Computational Methods
CMSC/AMSC/MAPL 460

Quadrature: Integration

Ramani Duraiswami,
Dept. of Computer Science

Some material adapted from the online slides of Eric Sandt and Dianne O’Leary
Numerical Integration

Idea is to do integral in small parts, like the way you first learned integration - a summation

Numerical methods just try to make it faster and more accurate
Basic Numerical Integration

- Weighted sum of function values

\[ \int_{a}^{b} f(x) \, dx \approx \sum_{i=0}^{n} c_i f(x_i) \]

\[ f(x) = c_0 f(x_0) + c_1 f(x_1) + \cdots + c_n f(x_n) \]
Numerical Integration

• Characterized by where the function is evaluated

• Newton-Cotes Closed Formulae -- Use both end points
  – Trapezoidal Rule : Linear
  – Simpson’s 1/3-Rule : Quadratic
  – Simpson’s 3/8-Rule : Cubic
  – Boole’s Rule : Fourth-order

• Newton-Cotes Open Formulae -- Use only interior points
  – midpoint rule
Trapezoid Rule

- **Straight-line approximation**

\[
\int_{a}^{b} f(x) \, dx \approx \sum_{i=0}^{I} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1)
\]

\[
= \frac{h}{2} [f(x_0) + f(x_1)]
\]
Example: Trapezoid Rule

Evaluate the integral \( \int_{0}^{4} xe^{2x} \, dx \)

- **Exact solution (integration by parts)**
  \[
  \int_{0}^{4} xe^{2x} \, dx = \left[ \frac{x}{2} e^{2x} - \frac{1}{4} e^{2x} \right]_{0}^{4} = \frac{1}{4} e^{2x} (2x - 1) \bigg|_{0}^{4} = 5216.926477
  \]

- **Trapezoidal Rule**
  \[
  I = \int_{0}^{4} xe^{2x} \, dx \approx \frac{4 - 0}{2} \left[ f(0) + f(4) \right] = 2(0 + 4e^{8}) = 23847.66
  \]
  \[
  \varepsilon = \frac{5216.926 - 23847.66}{5216.926} = -357.12\%
  \]
Simpson’s 1/3-Rule

Approximate the function by a parabola

\[ \int_{a}^{b} f(x) \, dx \approx \sum_{i=0}^{2} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2) \]

\[ = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] \]
**Simpson’s 3/8-Rule**

Approximate by a cubic polynomial

\[
\int_a^b f(x)\,dx \approx \sum_{i=0}^{3} c_i f(x_i) = c_0 f(x_0) + c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)
\]

\[
= \frac{3h}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]
\]
**Example: Simpson’s Rules**

Evaluate the integral \( \int_0^4 x e^{2x} \, dx \)

- **Simpson’s 1/3-Rule**

  \[
  I = \int_0^4 x e^{2x} \, dx \approx \frac{h}{3} \left[ f(0) + 4f(2) + f(4) \right] \\
  = \frac{2}{3} \left[ 0 + 4(2e^4) + 4e^8 \right] = 8240.411 \\
  \varepsilon = \frac{5216.926 - 8240.411}{5216.926} = -57.96\%
  \]

- **Simpson’s 3/8-Rule**

  \[
  I = \int_0^4 x e^{2x} \, dx \approx \frac{3h}{8} \left[ f(0) + 3f\left(\frac{4}{3}\right) + 3f\left(\frac{8}{3}\right) + f(4) \right] \\
  = \frac{3(4/3)}{8} \left[ 0 + 3(19.18922) + 3(552.33933) + 11923.832 \right] = 6819.209 \\
  \varepsilon = \frac{5216.926 - 6819.209}{5216.926} = -30.71\%
  \]
Midpoint Rule

Newton-Cotes Open Formula

\[ \int_{a}^{b} f(x) \, dx \approx (b - a) f(x_m) \]

\[ = (b - a) f\left(\frac{a + b}{2}\right) + \frac{(b - a)^3}{24} f^{''}(\eta) \]

\[ x \]

\[ a \]

\[ x_m \]

\[ b \]
Two-point Newton-Cotes Open Formula

Approximate by a straight line

\[ \int_a^b f(x)dx \approx \frac{b-a}{2} [f(x_1) + f(x_2)] + \frac{(b-a)^3}{108} f''(\eta) \]
Three-point Newton-Cotes Open Formula

Approximate by a parabola

\[
\int_a^b f(x) \, dx \approx \frac{b-a}{3} \left[ 2f(x_1) - f(x_2) + 2f(x_3) \right] + \frac{7(b-a)^5}{23040} f^{(m')}(\eta)
\]
Better Numerical Integration

• Composite integration
  – Composite Trapezoidal Rule
  – Composite Simpson’s Rule
• Richardson Extrapolation (next class)
• Romberg integration (next class)
Structure of quadrature programs

• Cost
  – Typically require several calls to function routine that is being integrated
  – So cost is in terms of function calls

• Accuracy
  – As a number
  – As the highest order polynomial that is integrated exactly
Error analysis

• All formulas thus far have form

\[ Q(f) = \sum_{i=1}^{m} c_i f(x_i) \]

• Define residue (or error function) as

\[ R(f) = I(f) - Q(f) \]

• We cannot calculate \( I(f) \) in general (as doing so would require us to know the right answer).
  – Instead we compute our error on a class of functions that form a basis in a function space … the polynomials
Error

- Trapezoidal rule is exact for constant and linear functions
- What about others?
- Let $T(f)$ denote trapezoidal rule result.
- Then for some $\xi \in [a,b]
  \[ I(f) - T(f) = -\frac{(b-a)^3}{12} f''(\xi) \]

- Similarly Simpson rule is exact for quadratics and has error proportional to third derivative
- We need 2 function evaluations for a 2\textsuperscript{nd} order error
  – 3 for a 3\textsuperscript{rd} order and so on …
Error analysis

- The formulas all have the form

\[ Q(f) = \sum_{i=1}^{m} \alpha_i f(t_i) \]

- The error function

\[ R(f) = I(f) - Q(f) \]

is a **linear operator**; i.e., for every two functions \( f \) and \( g \), and for every two scalars \( \beta \) and \( \gamma \),

\[ R(\beta f + \gamma g) = \beta R(f) + \gamma R(g) . \]

(We restrict \( f \) and \( g \) to lie in some function space; for example, we need a certain number of continuous derivatives in order for the polynomial error formula to apply.)
Formula for trapezoidal rule

If \( f(t) \) and its 1\(^{st} \) two derivatives are continuous on \([a, b]\), then

\[
\int_a^b f(t) dt - T = -\frac{(b-a)^3}{12} f''(\eta)
\]

where \( \eta \in [a, b] \).

**Proof:** The trapezoidal rule is computed by integrating the linear interpolant to \( f(t) \) at \( a \) and \( b \).

From our work on polynomial interpolation, we know that, for the linear interpolant,

\[
f(t) - p(t) = f[a, b, t](t - a)(t - b),
\]

so

\[
\int_a^b f(t) dt - T = \int_a^b f[a, b, t](t - a)(t - b) dt
\]
Recall the **Integral Mean Value Theorem**: If $w(t)$ doesn't change sign on $[a, b]$ then

$$
\int_{a}^{b} w(t)f(t) = f(\xi) \int_{a}^{b} w(t)dt
$$

for some point $\xi \in [a, b]$.

Therefore,

$$
\int_{a}^{b} f(t)dt - T = f[a, b, \xi] \int_{a}^{b} (t - a)(t - b)dt
= f[a, b, \xi](-\frac{1}{6}(b - a)^3)
$$

The result follows from the fact that

$$
f[a, b, \xi] = \frac{1}{2} f''(\eta) .
$$
How to reduce error?

- If \((b-a)\) is large error is higher
  - Use composite rules.

**Example:** Composite Trapezoidal Rule. Let’s divide \([a, b]\) into \(n\) pieces of equal length \(h = (b - a)/n\).

\[
\int_{a}^{b} f(t)dt \\
\approx \frac{h}{2}(f(a)+f(a+h)) + \frac{h}{2}(f(a+h)+f(a+2h))+\ldots+\frac{h}{2}(f(a+(n-1)h)+f(a+nh)) \\
= h\left[\frac{1}{2}f(a) + f(a + h) + f(a + 2h) + \ldots + f(a + (n - 1)h) + \frac{1}{2}f(b)\right] \\
\equiv T_n.
\]
Apply trapezoid rule to multiple segments over integration limits

Two segments

Three segments

Four segments

Many segments
Composite Trapezoid Rule

\[
\int_a^b f(x)\,dx = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx
\]

\[
= \frac{h}{2} \left[ f(x_0) + f(x_1) \right] + \frac{h}{2} \left[ f(x_1) + f(x_2) \right] + \cdots + \frac{h}{2} \left[ f(x_{n-1}) + f(x_n) \right]
\]

\[
= \frac{h}{2} \left[ f(x_0) + 2 f(x_1) + \cdots + 2 f(x_i) + \cdots + 2 f(x_{n-1}) + f(x_n) \right]
\]

\[
h = \frac{b-a}{n}
\]
Composite Trapezoid Rule

Evaluate the integral

\[ I = \int_0^4 xe^{2x} \, dx \]

\[ n = 1, h = 4 \Rightarrow I = \frac{h}{2} \left[ f(0) + f(4) \right] = 23847.66 \quad \varepsilon = -357.12\% \]

\[ n = 2, h = 2 \Rightarrow I = \frac{h}{2} \left[ f(0) + 2 f(2) + f(4) \right] = 12142.23 \quad \varepsilon = -132.75\% \]

\[ n = 4, h = 1 \Rightarrow I = \frac{h}{2} \left[ f(0) + 2 f(1) + 2 f(2) + 2 f(3) + f(4) \right] = 7288.79 \quad \varepsilon = -39.71\% \]

\[ n = 8, h = 0.5 \Rightarrow I = \frac{h}{2} \left[ f(0) + 2 f(0.5) + 2 f(1) + 2 f(1.5) + 2 f(2) + 2 f(2.5) + 2 f(3) + 2 f(3.5) + f(4) \right] = 5764.76 \quad \varepsilon = -10.50\% \]

\[ n = 16, h = 0.25 \Rightarrow I = \frac{h}{2} \left[ f(0) + 2 f(0.25) + 2 f(0.5) + \cdots + 2 f(3.5) + 2 f(3.75) + f(4) \right] = 5355.95 \quad \varepsilon = -2.66\% \]
**Composite Trapezoid Rule with Unequal Segments**

Evaluate the integral

\[ I = \int_{0}^{4} xe^{2x} \, dx \]

- \( h_1 = 2, \ h_2 = 1, \ h_3 = 0.5, \ h_4 = 0.5 \)

\[
I = \int_{0}^{2} f(x) \, dx + \int_{2}^{3} f(x) \, dx + \int_{3}^{3.5} f(x) \, dx + \int_{3.5}^{4} f(x) \, dx \\
= \frac{h_1}{2} [f(0) + f(2)] + \frac{h_2}{2} [f(2) + f(3)] \\
+ \frac{h_3}{2} [f(3) + f(3.5)] + \frac{h_4}{2} [f(3.5) + f(4)] \\
= \frac{2}{2} [0 + 2e^4] + \frac{1}{2} [2e^4 + 3e^6] + \frac{0.5}{2} [3e^6 + 3.5e^7] \\
+ \frac{0.5}{2} [3.5e^7 + 4e^8] = 5971.58 \quad \Rightarrow \varepsilon = -14.45\% 
\]
**Composite Simpson’s Rule**

Piecewise Quadratic approximations

\[ h = \frac{b - a}{n} \]
Composite Simpson’s Rule

Multiple applications of Simpson’s rule

\[ \int_{a}^{b} f(x) \, dx = \int_{x_0}^{x_2} f(x) \, dx + \int_{x_2}^{x_4} f(x) \, dx + \cdots + \int_{x_{n-2}}^{x_n} f(x) \, dx \]

\[ = \frac{h}{3} \left[ f(x_0) + 4f(x_1) + f(x_2) \right] + \frac{h}{3} \left[ f(x_2) + 4f(x_3) + f(x_4) \right] \]

\[ + \cdots + \frac{h}{3} \left[ f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \right] \]

\[ = \frac{h}{3} \left[ f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots \right. \]

\[ + 4f(x_{2i-1}) + 2f(x_{2i}) + 4f(x_{2i+1}) + \cdots \]

\[ + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \]
Composite Simpson’s Rule

Evaluate the integral

\[ I = \int_{0}^{4} x e^{2x} \, dx \]

- \( n = 2, \ h = 2 \)

\[
I = \frac{h}{3} [f(0) + 4f(2) + f(4)] \\
= \frac{2}{3} [0 + 4(2e^4) + 4e^8] = 8240.411 \quad \Rightarrow \varepsilon = -57.96\%
\]

- \( n = 4, \ h = 1 \)

\[
I = \frac{h}{3} [f(0) + 4f(1) + 2f(2) + 4f(3) + f(4)] \\
= \frac{1}{3} [0 + 4(e^2) + 2(2e^4) + 4(3e^6) + 4e^8] \\
= 5670.975 \quad \Rightarrow \varepsilon = -8.70\%
\]
**Composite Simpson’s Rule with Unequal Segments**

Evaluate the integral

$I = \int_0^4 x e^{2x} \, dx$

- $h_1 = 1.5$, $h_2 = 0.5$

$I = \int_0^3 f(x) \, dx + \int_3^4 f(x) \, dx$

$\quad = \frac{h_1}{3} \left[ f(0) + 4f(1.5) + 2f(3) \right]$

$\quad + \frac{h_2}{3} \left[ f(3) + 4f(3.5) + 2f(4) \right]$

$\quad = \frac{1.5}{3} \left[ 0 + 4(1.5e^3) + 3e^6 \right] + \frac{0.5}{3} \left[ 3e^6 + 4(3.5e^7) + 4e^8 \right]$

$\quad = 5413.23 \quad \Rightarrow \varepsilon = -3.76\%$
Error of composite trapezoid

The **Error formula** for the Composite Trapezoidal Rule is

\[ \int_{a}^{b} f(t)dt - T_n = - \sum_{i=1}^{n} \frac{h^3}{12} f''(\eta_i) \]

where \( \eta_i \in [a + (i - 1)h, a + ih] \). Since \( nh = b - a \), and

\[ \frac{1}{n} \sum_{i=1}^{n} f''(\eta_i) \]

is an average value of \( f'' \) on \([a, b]\), we obtain

\[ \int_{a}^{b} f(t)dt - T_n = - \frac{(b-a)h^2}{12} f''(\eta) \]

for some \( \eta \in [a, b] \).

- Error decreases by a factor of \((b-a)^2\)
Adaptive integration

- Other factor in the error is the second derivative
- Idea, keeping the error fixed, reduce the size of the interval where second derivative is high
- If we used the worst part of the domain to determine step size we would waste resources on the easy parts
- Idea of adaptive use different $h$ for different parts
Adaptive integration

- In general we do not have a graph to tell us where things are bad.
- Need a function which estimates the error locally.
- Idea: use two formulae: one more accurate, and one less accurate in each interval and estimate the error.
- Difference gives an estimate of the error locally.
- Where error is larger we need to do something.

Idea: use an initial mesh (black points), and then a mesh with more points (red and black points).

This gives us two estimates of the integral, $Q$ and $\tilde{Q}$. 
• If local error estimate is less than tolerance in a particular region we can stop dividing it.
• Otherwise split the interval in two pieces, and repeat the procedure
• Each sub-interval tolerance requirement needs to be half that of the parents
• Upon convergence each subinterval achieves success.
  – Some subintervals needed lots of points, others few
• Add up all sub interval answers and report to calling program
Adaptive methods

- Allow us to achieve a given tolerance at a given cost
Richardson Extrapolation

- Wikipedia
  http://en.wikipedia.org/wiki/Richardson_extrapolation
Richardson Extrapolation

For trapezoidal rule

\[ A = \int_{a}^{b} f(x)dx = A(h) + c_1 h^2 + \cdots \]

\[
\begin{align*}
    A &= A(h) + c_1 h^2 + c_2 h^4 \cdots \\
    A &= A(\frac{h}{2}) + c_1 (\frac{h}{2})^2 + c_2 (\frac{h}{2})^4 + \cdots \\
\end{align*}
\]

\[ \Rightarrow A = \frac{1}{3} \left[ 4A(\frac{h}{2}) - A(h) \right] - \frac{c_2}{4} h^4 + \cdots = B(h) + b_2 h^4 + \cdots \]

\[ k^{th} \text{ level of extrapolation} \]

\[
\begin{align*}
    A &= B(h) + b_2 h^4 \cdots \\
    A &= B(\frac{h}{2}) + b_2 (\frac{h}{2})^4 + \cdots \\
\end{align*}
\]

\[ \Rightarrow C(h) = \frac{1}{15} \left[ 16B(\frac{h}{2}) - B(h) \right] \]

\[
D(h) = \frac{4^k C(h/2) - C(h)}{4^k - 1}
\]
# Romberg Integration

## Accelerated Trapezoid Rule

\[
I_{j,k} = \frac{4^k I_{j+1,k} - I_{j,k}}{4^k - 1}; \quad k = 1, 2, 3, \ldots
\]

<table>
<thead>
<tr>
<th>Trapezoid</th>
<th>Simpson's</th>
<th>Boole's</th>
</tr>
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<tbody>
<tr>
<td>( k = 0 )</td>
<td>( k = 1 )</td>
<td>( k = 2 )</td>
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<tr>
<td>( O(h^2) )</td>
<td>( O(h^4) )</td>
<td>( O(h^6) )</td>
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</table>

| \( h \) | \( I_{0,0} \) | \( I_{0,1} \) | \( I_{0,2} \) | \( I_{0,3} \) | \( I_{0,4} \) |
| \( h/2 \) | \( I_{1,0} \) | \( I_{1,1} \) | \( I_{1,2} \) | \( I_{1,3} \) |
| \( h/4 \) | \( I_{2,0} \) | \( I_{2,1} \) | \( I_{2,2} \) |
| \( h/8 \) | \( I_{3,0} \) | \( I_{3,1} \) |
| \( h/16 \) | \( I_{4,0} \) |

\[
\begin{align*}
4I_{j+1,0} - I_{j,0} & \quad 16I_{j+1,1} - I_{j,1} & \quad 64I_{j+1,2} - I_{j,2} & \quad 256I_{j+1,3} - I_{j,3} \\
3 & \quad 15 & \quad 63 & \quad 255
\end{align*}
\]
# Romberg Integration

## Accelerated Trapezoid Rule

\[
I = \int_0^4 xe^{2x}\,dx = 5216.926477
\]

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<td>8240.41</td>
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<td>5224.84</td>
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<td>12142.2</td>
<td>5670.98</td>
<td>5229.14</td>
<td>\cellcolor{red}5217.01</td>
</tr>
<tr>
<td>(h = 1)</td>
<td>7288.79</td>
<td>5256.75</td>
<td>\cellcolor{red}5217.20</td>
<td></td>
</tr>
<tr>
<td>(h = 0.5)</td>
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<td>\cellcolor{red}5219.68</td>
<td></td>
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<td>(h = 0.25)</td>
<td>5355.95</td>
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<td></td>
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<td>(\varepsilon = )</td>
<td>(-2.66%)</td>
<td>(-0.0527%)</td>
<td>(-0.0053%)</td>
<td>(-0.00168%)</td>
</tr>
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</table>
Gaussian Quadratures

• **Newton-Cotes Formulae**
  - use evenly-spaced functional values
  - Did not use the flexibility we have to select the quadrature points

• In fact a quadrature point has several degrees of freedom.

\[ I(f) = \sum_{i=1}^{m} c_i f(x_i) \]

A formula with \( m \) function evaluations requires specification of \( 2m \) numbers \( c_i \) and \( x_i \)

• **Gaussian Quadratures**
  - select both these weights and locations so that a higher order polynomial can be integrated (alternatively the error is proportional to a higher derivatives)

• Price: functional values must now be evaluated at non-uniformly distributed points to achieve higher accuracy

• Weights are no longer simple numbers

• Usually derived for an interval such as \([-1,1]\)

• Other intervals \([a,b]\) determined by mapping to \([-1,1]\)
Gaussian quadrature

• More formally Gaussian quadrature is defined with a weight function

\[ I(f) = \int_a^b w(t) f(t) \, dt = \sum_{i=1}^m c_i f(t_i) \]

• Here the weight function is 1
• Special name: Gauss-Legendre quadrature
• Can define quadratures for other \( w(t) \) as long as

  • \( w(t) \geq 0 \) for \( t \in [a, b] \).

  • The moments

\[ \mu_k = \int_a^b w(t) t^k \, dt \]

exist and are finite for \( k = 0, 1, \ldots \).
Gauss-Legendre Quadrature on \([-1, 1]\)

\[
\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i) = c_1 f(x_1) + c_2 f(x_2) + \cdots + c_n f(x_n)
\]

- Two function evaluations:
  - Choose \((c_1, c_2, x_1, x_2)\) such that the method yields “exact integral” for \(f(x) = x^0, x^1, x^2, x^3\)

\[
n = 2 : \int_{-1}^{1} f(x)dx = c_1 f(x_1) + c_2 f(x_2)
\]
Finding quadrature nodes and weights

- One way is through the theory of orthogonal polynomials.
- Here we will do it via brute force
- Set up equations by requiring that the $2m$ points guarantee that a polynomial of degree $2m-1$ is integrated exactly.
- In general process is non-linear
  - (involves a polynomial function involving the unknown point and its product with unknown weight)
  - Can be solved by using a multidimensional nonlinear solver
  - Alternatively can sometimes be done step by step
Gauss-Legendre Quadrature on \([-1, 1]\)

\[ n = 2 : \quad \int_{-1}^{1} f(x) \, dx = c_1 f(x_1) + c_2 f(x_2) \]

Exact integral for \( f = x^0, x^1, x^2, x^3 \)

- Four equations for four unknowns

\[
\begin{align*}
\text{f} = 1 & \implies \int_{-1}^{1} 1 \, dx = 2 = c_1 + c_2 \\
\text{f} = x & \implies \int_{-1}^{1} x \, dx = 0 = c_1 x_1 + c_2 x_2 \\
\text{f} = x^2 & \implies \int_{-1}^{1} x^2 \, dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 \\
\text{f} = x^3 & \implies \int_{-1}^{1} x^3 \, dx = 0 = c_1 x_1^3 + c_2 x_2^3
\end{align*}
\]

\[
\begin{align*}
c_1 &= 1 \\
c_2 &= 1
\end{align*}
\]

\[
\begin{align*}
x_1 &= \frac{-1}{\sqrt{3}} \\
x_2 &= \frac{1}{\sqrt{3}}
\end{align*}
\]

\[
I = \int_{-1}^{1} f(x) \, dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)
\]
Error

- If we approximate a function with a Gaussian quadrature formula we cause an error proportional to $2n$ th derivative.
Gaussian Quadrature on $[-1, 1]$

\[ n = 3 : \int_{-1}^{1} f(x) \, dx = c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3) \]

- Choose \((c_1, c_2, c_3, x_1, x_2, x_3)\) such that the method yields “exact integral” for \(f(x) = x^0, x^1, x^2, x^3, x^4, x^5\)
Gaussian Quadrature on \([-1, 1]\)

\[ f = 1 \Rightarrow \int_{-1}^{1} x \, dx = 2 = c_1 + c_2 + c_3 \]

\[ f = x \Rightarrow \int_{-1}^{1} x \, dx = 0 = c_1 x_1 + c_2 x_2 + c_3 x_3 \]

\[ f = x^2 \Rightarrow \int_{-1}^{1} x^2 \, dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 + c_3 x_3^2 \]

\[ f = x^3 \Rightarrow \int_{-1}^{1} x^3 \, dx = 0 = c_1 x_1^3 + c_2 x_2^3 + c_3 x_3^3 \]

\[ f = x^4 \Rightarrow \int_{-1}^{1} x^4 \, dx = \frac{2}{5} = c_1 x_1^4 + c_2 x_2^4 + c_3 x_3^4 \]

\[ f = x^5 \Rightarrow \int_{-1}^{1} x^5 \, dx = 0 = c_1 x_1^5 + c_2 x_2^5 + c_3 x_3^5 \]

\[ \Rightarrow \begin{cases} 
  c_1 = 5/9 \\
  c_2 = 8/9 \\
  c_3 = 5/9 \\
  x_1 = -\sqrt{3}/5 \\
  x_2 = 0 \\
  x_3 = \sqrt{3}/5 
\end{cases} \]
Gaussian Quadrature on $[-1, 1]$

Exact integral for $f = x^0, x^1, x^2, x^3, x^4, x^5$

$$I = \int_{-1}^{1} f(x)dx = \frac{5}{9} f(-\sqrt{\frac{3}{5}}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{\frac{3}{5}})$$
Gaussian Quadrature on \([a, b]\)

Coordinate transformation from \([a,b]\) to \([-1,1]\)

\[
t = \frac{b-a}{2} x + \frac{b+a}{2}
\]

\[
\begin{cases}
x = -1 \Rightarrow t = a \\
x = 1 \Rightarrow t = b
\end{cases}
\]

\[
\int_a^b f(t) dt = \int_{-1}^{1} f\left( \frac{b-a}{2} x + \frac{b+a}{2} \right) \left( \frac{b-a}{2} \right) dx = \int_{-1}^{1} g(x) dx
\]
Example: Gaussian Quadrature

Evaluate \( I = \int_0^4 te^{2t} \, dt = 5216926477 \)

Coordinate transformation

\[
t = \frac{b-a}{2} x + \frac{b+a}{2} = 2x + 2; \quad dt = 2dx
\]

\[
I = \int_0^4 te^{2t} \, dt = \int_{-1}^{1} (4x + 4)e^{4x+4} \, dx = \int_{-1}^{1} f(x) \, dx
\]

Two-point formula

\[
I = \int_{-1}^{1} f(x) \, dx = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = (4 - \frac{4}{\sqrt{3}})e^{\frac{4-4}{\sqrt{3}}} + (4 + \frac{4}{\sqrt{3}})e^{\frac{4+4}{\sqrt{3}}}
\]

\[
= 9.167657324 + 3468.376279 = 3477.543936 \quad (\varepsilon = 33.34\%)
\]
Example: Gaussian Quadrature

Three-point formula

\[ I = \int_{-1}^{1} f(x)dx = \frac{5}{9} f(-\sqrt{0.6}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{0.6}) \]
\[ = \frac{5}{9} (4 - 4\sqrt{0.6}) e^{4-\sqrt{0.6}} + \frac{8}{9} (4) e^4 + \frac{5}{9} (4 + 4\sqrt{0.6}) e^{4+\sqrt{0.6}} \]
\[ = \frac{5}{9} (2.221191545) + \frac{8}{9} (218.3926001) + \frac{5}{9} (8589.142689) \]
\[ = 4967.106689 \quad (\varepsilon = 4.79\%) \]

Four-point formula

\[ I = \int_{-1}^{1} f(x)dx = 0.34785 [f(-0.861136) + f(0.861136)] + 0.652145 [f(-0.339981) + f(0.339981)] \]
\[ = 5197.54375 \quad (\varepsilon = 0.37\%) \]
Other rules

• Gauss-Lobatto:
  – requiring end points be included in the formula

• Gauss-Radau
  – Require one end point be in the formula
Higher dimensions

• Can take similar approach (fit polynomials and evaluate)
• However, as dimensionality increases number of points needed increases exponentially in dimension
• Very high dimensions: only practical way is “Monte-Carlo” integration
• Evaluates integrals probabilistically
• In this case expected value is the computed integral
• Error is the variance of the estimate.