

*Computational Methods*  
CMSC/AMSC/MAPL 460

Gaussian Quadrature

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# 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

# Error

- Trapezoidal rule is exact for constant and linear functions
- What about others?
- Let  $T(f)$  denote trapezoidal rule result.
- Then  $I(f) - T(f) = -(b-a)^3/12 f''(\xi)$  for some  $\xi \in [a, b]$
- Similarly Simpson rule is exact for quadratics and has error proportional to third derivative
- ... and so on.
- We need 2 function evaluations for a 2<sup>nd</sup> order error
  - 3 for a 3<sup>rd</sup> order and so on ...
- Error and derivatives ...

# 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.

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

A formula with  $m$  function evaluations requires specification of  $2m$  numbers  $c_i$  and  $x_i$

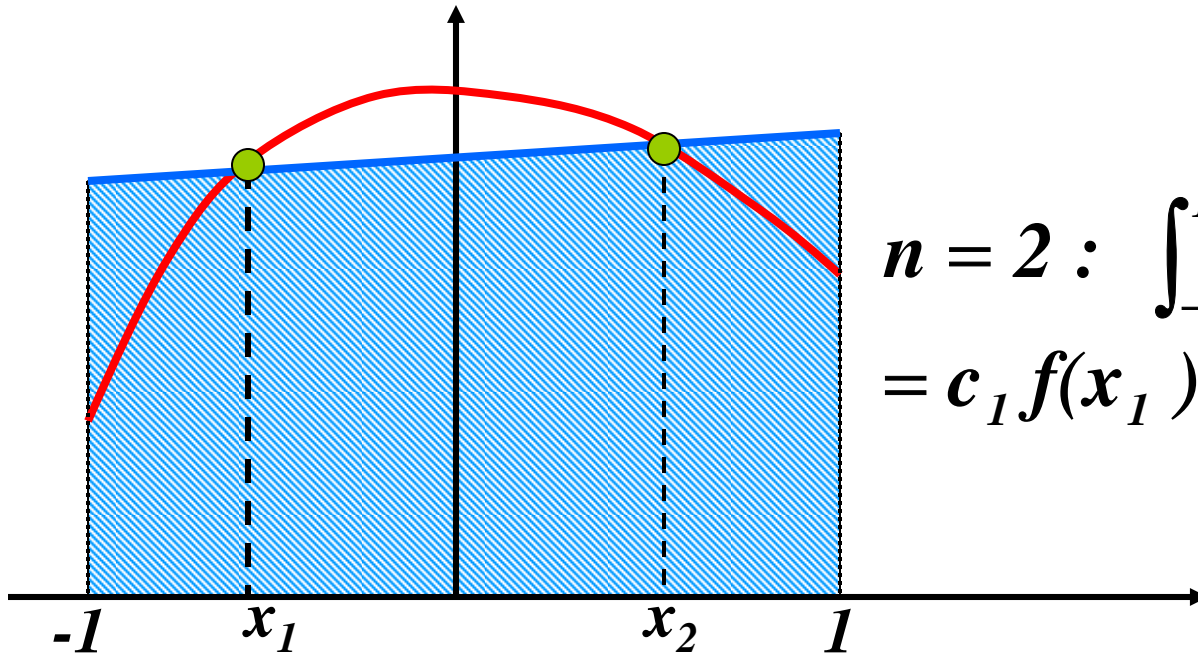
- **Gaussian Quadratures**

- 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 on $[-1, 1]$

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

- 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

# *Gaussian Quadrature on [-1, 1]*

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

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

– Four equations for four unknowns

$$\left\{ \begin{array}{l} f = 1 \Rightarrow \int_{-1}^1 1 dx = 2 = c_1 + c_2 \\ f = x \Rightarrow \int_{-1}^1 x dx = 0 = c_1 x_1 + c_2 x_2 \\ f = x^2 \Rightarrow \int_{-1}^1 x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 \\ f = x^3 \Rightarrow \int_{-1}^1 x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3 \end{array} \right.$$

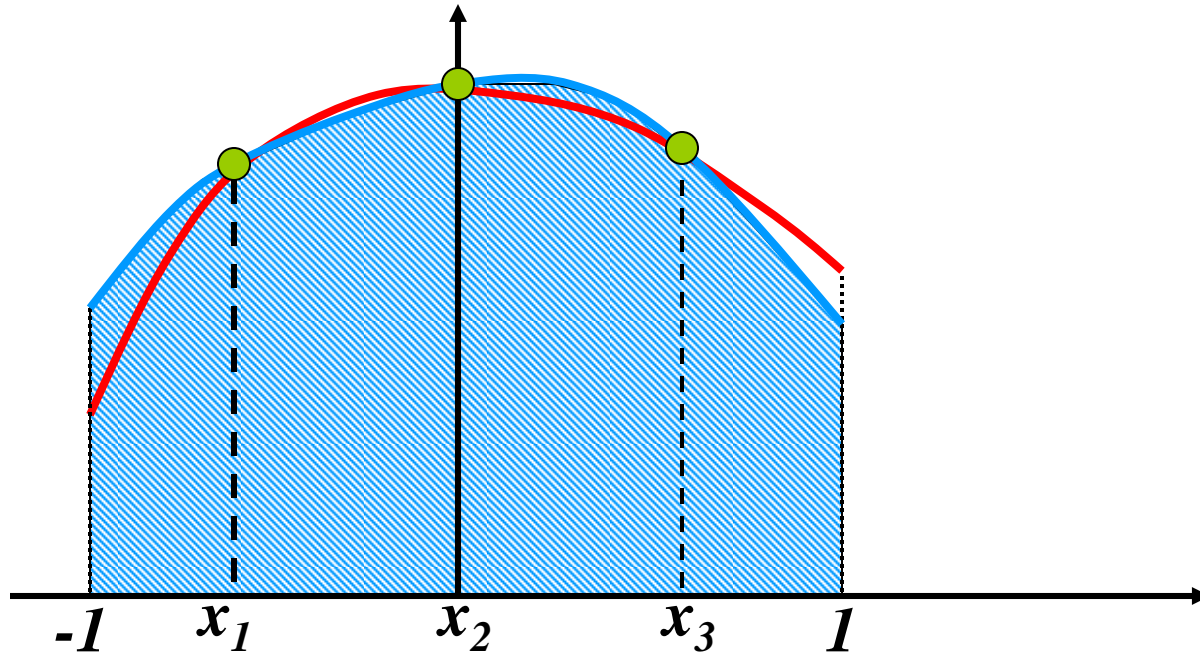
$$I = \int_{-1}^1 f(x) dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

# 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]*

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

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

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

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

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

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

$$\Rightarrow \begin{cases} c_1 = 5/9 \\ c_2 = 8/9 \\ c_3 = 5/9 \\ x_1 = -\sqrt{3/5} \\ x_2 = 0 \\ x_3 = \sqrt{3/5} \end{cases}$$

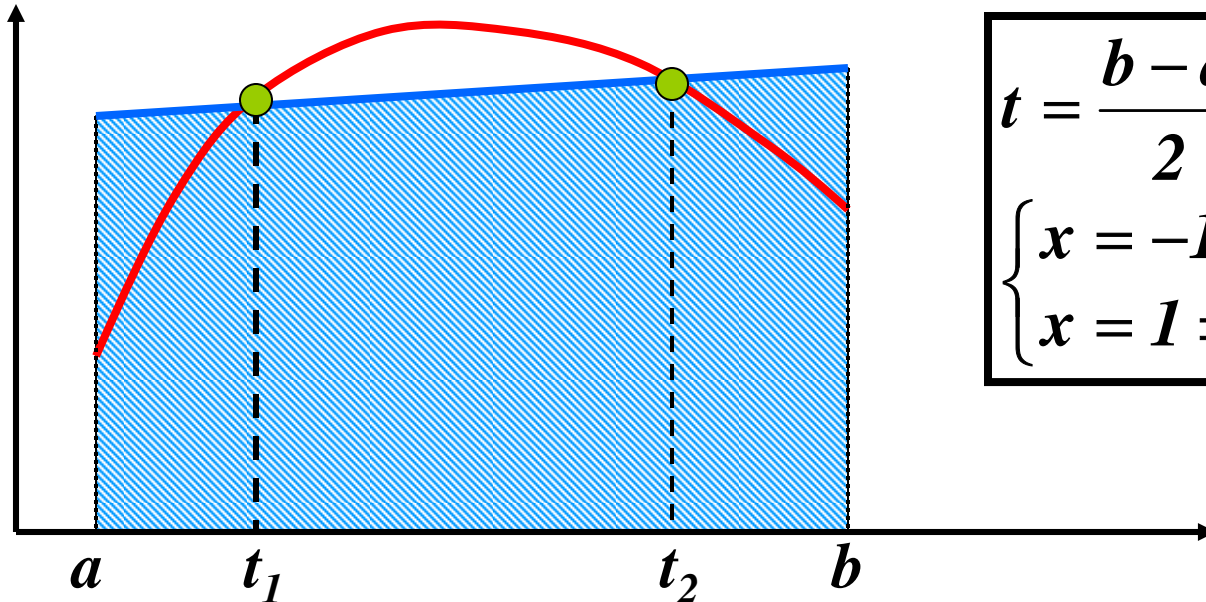
# *Gaussian Quadrature on [-1, 1]*

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

$$I = \int_{-1}^1 f(x) dx = \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$$

# *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  $I = \int_0^4 te^{2t} dt = 5216.926477$

**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**

$$\begin{aligned} I &= \int_{-1}^1 f(x) dx = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = \left(4 - \frac{4}{\sqrt{3}}\right)e^{4-\frac{4}{\sqrt{3}}} + \left(4 + \frac{4}{\sqrt{3}}\right)e^{4+\frac{4}{\sqrt{3}}} \\ &= 9.167657324 + 3468.376279 = 3477.543936 \quad (\varepsilon = 33.34\%) \end{aligned}$$

# *Example: Gaussian Quadrature*

## **Three-point formula**

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

## **Four-point formula**

$$\begin{aligned} I &= \int_{-1}^1 f(x) dx = 0.34785 [f(-0.861136) + f(0.861136)] \\ &\quad + 0.652145 [f(-0.339981) + f(0.339981)] \\ &= 5197.54375 \quad (\varepsilon = 0.37\%) \end{aligned}$$

# 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.