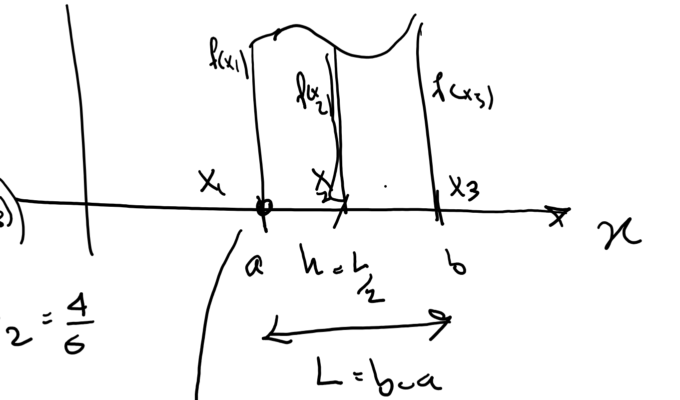
FEM2021/11/19

Friday, November 19, 2021 2:53 PM

NC scheme continued:
3 point rule: Simpson's rule

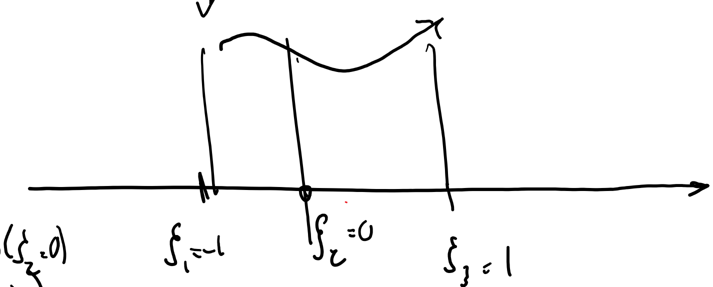
$$\underbrace{\int_a^b f(x)\,dx}_{\text{answer}} = L\,\Big(\overset{1/6}{\omega_1} f(x_1) + \overset{4/6}{\omega_2} f(x_2) + \overset{1/6}{\omega_3} f(x_3)\Big)$$

$$\omega_1 = \omega_3 = \frac{1}{6}, \quad \omega_2 = \frac{4}{6}$$



Why?

Let's write Simpson's rule for ξ coordinate



$$\int_{-1}^{1} f(\xi)\,d\xi = \underbrace{[1-(-1)]}_{\text{Length in } \xi}\Big(\omega_1 f(\xi_1 = -1) + \omega_2 f(\xi_2 = 0) + \omega_3 f(\xi_3 = 1)\Big)$$

$$\int_{-1}^{1} f(\xi)\,d\xi = \underbrace{2\,(\omega_1 f(-1) + \omega_2 f(0) + \omega_3 f(1))}$$ (*)

Let's derive $\omega_1, \omega_2, \omega_3$

3 unknown $\omega_1, \omega_2, \omega_3$: We need three equations,

if $f(\xi)$ is a polynomial up to what order could we ensure that the integral is exact:

$$f(\xi) = \underbrace{\alpha_0 + \alpha_1 \xi + \alpha_2 \xi^2}_{\text{3-equations}} + \alpha_3 \xi^3 + \cancel{\alpha_4 \xi^4 + \dots}$$

integrating 1 exactly $\longrightarrow \int_{-1}^{1} 1\,d\xi = 2 = 2\,(\omega_1 \overset{1}{f(-1)} + \omega_2 \overset{1}{f(0)} + \omega_3 \overset{1}{f(1)})$

" ξ " $\longrightarrow \int_{-1}^{1} \xi\,d\xi = 0 = 2\,(\omega_1 \overset{-1}{f(-1)} + \omega_2 \overset{0}{f(0)} + \omega_3 \overset{1}{f(1)})$

" ξ^2 " $\longrightarrow \int_{-1}^{1} \xi^2\,d\xi = \frac{\xi^3}{3}\Big|_{-1}^{1} = \frac{2}{3} = 2\,(\omega_1 \overset{1}{f(-1)} + \omega_2 \overset{0}{f(0)} + \omega_3 \overset{1}{f(1)})$ $\longrightarrow$

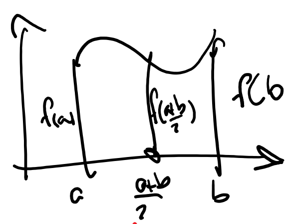
$$\begin{cases} (a)\ \ \omega_1 + \omega_2 + \omega_3 = 1 \\ (b)\ -\omega_1 + \omega_3 = 0 \\ (c)\ \ \omega_1 + \omega_3 = \frac{1}{3} \end{cases}$$

(side note for NC scheme by $\int f(\xi)\,d\xi$
$f(\xi) = 1 \longrightarrow \boxed{\sum_{i=1} \omega_i = 1}$

b,c $\quad w_1 = w_3 = \frac{1}{6}$ @ $\rightarrow w_2 = \frac{4}{6}$

Simpson's rule

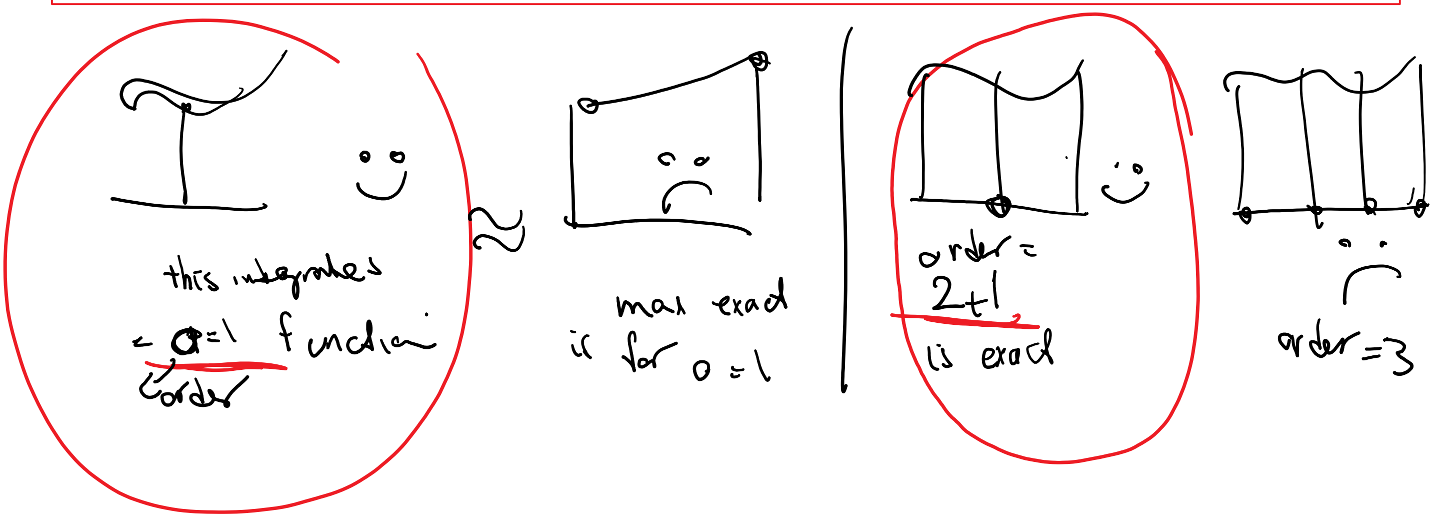
$$\int_a^b f(x)\,d\xi = \underbrace{(b-a)}_{L}\left(\frac{1}{6}f(a) + \frac{4}{6}f\left(\frac{a+b}{2}\right) + \frac{1}{6}f(b)\right)$$



What is the maximum polynomial order Simpson's rule can integrate exactly? 2 + 1

bonus

any NC scheme that has odd # pts (ending with a pt @ the center) there is an additional bonus ~ the order it can integrate



So, in NC we use odd # point schemes.

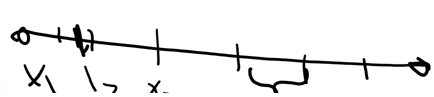
HW5, problem 1

$$\int_a^b f(x)\,dx = \underbrace{C_0 h \sum_{i=1}^{n} W_i f(x_i)}_{\text{quadrature scheme}} + \underbrace{C_1 h^{k+1} f^{(k)}(\xi)}_{\text{estimate of error}}$$

Newton-Cotes

FYI

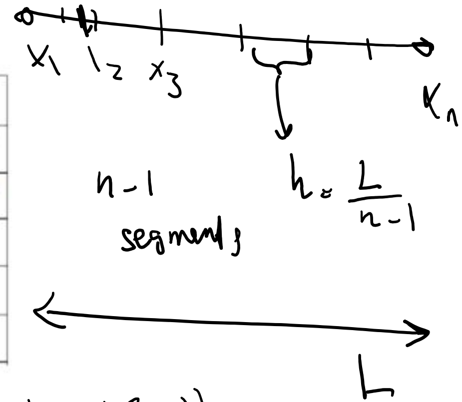
NOT compute



NOT compute

Newton-Cotes

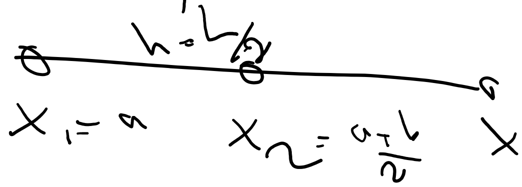
n	C_0	W_1	W_2	W_3	W_4	W_5	C_1	k	Name
1	1	1					1/2	1	Rectangle
2	1/2	1	1				–1/12	2	Trapezium
3	1/3	1	4	1			–1/90	4	Simpson
4	3/8	1	3	3	1		–3/80	4	4-point
5	2/45	7	32	12	32	7	–8/945	6	5-point



$$\int_a^b f(x)dx = \frac{1}{3}\cdot\left(\frac{L}{3-1}\right)\left(1 f(x_1) + 4 f(x_2) + 1 f(x_3)\right)$$

$$= L\left(\frac{1}{6} f(x_1) + \frac{4}{6} f(x_2) + \frac{1}{6} f(x_3)\right)$$

we obtained this before.



You can also use this table from Bathe's book:

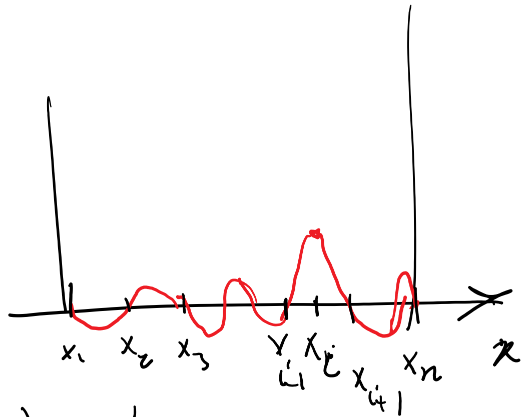
TABLE 5.5 *Newton-Cotes numbers and error estimates*

Number of intervals n	C_0^n	C_1^n	C_2^n	C_3^n	C_4^n	C_5^n	C_6^n	Upper bound on error R_n as a function of the derivative of F
1	$\frac{1}{2}$	$\frac{1}{2}$						$10^{-1}(b-a)^3F^{\text{II}}(r)$
2	$\frac{1}{6}$	$\frac{4}{6}$	$\frac{1}{6}$					$10^{-3}(b-a)^5F^{\text{IV}}(r)$
3	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$				$10^{-3}(b-a)^5F^{\text{IV}}(r)$
4	$\frac{7}{90}$	$\frac{32}{90}$	$\frac{12}{90}$	$\frac{32}{90}$	$\frac{7}{90}$			$10^{-6}(b-a)^7F^{\text{VI}}(r)$
5	$\frac{19}{288}$	$\frac{75}{288}$	$\frac{50}{288}$	$\frac{50}{288}$	$\frac{75}{288}$	$\frac{19}{288}$		$10^{-6}(b-a)^7F^{\text{VI}}(r)$
6	$\frac{41}{840}$	$\frac{216}{840}$	$\frac{27}{840}$	$\frac{272}{840}$	$\frac{27}{840}$	$\frac{216}{840}$	$\frac{41}{840}$	$10^{-9}(b-a)^9F^{\text{VIII}}(r)$

To obtain weights of an n-point NC scheme, we need to solve an n x n linear system.
Not really!

$$\int_a^b f(x)dx = L(\omega_1 f(x_1) + \dots + \omega_n f(x_n))$$

find ω_i's

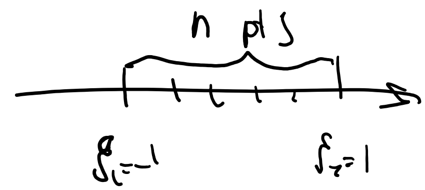


Let's ~~choose~~ $f(x) = L_i(x)$

$$\int_a^b L_i(x)dx = L\cdot(\omega_1 \underbrace{L_i(x_1)}_{0} + \dots + \omega_{i-1} \underbrace{L_i(x_{i-1})}_{0} + \omega_i \underbrace{L_i(x_i)}_{1} + \omega_{i+1} \underbrace{L_i(x_{i+1})}_{0} + \dots + \omega_n \underbrace{L_i(x_n)}_{0})$$

$$\omega_i = \frac{1}{L}\int_a^b L_i(x)dx$$

and it's better to use ξ axis



$$\omega_i = \frac{1}{2}\int_{-1}^{1} L_i(\xi)d\xi$$

Summary:
NC with n points -> we have n unknown w's -> n polynomial coefficients -> It can integrate polynomial order n - 1 exactly (or with bonus polynomial order n when n is odd)

NC

#pts (n)

polynomial order that can be integrated exactly

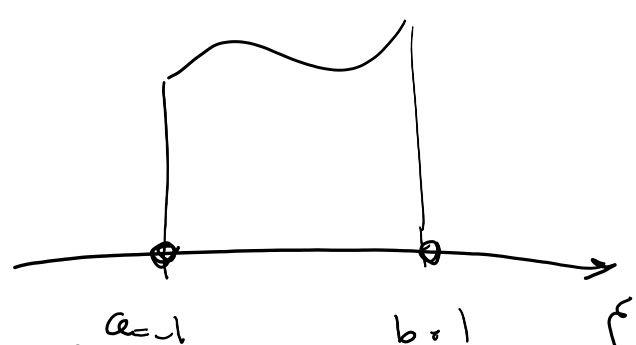
$$(o) = \begin{cases} n-1 & n \text{ even} \\ n & n \text{ odd} \end{cases}$$

Gauss quadrature:
In Newton-Cotes every point is worth one unknown -> w_i

In Gauss point every point is worth TWICE!

2 pt scheme

NC



$\int f(\xi)d\xi = (2)(\omega_1 f(-1) \quad \omega_2 f(1))$

$$\int f(\xi)\,d\xi \approx (2)\left(\omega_1 f(\underset{\xi_1}{-1}) + \omega_2 f(\underset{\xi_2}{1})\right) \qquad a=-1 \quad b=1 \quad \xi$$

2 ω's → we can integrate $f(\xi) = \alpha_0 + \alpha_1 \xi$ exactly

Gauss: Why should we fix the pts let ξ_1, ξ_2 be unknowns to begin with

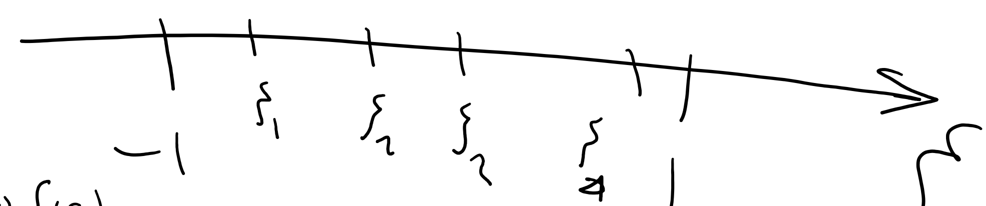
Gauss Quadrature is always expressed in $\xi \in [-1, 1]$ domain (parent geometry)

$$\int_{-1}^{1} f(\xi)\,d\xi = \cancel{\underbrace{(1-(-1))}_{2}}\left(\sum \omega_i f(\xi_i)\right)$$

ω_i: quadrature weights

ξ_i: quadrature pts

In Gauss Quadrature we don't have this factor



$$\int_{-1}^{1} f(\xi)\,d\xi = \sum \omega_i f(\xi_i)$$

Gauss table

TABLE 5.6 *Sampling points and weights in Gauss-Legendre numerical integration (interval −1 to +1)*

n	r_i			α_i		
1	0.	(15 zeros)		2.	(15 zeros)	
2	±0.57735	02691	89626	1.00000	00000	00000
3	±0.77459	66692	41483	0.55555	55555	55556
	0.00000	00000	00000	0.88888	88888	88889
4	±0.86113	63115	94053	0.34785	48451	37454
	±0.33998	10435	84856	0.65214	51548	62546
5	±0.90617	98459	38664	0.23692	68850	56189
	±0.53846	93101	05683	0.47862	86704	99366
	0.00000	00000	00000	0.56888	88888	88889
6	±0.93246	95142	03152	0.17132	44923	79170

2 pt

Gauss scheme

$\omega_1 = 1, \ \xi = -.577...26$

$\xi_2 = 0$, $\omega_2 = .88$

$\xi_3 = .7745$, $\omega_3 = .55$

$\xi_1 = -.7745...$, $\omega_1 = .55$

-1

1

5	±0.90617	98459	38664	0.23692	68850	56189	
	±0.53846	93101	05683	0.47862	86704	99366	
	0.00000	00000	00000	0.56888	88888	88889	
6	±0.93246	95142	03152	0.17132	44923	79170	
	±0.66120	93864	66265	0.36076	15730	48139	
	±0.23861	91860	83197	0.46791	39345	72691	

$\omega_1 = 1,\ \xi_1 = -.577\ldots 26$

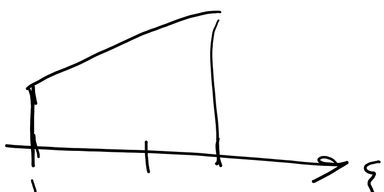
$\omega_2 = 1,\ \xi_2 = +$

$\omega_1 \approx .55$

$n = 2$

Comparison of NC and Gauss schemes with 2 points

NC

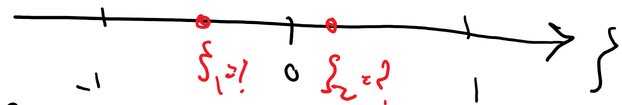


$\xi_1 = -1 \qquad \xi_2 = 1$

$$\int_{-1}^{1} f(\xi)\,d\xi = 2\left(\tfrac{1}{2} f(\xi_1) + \tfrac{1}{2} f(\xi_2)\right) = f(-1) + f(1)$$

Integrates $\boxed{\text{order} = 1}$ exactly

Gauss



$$\int f(\xi)\,d\xi = \omega_1 f(\xi_1) + \omega_2 f(\xi_2)$$

unknowns : 4 $\quad \omega_1, \omega_2 + \underbrace{\xi_1, \xi_2}$ 4 unknowns

$$f(\xi) = \underbrace{\alpha_0 1 + \alpha_1 \xi + \alpha_2 \xi^2 + \alpha_3 \xi^3}_{4 \text{ eqns}} + \cdots$$

We'll be able to integrate up to $\boxed{\text{order} = 3}$ exactly

Gauss scheme integrates $1, \xi, \xi^2, \xi^3$ exactly

$f(\xi) = 1 \;\rightarrow\; \int_{-1}^{1} f(\xi)\,d\xi = \int_{-1}^{1} 1\,d\xi = 2 = \omega_1 f(\xi_1) + \omega_2 f(\xi_2) \qquad \omega_1 + \omega_2 = 2 \quad (1)$

$f(\xi) = \xi \qquad \int_{-1}^{1} f(\xi)\,d\xi = \int_{-1}^{1} \xi\,d\xi = 0 = \quad \text{''} \quad = \qquad \omega_1 \xi_1 + \omega_2 \xi_2 = 0 \quad (2)$

$f(\xi) = \xi^2 ; \qquad \int_{-1}^{1} f(\xi)\,d\xi = \int_{-1}^{1} \xi^2\,d\xi = \frac{2}{3} = \quad \text{''} \quad = \qquad \omega_1 \xi_1^2 + \omega_2 \xi_2^2 = 2/3 \quad (3)$

$f(\xi) = \xi^3 \qquad \int_{-1}^{1} f(\xi)\,d\xi = \int \xi^3\,d\xi = 0 = \quad \text{''} \quad = \qquad \omega_1 \xi_1^3 + \omega_2 \xi_2^3 = 0 \quad (4)$

4 eqn, 4 unknown nonlinear system

Multiply (2) by ξ_1^2 :

$$\omega_1 \xi_1^3 + \omega_2 \xi_1^2 \xi_2 = 0$$

(4)

$$\omega_1 \xi_1^3 + \omega_2 \xi_2^3 = 0$$

$$\omega_2 \xi_2 (\xi_1 - \xi_2)(\xi_1 + \xi_2) = 0 \longrightarrow$$

$\cancel{\omega_2 = 0}$

$\cancel{\xi_2 = 0}$

$\cancel{\xi_1 = \xi_2}$

$\boxed{\xi_1 = -\xi_2}$ → plug in (2)

$\omega_1 \xi_1 + \omega_2 \xi_2 = 0$

$\omega_1\xi_1 + \omega_2\xi_2 = 0$

$\longrightarrow (\omega_1 - \omega_2)\xi_1 = 0$, $\xi_1 \neq 0$

(1) $\left.\begin{array}{l}\omega_1 - \omega_2 = 0\\ \omega_1 + \omega_2 = 2\end{array}\right\} \longrightarrow \boxed{\omega_1 = \omega_2 = 1}$

$\xi_1, \xi_2 = ?$ eq (3) $\underset{1}{\omega_1}\xi_1^2 + \underset{1}{\omega_2}\xi_2^2 = \frac{2}{3}$, $\xi_2 = -\xi_1$ $\longrightarrow 2\xi_1^2 = \frac{2}{3}$

$\longrightarrow \xi_1 = \mp\frac{1}{\sqrt{3}}$ want to have $\xi_2 > \xi_1$

Gauss Quadrature with 2 pts

$\xi = -1$ $\xi_1 = -\frac{1}{\sqrt{3}}$ $\xi_2 = \frac{1}{\sqrt{3}}$ $\xi = 1$

$\omega_1 = 1$ $\omega_2 = 1$

$\int_{-1}^{1} f(\xi)\, d\xi \approx \omega_1 f(\xi_1) + \omega_2 f(\xi_2)$ the error $\propto f^{(iv)}(\tilde{\xi})$

$=$ for f being a polynomial of order ≤ 3

How to use the table in HW5:

$\frac{1}{\sqrt{3}}$ ω

Gauss Points ($\pm x_i$)	Weights (w_i)
n = 2	
0.57735 02691 89626	1.00000 00000 00000
n = 3	
0.00000 00000 00000	0.88888 88888 88888
0.77459 66692 41483	0.55555 55555 55555
n = 4	
0.33998 10435 84856	0.65214 51548 62546
0.86113 63115 94053	0.34785 48451 37454
n = 5	
0.00000 00000 00000	0.56888 88888 88889
0.53846 93101 05683	0.47862 86704 99366
0.90617 98459 38664	0.23692 68850 56189

ξ $-.577$ $.577$
ω 1 1

ξ's $-.77\ldots$ $.83$ 0 $.7745$
ω's $0.5\bar{5}$ $0.\bar{8}$ $0.5\bar{5}$

1. $\boxed{\textbf{50 Points}}$ Use a 3 point Gauss and 5 point Newton-Cotes quadrature rule to evaluate the following integral and obtain their respective errors with respect to exact value of the integral $I_e = \tan^{-1}(2) - \tan^{-1}(-1)$. Quadrature points and weights are given in fig. 1.

$$I = \underbrace{\int_{-1}^{2} \frac{dx}{1+x^2}} = \int_{-1}^{1} \underbrace{\left[\frac{1}{[1+x(\xi)]^2} J \right]}_{g(\xi)} d\xi$$

$x_a = -1$ $\quad$ $x_b = 2$

$\xi_a = -1$ $\quad$ $\xi_b = 1$

$$J = \frac{L_x}{L_\xi} = \frac{3}{2}$$

$$X(\xi) = x_a \underbrace{N_1^L(\xi)}_{\frac{1-\xi}{2}} + x_b \underbrace{N_2^L(\xi)}_{\frac{1+\xi}{2}}$$

$$\int_{-1}^{1} g(\xi)\, d\xi = \sum_{i=1}^{n} w_i\, g(\xi_i)$$

Derivation of Gauss points is difficult -> it results in an n x n nonlinear system of equations.

Extra credit assignment

(b) $\boxed{\textbf{35 Points}}$ In many instances we are dealing with more general integrals of the form $I = \int_{-\infty}^{\infty} f(\xi)\rho(\xi)d\xi$ $(\rho(\xi) \geq 0)$. For example Gauss integration is a special case where $\rho = \chi_{[-1\ 1]}$. Also in probability theory expected value of a quantity is defined as $\mathbb{E}(f(\xi)) = \int_{-\infty}^{\infty} f(\xi)\rho(\xi)d\xi$ where $\rho(\xi)$ is the *probability density function* (PDF) of the random variable ξ. In the context of FEM formulation, the integrals of latter form are encountered in the solution of stochastic PDEs. Ideally we want to derive quadrature rules for these more general cases as $I = \int_{-\infty}^{\infty} f(\xi)\rho(\xi)d\xi \quad \Rightarrow \mathrm{Q}(I) = \Sigma_{i=1}^{n} w_i f(\xi_i)$ where again ξ_i are quadrature points and w_i are quadrature weights. Given that we can define an inner-product of the form $< f, g >_\rho = \int_{-\infty}^{\infty} f(\xi)g(\xi)\rho(\xi)d\xi$ we can use any orthonormalization scheme such as Gram-Schmidt to form an orthonormal basis of Q_i (Q_i being a polynomial of order i) for polynomial functions. That is,

$$< Q_i, Q_j >_\rho = \delta_{ij} \quad \text{that is} \quad \int_{-\infty}^{\infty} Q_i(\xi)Q_j(\xi)\rho(\xi)d\xi = \delta_{ij} \tag{5}$$

n	$P_n(x)$	roots
0	1	
1	x	0
2	$\frac{1}{2}(3x^2-1)$	$\mp \frac{1}{\sqrt{3}}$
3	$\frac{1}{2}(5x^3-3x)$	$0, \pm \sqrt{3/5}$
4	$\frac{1}{8}(35x^4-30x^2+3)$	
5	$\frac{1}{8}(63x^5-70x^3+15x)$	
6	$\frac{1}{16}(231x^6-315x^4+105x^2-5)$	
7	$\frac{1}{16}(429x^7-693x^5+315x^3-35x)$	
8	$\frac{1}{128}(6435x^8-12012x^6+6930x^4-1260x^2+35)$	
9	$\frac{1}{128}(12155x^9-25740x^7+18018x^5-4620x^3+315x)$	

7	$\frac{1}{16}(429x^7 - 693x^5 + 315x^3 - 35x)$
8	$\frac{1}{128}(6435x^8 - 12012x^6 + 6930x^4 - 1260x^2 + 35)$
9	$\frac{1}{128}(12155x^9 - 25740x^7 + 18018x^5 - 4620x^3 + 315x)$
10	$\frac{1}{256}(46189x^{10} - 109395x^8 + 90090x^6 - 30030x^4 + 3465x^2 - 63)$

Figure 4: Legendre polynomials (Source: http://en.wikipedia.org/wiki/Legendre_polynomials)

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	±0.33998	10435	84856	0.65214	51548	62546
5	±0.90617	98459	38664	0.23692	68850	56189
	±0.53846	93101	05683	0.47862	86704	99366
	0.00000	00000	00000	0.56888	88888	88889
6	±0.93246	95142	03152	0.17132	44923	79170
	±0.66120	93864	66265	0.36076	15730	48139
	±0.23861	91860	83197	0.46791	39345	72691

roots of Legendre polynomials are Gauss pts

Summary of NC and Gauss integration schemes

$\boxed{n \rightarrow O}$	# of quadrature pts n	max poly. order that is exactly integrated O
Newton Cotes	n	$O = \begin{cases} n-1 & n \text{ even} \\ n & \end{cases}$
Gauss	n	$2n-1$

$\boxed{O \rightarrow n}$

NC

n	O
1	0+1
2	1

1

Gauss

$O = 2n-1$

NC

1	o+1
2	1
3	2+1
4	3

1

3

$o = 2n - 1$

$\rightarrow n = \frac{o+1}{2}$

integran

$n = \text{ceil}\left(\frac{o+1}{2}\right)$

$o \rightarrow n$

NC

$$n = \begin{cases} o & o \text{ odd} \\ \boxed{o+1 \quad o \text{ even}} \end{cases}$$

often the case

G

$$n = \text{ceil}\left(\frac{o+1}{2}\right)$$

What is the integration order and how many Gauss points needed?

$$K^e_{3\times3} = \int_{\xi=-1}^{1} \frac{EA(\xi)}{\underbrace{2\xi(x_{ave} - x^3) + \frac{L_e}{2}}_{J(\xi)}} \begin{bmatrix} \xi - \frac{1}{2} \\ \xi + \frac{1}{2} \\ -2\xi \end{bmatrix} \underbrace{\left[\xi - \frac{1}{2},\ \xi + \frac{1}{2},\ -2\xi\right]}_{B_\xi} d\xi$$

order $p-1$

element

ignore these

$o = 2$

$o = 2$

$n = \text{ceil}\left(\frac{o+1}{2}\right) = 2$

Gauss

$\xi_1 = \frac{-1}{\sqrt{3}}$ $\quad \xi_2 = \frac{1}{\sqrt{3}}$

NC

$n = o + 1 = 3$

NC

NC

$\xi_1 = -1$ $\xi_2 = 0$ $\xi_3 = 1$