Richardson Extrapolation

For trapezoidal rule

$$A=\int_a^b f(x)dx = A(h)+c_1h^2+\cdots$$

$$\begin{cases} A = A(h)+c_1h^2+c_2h^4\cdots \\ A = A(\frac{h}{2})+c_1(\frac{h}{2})^2+c_2(\frac{h}{2})^4+\cdots \end{cases}$$

$$\Rightarrow A=\frac{1}{3}\left[4A(\frac{h}{2})-A(h)\right]-\frac{c_2}{4}h^4+\cdots = B(h)+b_2h^4+\cdots$$

– k^{th} **level of extrapolation**

$$\left.\begin{cases} A = B(h)+b_2h^4\cdots \\ A = B(\frac{h}{2})+b_2(\frac{h}{2})^4+\cdots \end{cases}\right\} \Rightarrow C(h)=\frac{1}{15}\left[16B(\frac{h}{2})-B(h)\right]$$

$$D(h)=\frac{4^kC(h/2)-C(h)}{4^k-1}$$

Romberg Integration

Accelerated Trapezoid Rule

$$I_{j,k}=\frac{4^kI_{j+1,k}-I_{j,k}}{4^k-1};\quad k=1,2,3,\cdots$$

	Trapezoid	Simpson's	Boole's		
	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$
	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$	$O(h^{10})$
h	$I_{0,0}$	$I_{0,1}$	$I_{0,2}$	$I_{0,3}$	$I_{0,4}$
$h/2$	$I_{1,0}$	$I_{1,1}$	$I_{1,2}$	$I_{1,3}$	
$h/4$	$I_{2,0}$	$I_{2,1}$	$I_{2,2}$		
$h/8$	$I_{3,0}$	$I_{3,1}$			
$h/16$	$I_{4,0}$				
		$\frac{4I_{j+1,0}-I_{j,0}}{3}$	$\frac{16I_{j+1,1}-I_{j,1}}{15}$	$\frac{64I_{j+1,2}-I_{j,2}}{63}$	$\frac{256I_{j+1,3}-I_{j,3}}{255}$

Romberg Integration

Accelerated Trapezoid Rule

$$I = \int_0^4 xe^{2x}dx = 5216.926477$$

	Trapezoid	Simpson's	Boole's		
	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$
	$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$	$O(h^{10})$
$h=4$	23847.7	8240.41	5499.68	5224.84	5216.95
$h=2$	12142.2	5670.98	5229.14	5217.01	
$h=1$	7288.79	5256.75	5217.20		
$h=0.5$	5764.76	5219.68			
$h=0.25$	5355.95				
$\varepsilon=$	-2.66%	-0.0527%	-0.0053%	-0.00168%	-0.00050%

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.

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

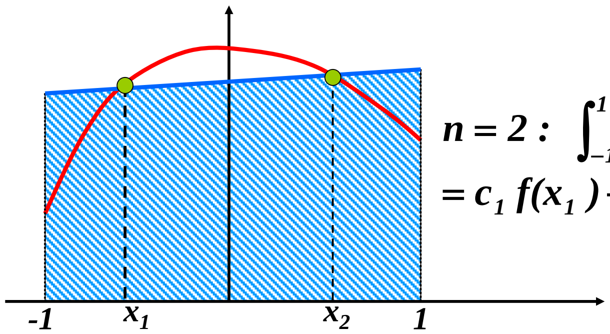
A formula with m function evaluations requires specification of $2m$ numbers c_i and x_i

- **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]

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

- Two function evaluations:
  - Choose (c1, c2, x1, x2) 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**

$$\begin{cases} f = 1 \Rightarrow \int_{-1}^{1} 1dx = 2 = c_1 + c_2 \\ f = x \Rightarrow \int_{-1}^{1} xdx = 0 = c_1 x_1 + c_2 x_2 \\ f = x^2 \Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 \\ f = x^3 \Rightarrow \int_{-1}^{1} x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3 \end{cases}$$

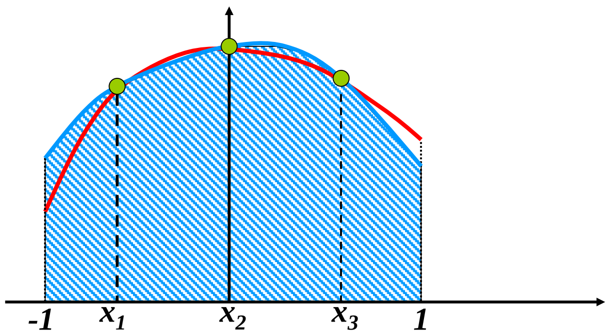
$$I = \int_{-1}^{1} f(x)dx = f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}})$$

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]

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

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

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

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

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

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

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

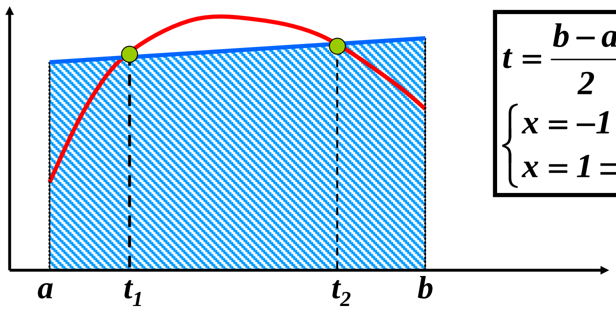
Gaussian Quadrature on [-1, 1]

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]



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

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

$$\int_a^b f(t)dt = \int_{-1}^{1} f(\frac{b-a}{2}x + \frac{b+a}{2})(\frac{b-a}{2})dx = \int_{-1}^{1} g(x)dx$$

Example: Gaussian Quadrature

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

Coordinate transformation

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

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

Two-point formula

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

Example: Gaussian Quadrature

Three-point formula

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

Four-point formula

$$I = \int_{-1}^{1} f(x)dx = 0.34785\left[f(-0.861136) + f(0.861136)\right]$$
$$+ 0.652145\left[f(-0.339981) + f(0.339981)\right]$$
$$= 5197.54375 \qquad (\varepsilon = 0.37\%)$$

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.