Numerical Integration of a Function

- If we evaluate the function at 2 points, what should be the location of these points such that the error is minimized?
- Standard domain $\int_{-1}^{1} f(z)dz \approx \widetilde{I}_z = c_0 f(z_0) + c_1 f(z_1)$
- Four adjustable parameters, c_0, z_0 and c_1, z_1
- May integrate polynomials of degree 3 exactly
- How to obtain these parameters?
- One option: Using $f(z)$ as $1, z, z^2, z^3$

Integration of a Function: Standard Domain

- We get:

$$c_0 + c_1 = 2; c_0 z_0 + c_1 z_1 = 0; c_0 z_0^2 + c_1 z_1^2 = \frac{2}{3}; c_0 z_0^3 + c_1 z_1^3 = 0$$

resulting in

$$z_0 = -\frac{1}{\sqrt{3}}; z_1 = \frac{1}{\sqrt{3}}; c_0 = 1; c_1 = 1$$

- 2-point Gauss Quadrature

General Methodology

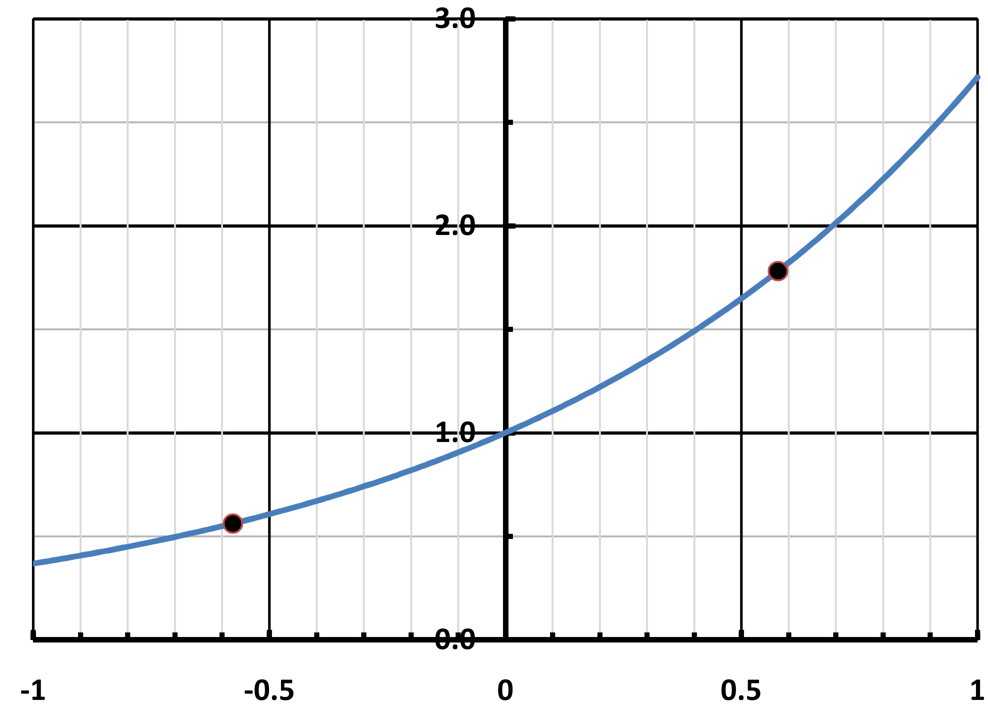
- Let the *exactly integrable polynomial* be

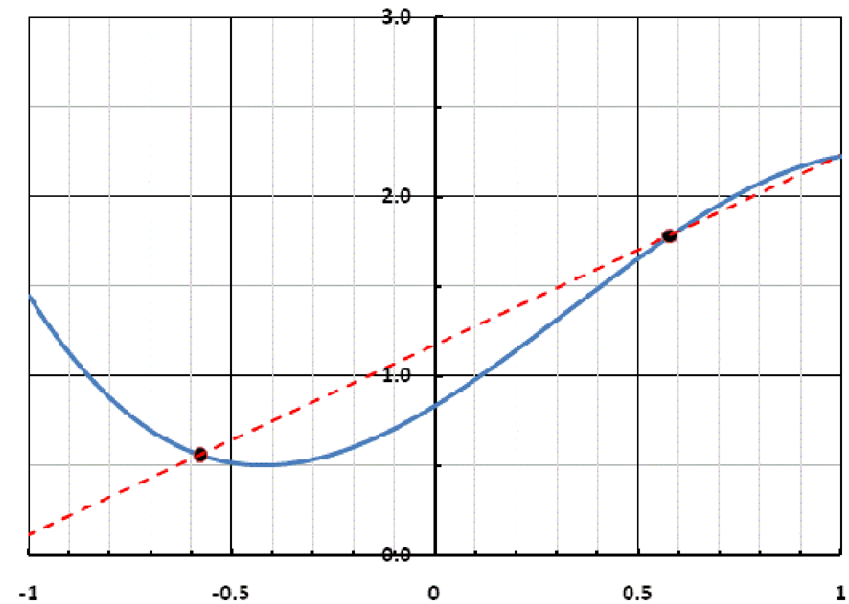
$$f_3(z) = \frac{z - z_1}{z_0 - z_1} f(z_0) + \frac{z - z_0}{z_1 - z_0} f(z_1) + (a + bz)(z - z_0)(z - z_1)$$

  a and *b* are arbitrary constants

- This function satisfies

$$f_3(z_0) = f(z_0) \quad \text{and} \quad f_3(z_1) = f(z_1)$$

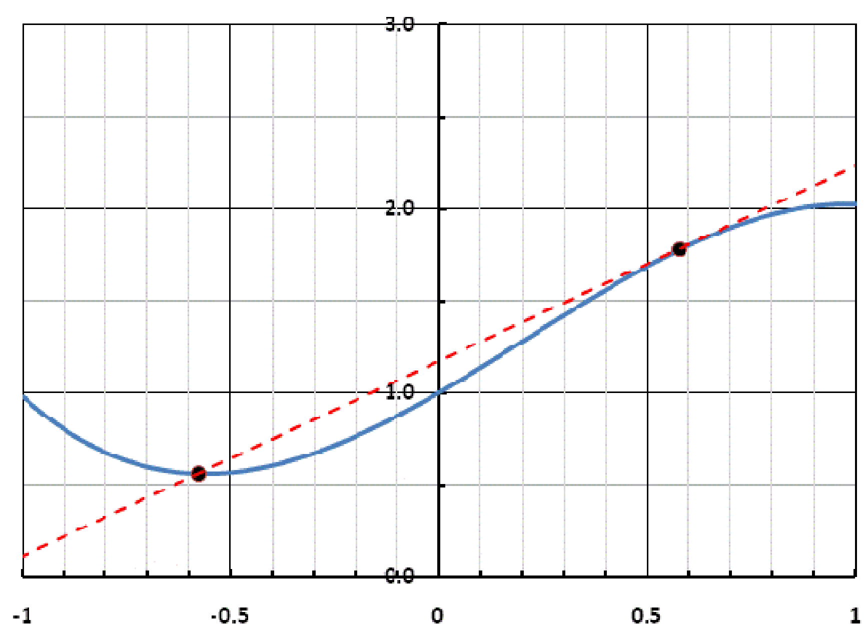




$$\int_{-1}^{1} f(z)dz \approx \widetilde{I}_z = c_0 f\left(z_0\right) + c_1 f\left(z_1\right)$$

$$f_3(z) = \frac{z - z_1}{z_0 - z_1} f(z_0) + \frac{z - z_0}{z_1 - z_0} f(z_1)$$

$$+ (a + bz)(z - z_0)(z - z_1)$$



Gauss Quadrature: General Form

- Since the cubic polynomial is exactly integrable

$$\int_{-1}^{1} \frac{z-z_1}{z_0-z_1} f(z_0) + \frac{z-z_0}{z_1-z_0} f(z_1) + (a+bz)(z-z_0)(z-z_1)\,dz$$
$$= c_0 f\left(z_0\right) + c_1 f\left(z_1\right)$$

Which implies that $c_0 = \int_{-1}^{1} \frac{z-z_1}{z_0-z_1}\,dz$ and $c_1 = \int_{-1}^{1} \frac{z-z_0}{z_1-z_0}\,dz$

And, for any arbitrary *a* and *b*:

$$\int_{-1}^{1} (a+bz)(z-z_0)(z-z_1)\,dz = 0$$

Gauss-Legendre Quadrature

- Recall the first few Legendre polynomials:

$P_0(x)=1$; $P_1(x) = x$; $P_2(x) = (-1+3x^2)/2$

$P_3(x) = (-3x+5x^3)/2$; $P_4(x) = (3-30x^2+35x^4)/8$

- Any of these is orthogonal to all lower degree polynomials. Earlier we had seen that $P_2(z)$ is orthogonal to $P_0(z)$, and $P_1(z)$, *i.e.*,

$$\int_{-1}^{1} P_2(z)P_0(z)dz = \int_{-1}^{1} P_2(z)P_1(z)dz = 0$$

- It implies that $P_2(z)$ is orthogonal to 1 and z

Gauss-Legendre Quadrature

- Therefore, if we want the quadratic $(z-z_0)(z-z_1)$ to be orthogonal to all linear functions, we should choose z_0 and z_1 as the roots of $(-1+3z^2)=0$
- Which gives us $-1/\sqrt{3}$, and $1/\sqrt{3}$
- The weights are obtained from

$$c_0 = \int_{-1}^{1} \frac{z - \frac{1}{\sqrt{3}}}{-\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}} dz = \left[\frac{z}{2} - \frac{\sqrt{3}}{4} z^2\right]_{-1}^{1} = 1 \quad \text{and} \quad c_1 = \int_{-1}^{1} \frac{z + \frac{1}{\sqrt{3}}}{\frac{1}{\sqrt{3}} + \frac{1}{\sqrt{3}}} dz = 1$$

Gauss-Legendre Quadrature

- Similarly, for three Gauss points, we need the zeroes of $(-3z+5z^3)$, which are $0, \pm\sqrt{\frac{3}{5}}$

$$L_0(z)=\frac{z\left(z-\sqrt{\frac{3}{5}}\right)}{\sqrt{\frac{3}{5}}\times 2\sqrt{\frac{3}{5}}}=-\frac{5}{6}\sqrt{\frac{3}{5}}z+\frac{5}{6}z^2;L_1(z)=1-\frac{5}{3}z^2;L_2(z)=\frac{5}{6}\sqrt{\frac{3}{5}}z+\frac{5}{6}z^2$$

$$c_0=\int_{-1}^{1}L_0(z)dz=\left[-\frac{5z^2}{12}\sqrt{\frac{3}{5}}+\frac{5}{18}z^3\right]_{-1}^{1}=\frac{5}{9};c_1=\frac{8}{9};c_2=\frac{5}{9}$$

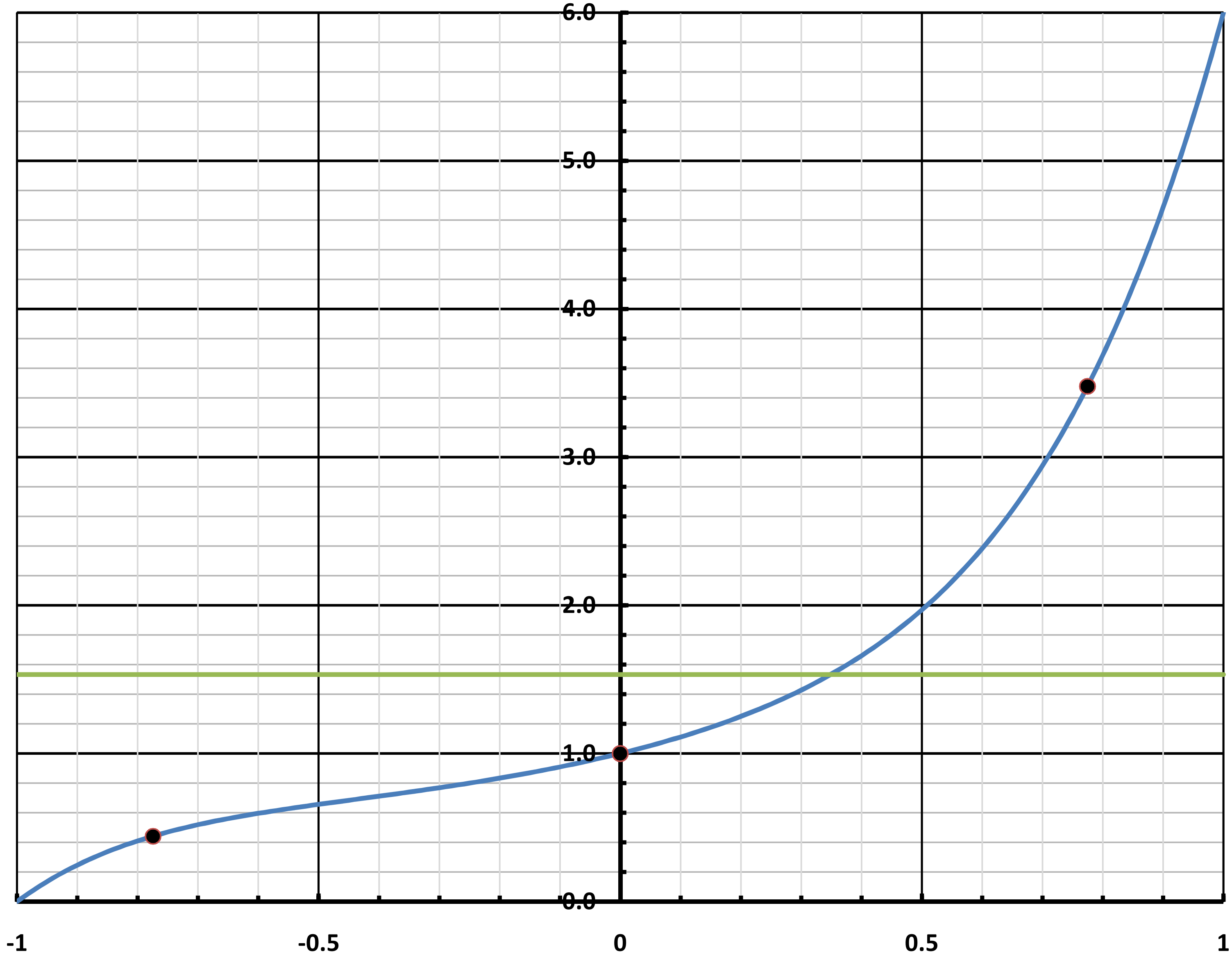
- Since the *c*'s are weights, it is common to use the symbol, W

Gauss-Legendre Quadrature Weights

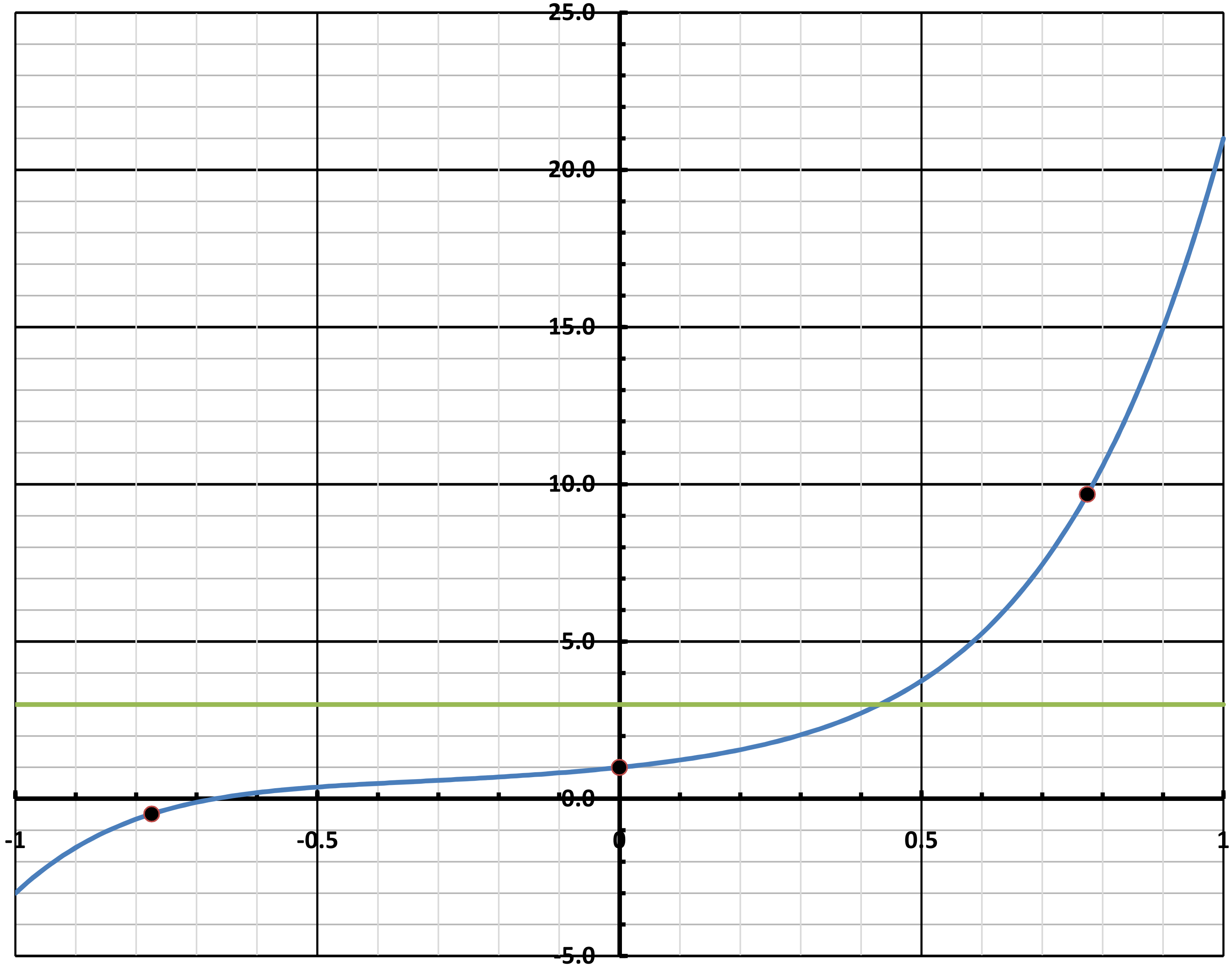
- The weights may be related to the Legendre polynomials, $P_n(z)$:

$$W_i = \frac{2\left(1 - z_i^2\right)}{\left[(n+1)P_n(z_i)\right]^2}$$

- For example, with 3 Gauss points (n=2), $P_2(z) = (-1+3z^2)/2$; the z's are $-\sqrt{0.6}$, 0, $\sqrt{0.6}$
- The value of $P_2(z)$ at these points are 0.4, -0.5, and 0.4, respectively.
- The weights are 5/9, 8/9, and 5/9, as before.



$$f(x) = 1 + x + x^2 + x^3 + x^4 + x^5$$



$$f(x) = 1 + 2x + 3x^2 + 4x^3 + 5x^4 + 6x^5$$

Abscissa, Weight, and Error for the Gauss-Legendre Quadrature points

n	Abscissa	Weight	Error
0	0.00000	2.0000	$\dfrac{f''(\xi)}{3}$
1	±0.57735	1.0000	$\dfrac{f^{iv}(\xi)}{135}$
2	0.00000	0.88889	$\dfrac{f^{vi}(\xi)}{15750}$
	±0.77460	0.55556	
3	±0.33998	0.65215	$\dfrac{f^{(8)}(\xi)}{3472875}$
	±0.86114	0.34785	
4	0.00000	0.56889	$\dfrac{f^{(10)}(\xi)}{1237732650}$
	±0.53847	0.47863	
	±0.90618	0.23693	

Weighted Gauss Quadrature

- Instead of integral of the function, we need the integral with a weight-function

$$\int_{-1}^{1} w(z) f(z) dz \approx \widetilde{I} = \sum_{i=0}^{n} W_i f(z_i)$$

- Recall the Tchebycheff polynomials, where the weight was $1/\sqrt{1-z^2}$
- Using this weight function, we get the Gauss-Tchebycheff quadrature
- Of course, we could treat *w*(*z*)*f*(*z*) as a single function and use Gauss-Legendre quadrature

Gauss-Tchebycheff quadrature

- The quadrature points are the zeroes of Tchebycheff polynomial of degree n+1
- These zeroes are given by

$$z_i = \cos\left[\frac{2n-2i+1}{n+1}\frac{\pi}{2}\right] \qquad\qquad i = 0,1,2,\ldots,n$$

- And all the weights turn out to be equal to $\pi/(n+1)$

Gauss Quadrature: Example

- Estimate $I = \int_1^2 \frac{1}{xe^x} dx$ (T.V. = 0.170483)
- First, convert to standard domain: z=2(x−1.5)
- Use 2-point Gauss-Legendre:

i	z	W	x	f
0	−1/√3	1	1.5−1/2√3	0.245849
1	1/√3	1	1.5+1/2√3	0.093467

resulting in I_z=0.339315 and I_x=0.169658

- Error in I_x = 8.25x10^{-4}. In I_z= 1.65x10^{-3}
- Recall: $E = \frac{f^{iv}(\zeta)}{135}$. 4th derivative (z) varies from 0.04 to 1.5. Theoretical error: 0.0003 to 0.011

Gauss Quadrature: Example

- Use 3-point Gauss-Legendre:

i	z	W	x	f
0	$-\sqrt{0.6}$	5/9	$1.5-\sqrt{0.6}/2$	0.295380
1	0	8/9	1.5	0.148753
2	$\sqrt{0.6}$	5/9	$1.5+\sqrt{0.6}/2$	0.080263

resulting in I_z=0.340916 and I_x=0.170458

- Error in I_x = $2.5\text{x}10^{-5}$. In I_z= $5\text{x}10^{-5}$

Gauss-Tchebycheff Quadrature: Example

- Estimate (same as before, but weighted)

$$I_z = \int_{-1}^{1} \frac{e^{-(z/2+1.5)}}{\sqrt{1-z^2}\,(z/2+1.5)}\,dz \qquad \text{(T.V. = 0.571946)}$$

- Use 2-point Gauss-Tchebycheff (n=1), $T_2(z) = 2z^2-1$; the z's are $\pm\sqrt{0.5}$:

i	z	W	x	f
0	$-1/\sqrt{2}$	$\pi/2$	$1.5-1/2\sqrt{2}$	0.277173
1	$1/\sqrt{2}$	$\pi/2$	$1.5+1/2\sqrt{2}$	0.084529

resulting in I_z=0.568160

- Error in I_z= $3.79\text{x}10^{-3}$

Gauss-Tchebycheff Quadrature: Example

- Use 3-points, $T_3(z) = 4z^3 - 3z$; the z's are $-\sqrt{0.75}, 0, \sqrt{0.75}$:

i	z	W	x	f
0	$-\sqrt{0.75}$	$\pi/3$	$1.5-\sqrt{0.75}/2$	0.322444
1	0	$\pi/3$	1.5	0.148753
2	$\sqrt{0.75}$	$\pi/3$	$1.5+\sqrt{0.75}/2$	0.074863

resulting in I_z=0.571833

- Error in I_z= 1.13×10^{-4}

Numerical Integration: Improper Integrals

- Estimate $I = \int_a^b f(x)dx$ for a known function
- We have assumed:
  - a and b are finite
  - $f(x)$ is defined and is continuous in (a,b)
- Improper Integral: When any (or both) of these assumptions is violated
- E.g.,

$$I = \int_1^\infty e^{-x^2} dx \qquad I = \int_0^1 \frac{\cos x}{\sqrt{x}} dx$$

Improper Integrals: Convergence

- An improper integral may or may not converge (i.e., have a finite value)
- We assume that it converges! How to find it?
  - If the domain is unbounded, we use a transformation of variable to make it finite

$$I = \int_1^{\infty} e^{-x^2} dx : z = \frac{1}{x} \Rightarrow I = \int_0^1 \frac{e^{-\frac{1}{z^2}}}{z^2} dz$$

  - If $f(x)$ is undefined at one end, a semi-open method could be used (or variable transform)

$$I = \int_0^1 \frac{\cos x}{\sqrt{x}} dx : z = \sqrt{x} \Rightarrow I = \int_0^1 2\cos z^2 dz$$

Improper Integrals: Evaluation

- If $f(x)$ is undefined at both ends, an open method could be used
- If $f(x)$ is undefined at some point within (a,b), we may need to split the integral into two parts
- Sometimes both the domain and the range could be unbounded. E.g.,

$$I = \int_0^{\infty} \frac{\cos x}{\sqrt{x}}\, dx$$

Improper Integrals: Example

- The complementary error function is defined as

$$erfc(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt$$

- Estimate the value of *erfc*(1) (T.V.=0.157299)
- Transformation: $y=1/t$

$$I = \int_1^{\infty} e^{-t^2} dt \Rightarrow I = \int_0^1 \frac{e^{-\frac{1}{y^2}}}{y^2} dy$$

- Note that $f(y)$ is undefined at $y=0$ (limit does exist). Trapezoidal, Simpson… cannot be used!
- Use 3-point Gauss-quadrature

Improper Integrals: Example

- 3-point Gauss-quadrature

i	z	W	y	f
0	$-\sqrt{0.6}$	5/9	$(-\sqrt{0.6}+1)/2$	0.000000
1	0	8/9	0.5	0.073263
2	$\sqrt{0.6}$	5/9	$(\sqrt{0.6}+1)/2$	0.356644

- I_z=0.263258; I_y=0.131629; erfc(1)=0.148527
- Error = 8.77×10^{-3}