2}{6} f'''(\eta), \quad x_{i-1} < \eta < x_{i+1} + 1 \]
Second Derivatives

\[ f(x + h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x)(\eta_1) \]
\[ f(x - h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x)(\eta_2) \]

Thus

\[ f(x + h) + f(x - h) = 2f(x) + h^2f''(x) + \frac{h^4}{4!}[f^{(4)}(x)(\eta_1) + f^{(4)}(x)(\eta_2)] \]
\[ f''(x) \approx \frac{1}{h^2}[f(x + h) - 2f(x) + f(x - h)] \]

with truncation error of the \( O(h^4) \)
Partial Derivatives

- Generally, interested in partial derivatives of functions of 2 variables, \((x_i, y_j)\), based on a mesh of points.
- Subscripts denote partial derivatives.

\[
\begin{align*}
    u_x(x_i, y_j) &\approx \frac{1}{2h} \left[ -u_{i-1,j} + u_{i+1,j} \right] \quad u_x \approx \frac{1}{2h} \begin{array}{ccc} 1 & 0 & 1 \\ i-1 & i & i+1 \end{array} \\
    u_{xx}(x_i, y_j) &\approx \frac{1}{h^2} \left[ u_{i-1,j} - 2u_{ij} + u_{i+1,j} \right] \quad u_{xx} \approx \frac{1}{h^2} \begin{array}{ccc} 1 & -2 & 1 \\ i-1 & i & i+1 \end{array}
\end{align*}
\]
Partial Derivatives (contd)

- Laplacian operator: \( \Delta^2 u = u_{xx} + u_{yy} \)
- Biharmonic Operator: \( \Delta^4 u = u_{xxxx} + u_{xxyy} + u_{yyyy} \)
Using Interpolating Polynomials

- Given a function in discrete form, the data can be interpolated to fit an nth order polynomial.
- For those functions that are in analytical form, but difficult to differentiate, the function can be discretized and fitted by a polynomial.

\[ f(x) = b_n x^n + b_{n-1} x^{n-1} + \cdots + b_1 x + b_0 \]

whose derivative is

\[ \frac{df(x)}{dx} = nb_n x^{n-1} + (n - 1)b_{n-2} x^{n-2} + \cdots + b_1 \]
Power Series Type Interpolating Polynomial

Consider the \( n \)th order polynomial passing through \((n+1)\) points; the \((n+1)\) coefficients can be uniquely determined.

**Example**

\[
f(x) = a_0 + a_1 x + a_2 x^2
\]

Consider \( f(x_i), f(x_i + h), f(x_i + 2h) \)

\[
f(x_i) = a_0 + a_1 x_i + a_2 x_i^2
\]
\[
f(x_i + h) = a_0 + a_1 (x_i + h) + a_2 (x_i + h)^2
\]
\[
f(x_i + 2h) = a_0 + a_1 (x_i + 2h) + a_2 (x_i + 2h)^2
\]
Example (contd)

For the 3 points, \( x_i = 0, h, 2h, \)

\[
\begin{align*}
  f_i &= a_0 \\
  f_{i+1} &= a_0 + a_1 h + a_2 h^2 \\
  f_{i+2} &= a_0 + 2a_1 h + 4a_2 h^2
\end{align*}
\]

which has the solution,

\[
\begin{align*}
  a_0 &= f_i \\
  a_1 &= \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} \\
  a_2 &= \frac{f_{i+2} - 2f_{i+1} + f_i}{2h^2}
\end{align*}
\]
**Example (contd)**

\[ f(x) = a_0 + a_1 x + a_2 x^2 \]

\[ f'(x_i) = f'_i = f'(x_i = 0) \]
\[ = a_1 + 2a_2 x_i \]
\[ = a_1 \]
\[ = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} \]

Similarly, second derivatives can also be obtained.
Numerical Integration

Integration can be thought of as considering some continuous function $f(x)$ and the area $A$ subtended by it; for instance, within a particular interval

$$A = \int_a^b f(x)\,dx$$

Numerical Integration is needed when $f(x)$ does not have a known analytical solution, or, if $f(x)$ is only defined at discrete points.

There are two approaches to a numerical solution:

⇒ Fitting polynomials to $f(x)$ and integrating using analytical calculus,

⇒ Area under $f(x)$ can be approximated using geometric shapes defined by adjacent points.
Interpolation Approach

We can derive an $n$th order polynomial (for instance, Gregory-Newton method), which has the general form as

$$f(x) = b_1 x^n + b_2 x^{n-1} + \cdots + b_n x + b_{n+1}$$

After the $b_i$s are determined, this can be integrated as

$$\int f(x) \, dx = \frac{b_1 x^{n+1}}{n+1} + \frac{b_2 x^n}{n} + \cdots + \frac{b_n x^2}{2} + b_{n+1} x$$

which can be solved for, within the limits of the integration.
Basic Numerical Integration (Newton-Cotes Closed Formulas)

- **Trapezoid Rule**: Approximates function by a straightline to compute area under curve.

\[ \int_{a}^{b} f(x) \, dx \approx \frac{h}{2} \left[ f(x_0) + f(x_1) \right] \]

- Solution is exact, for polynomials of degree \( \leq 1 \), i.e. linear functions.

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**Example 11.5** Integral of \( e^{-x^2} \) Using the Basic Trapezoid Rule

Consider now a very important function for which the exact value of the integral is not known:

\[ f(x) = \exp(-x^2), \quad x_0 = a = 0, \quad x_1 = b = 2. \]

Using the trapezoid rule, we find (since \( (b-a)/2 = 1 \) for this example) that

\[ \int_{0}^{2} \exp(-x^2) \, dx \approx [\exp(-0^2) + \exp(-2^2)] = 1 + \exp(-4) = 1.0183. \]

The function and the straight-line approximation are shown in Fig. 11.4.
Basic Numerical Integration (Newton-Cotes Closed Formulas)

- **Simpson’s Rule**: Instead of a linear approximation, use a quadratic polynomial:

\[ h = \frac{b - a}{2}, \quad x_0 = a, \quad x_1 = x_0 + h = \frac{b + a}{2}, \quad x_2 = b \]

Approximate integral is given by

\[ \int_a^b f(x)\,dx \approx \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] \]
Basic Simpson’s Rule: Example 1

Example 11.6 Approximating $\pi/4$ Using the Basic Simpson’s Rule

Since the exact value of the integral $\int_0^1 \frac{1}{1 + x^2} \, dx$ is $\arctan(1) = \pi/4 \approx 0.7853 \ldots$, we can approximate $\pi/4$ by approximating the integral numerically. Using Simpson’s rule with $f(x) = \frac{1}{1 + x^2}$, $a = 0$, and $b = 1$ gives $h = 1/2$, and

$$\int_0^1 \frac{1}{1 + x^2} \, dx \approx \frac{1}{6} \left[ f(0) + 4f(1/2) + f(1) \right] = \frac{1}{6} \left[ 1 + (4) \frac{4}{5} + \frac{1}{2} \right] = \frac{47}{60} \approx 0.78333.$$

The graph of $f(x) = \frac{1}{1 + x^2}$ and the quadratic polynomial that passes through the points (0,1), (1/2, 4/5), and (1,1/2) are shown in Fig. 11.5. It is not surprising that the approximate value of the integral from Simpson’s rule is quite good, because the two functions are very similar.

![Graph of $f(x) = \frac{1}{1 + x^2}$ and the quadratic polynomial that passes through the points (0,1), (1/2, 4/5), and (1,1/2).]
Basic Simpson’s Rule: Example 2

Example 11.7 Integral of $e^{-x^2}$ Using the Basic Simpson’s Rule

Consider again the integral of the function $f(x) = \exp(-x^2)$, on $[0, 2]$.
The required values for applying Simpson’s rule are

$$h = \frac{b - a}{2} = 1, \quad x_0 = a = 0, \quad x_1 = (2 + 0)/2 = 1, \quad x_2 = b = 2,$$

which gives

$$\int_0^2 \exp(-x^2) \, dx \approx \frac{1}{3} [\exp(-0^2) + 4 \exp(-1^2) + \exp(-2^2)] = .8299.$$

The graphs of $f(x) = \exp(-x^2)$ and the quadratic polynomial passing through the points $(0, 1), (1, \exp(-1))$, and $(2, \exp(-4))$ are shown in Fig. 11.6.
Improved Numerical Integration

- Improve the accuracy by applying lower order methods repeatedly on several subintervals.
- Known as composite integration
- Simpson, Trapezoid rules use equal subintervals; using unequal (adaptive) intervals leads to Gaussian Quadrature methods.
Composite Trapezoid Rule

- Approximates the area under the function $f(x)$ by a set of discrete trapezoids fitted between each pair of points of the dependent variable (and the X axis)

$$\int_{x_1}^{x_n} f(x) \, dx \approx \sum_{i=1}^{n-1} (x_{i+1} - x_i) \frac{f(x_{i+1}) + f(x_i)}{2}$$

If the intervals are the same, $h = (b - a)/n$, we get

$$\int_{x_1}^{x_n} f(x) \, dx \approx \frac{b - a}{2n} [f(a) + 2f(x_1) + \ldots + f(b)]$$
Example 11.9 Integral of $1/x$ Using the Trapezoid Rule

Consider the problem of finding

$$\int_1^2 \frac{dx}{x} = \frac{h}{2} [f(a) + 2f(x_1) + \ldots + 2f(x_{n-1}) + f(b)].$$

For $n = 2$ subintervals, $h = (2 - 1)/2 = 0.5$, and the composite trapezoid rule gives

$$I_1 = \frac{1}{4} [f(1) + 2f(1.5) + f(2)] = \frac{1}{4} \left[ \frac{1}{1} + \frac{2}{1.5} + \frac{1}{2} \right] = \frac{17}{24} = 0.7083.$$

The function and the two straight-line approximations are shown in Fig. 11.8.

For $n = 2^2 = 4$ subintervals, $h = 1/4$, and the composite trapezoid rule gives

$$I_2 = \frac{1}{8} [f(1) + 2f(5/4) + 2f(3/2) + 2f(7/4) + f(2)] = \frac{1}{8} \left[ 1 + \frac{8}{5} + \frac{4}{3} + \frac{8}{7} + \frac{1}{2} \right]$$

$$= 0.6970 \ldots .$$

For $n = 2^3 = 8$ subintervals, $h = 1/8$, and the composite trapezoid rule yields

$$I_3 = \frac{1}{16} [f(1) + 2f(9/8) + 2f(5/4) + 2f(11/8) + 2f(13/8) + 2f(15/8) + 2f(7/4) + f(2)]$$

$$= 0.6941 \ldots .$$

The exact value of the integral is $\ln(2) = 0.693147 \ldots$. 

**FIGURE 11.8** $y = 1/x$ and trapezoid rule approximations on $[1, 1.5]$ and $[1.5, 2]$. 

**ITCS 4133/5133: Numerical Comp. Methods**

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Numerical Differentiation and Integration
Composite Trapezoid Rule: Algorithm

Input
- f(x) function to be integrated
- a lower limit of integral
- b upper limit of integral
- n number of subintervals

Begin computations
h = (b - a)/n
S = 0
For i = 1 to n - 1
    x_i = a + hi
    S = S + f(x_i)
End
I = (h/2) * (f(a) + f(b) + 2S)
Return I
Composite Trapezoid Rule: Notes

⇒ \( \frac{f(x_{i+1}) + f(x_i)}{2} \) represents the average height of the trapezoid.

⇒ Linear approximation between pairs of successive points used; error is proportional to the distance between sample points.

**Error**

⇒ Error in the trapezoidal can be approximated by Taylor’s series

\[
\frac{x_{i+1} - x_i}{2} f''(x)
\]

where \( f''(x) \) is evaluated at the value of \( x \) that maximizes the second derivative between the two sample points.
Composite Simpson’s Rule

- Uses the same idea as the composite Trapezoid rule, by using multiple sub-intervals to improve the Simpson rule approximation.
- For 2 subintervals, Simpson’s rule has the following form:

\[
\int_a^b f(x)\,dx = \int_a^{x_2} f(x)\,dx + \int_{x_2}^b f(x)\,dx
\]

\[
\approx \frac{h}{3} [f(a) + 4f(x_1) + f(x_2)] + \frac{h}{3} [f(x_2) + 4f(x_3) + f(b)]
\]

\[
\approx \frac{h}{3} [f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(b)]
\]
Composite Simpson’s Rule (contd)

■ For \( n \) (\( n \) must be even) subintervals, \( h = (b - a)/n \) we get

\[
\int_a^b f(x) \, dx = \frac{h}{3} [f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \ldots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(b)]
\]

■ \( n \) must be even number of subintervals.

■ **Error Bound:** Based on the 4th derivative:

\[
Error = \frac{(x_{i+1} - x_i)^5}{90} f^{(4)}(x_i)
\]

where \( f^{(4)}(x_i) \) is evaluated at the value of \( x \) that maximizes the 4th derivative between the two sample points.
Composite Simpson’s Rule: Example

Example 11.10 Integral of $e^{-x^2}$ Using Simpson’s Rule

For $n = 4$ and $f(x) = e^{-x^2}$, the integral of $f$ is approximately 0.84232. The function and the two quadratic approximations are shown in Fig. 11.9.

FIGURE 11.9 $y = e^{-x^2}$ and Simpson’s rule approximations for $n = 4$. 
Composite Simpson’s Rule: Algorithm

```
Input
  f(x)         function to be integrated
  a            lower limit of integral
  b            upper limit of integral
  n            number of subintervals (must be even)

Begin computations
h = (b - a) / n
m = n / 2
S1 = 0
S2 = 0
For k = 0 to m - 1
  x(2k+1) = a + h(2k+1)
  S1 = S1 + f(x(2k+1))
End
For k = 1 to m - 1
  x(2k) = a + h(2k)
  S2 = S2 + f(x(2k))
End
I = (h/3) ( f(a) + f(b) + 2 S1 + 4 S2)
Return
  I
```
Romberg Integration

- Simpson’s rule improves on Trapezoid rule with additional evaluations of $f(x)$, required to fit a more accurate polynomial.
- More evaluations will further improve the integral, leading to the Romberg Integration.

\[
I_{01} = \frac{b - a}{2} (f(a) + f(b))
\]

A second estimate can be obtained with subdividing the interval $ab$ into 2 equal intervals is given by

\[
I_{11} = \frac{b - a}{2} \left( \frac{1}{2} f(a) + f(m) + \frac{1}{2} f(b) \right)
\]

\[
= \frac{1}{2} \left[ I_{01} + (b - a) f \left( a + \frac{b - a}{2} \right) \right]
\]
Romberg Integration (contd.)

A third estimate, $I_{21}$, using 3 intermediate points $m_1, m_2, m_3$ is given by

$$I_{21} = \frac{b-a}{2} \left[ \frac{1}{4} f(a) + \frac{1}{2} f(m_1) + \frac{1}{2} f(m_2) + \frac{1}{2} f(m_3) + \frac{1}{4} f(b) \right]$$

$$= \frac{1}{2} \left[ I_{11} + \frac{b-a}{2} \sum_{k=1, k\neq 2}^{3} f \left( a + \frac{b-a}{4} k \right) \right]$$

This leads to the recursive relationship

$$I_{i1} = \frac{1}{2} \left[ I_{i-1,1} + \frac{b-a}{2^{i-1}} \sum_{k=1, k\neq 2}^{2^i-1} f \left( a + \frac{b-a}{2^i} k \right) \right], \text{ for } i = 1, 2, \ldots$$
Romberg Integration (contd.)

\[ I_{i1} = \frac{1}{2} \left[ I_{i-1,1} + \frac{b - a}{2^{i-1}} \sum_{k=1,3,5}^{2^{i-1}} f \left( a + \frac{b - a}{2^i} k \right) \right] \], for \( i = 1, 2, \ldots \)

We can combine these estimates using Richardson’s formula,

\[ I_{ij} = \frac{4^{j-1} I_{i+1,j-1} - I_{i,j-1}}{4^{j-1} - 1} \]

for \( i = 0, 1, \ldots, N - j + 1, j = 1, 2, \ldots N \). The estimates form an upper triangular matrix:

\[
\begin{bmatrix}
I_{01} & I_{02} & I_{03} & I_{04} & \cdots & I_{0,N-1} & I_{0,N} & I_{0,N+1} \\
I_{11} & I_{12} & I_{13} & \cdots & I_{1,N-1} & I_{1,N} \\
I_{21} & I_{22} & \cdots & \cdots & I_{2,N-1} \\
I_{31} & \cdots & \cdots & \cdots & \cdots \\
\vdots & \cdots & \cdots & \cdots & \cdots & I_{N-2,3} \\
\vdots & \cdots & \cdots & \cdots & \cdots & \cdots & I_{N-1,2} \\
I_{N1} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}
\]
Romberg Integration (contd.)

Algorithm (To solve for $I_{0,N}$)

- Determine $I_{01}$ (Trapezoid formula)
- Determine $I_{i1}$, for $i = 1, 2, \ldots$
- Determine $I_{i2}, I_{i3}$, etc., using Richardson’s formula.