§6.1 Numerical Integration

- Given *f(x)*, compute $\int_b^a f(x)dx$.
- Process is called quadrature and is usually more accurate than numerical differentiation.
- Goal: Approximate the definite integral $\int_b^a f(x)dx$ by $I = \sum_{i=0}^{n} A_i f(x_i)$.

weight

nodal abscissa

- Quadrature rules are derived from poly. interpolation of *f(x)*.

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Numerical Integration

- Two groups of rules: Newton-Coates and Gaussian Quadrature.
- Properties:

Newton-Coates	**Gaussian Quadrature**
equally-spaced abscissas	abscissas chosen to yield best accuracy
f(*x*) computed at equal intervals	f(x) may be expensive to compute
f(*x*) cheap to compute	can handle singularities, e.g.,
based on local interpolation	$\int_0^1 \frac{g(x)}{\sqrt{1-x^2}} dx.$

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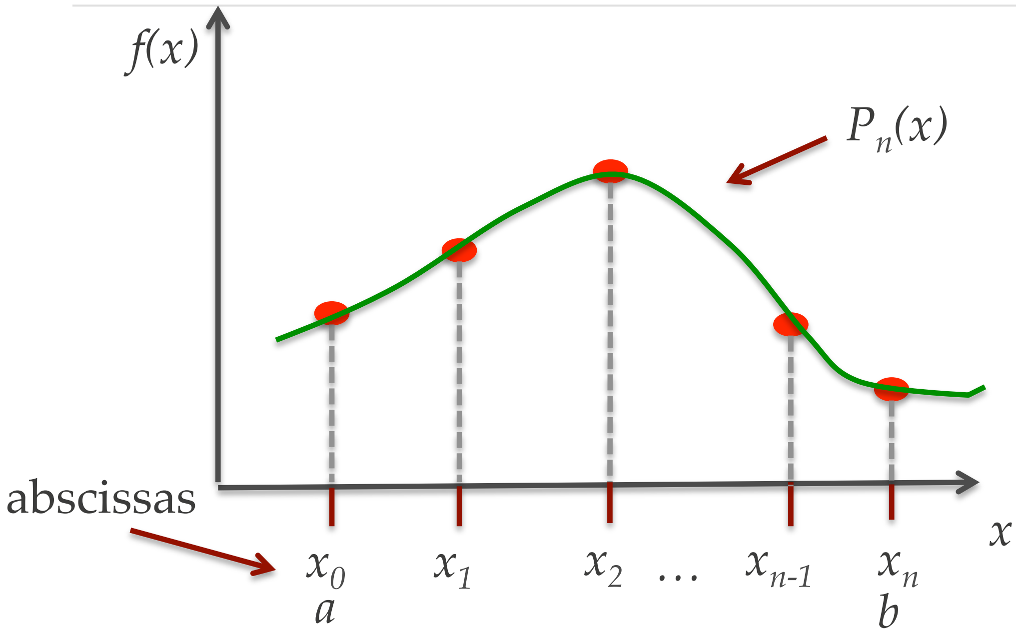
§6.2 Newton-Cotes Formulas



Use Lagrange interpolation with

$$P_n(x) = \sum_{i=0}^{n} f(x_i) l_i(x).$$

Divide (a,b) into n equal subintervals of length $h=(b-a)/n$ and construct a polynomial approx. of $f(x)$.

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Newton-Cotes Formulas

- Using Lagrange interpolation we can produce this formula:

$$I = \int_a^b P_n(x)dx = \sum_{i=0}^{n}\left[f(x_i)\int_a^b l_i(x)dx\right] = \sum_{i=0}^{n} A_i f(x_i),$$

where $A_i = \int_a^b l_i(x)dx, i = 0,1,2,\ldots,n.$

- Cases:

n=1 : Trapezoidal Rule

n=2 : Simpson's Rule

n=3 : Simpson's 3/8 Rule

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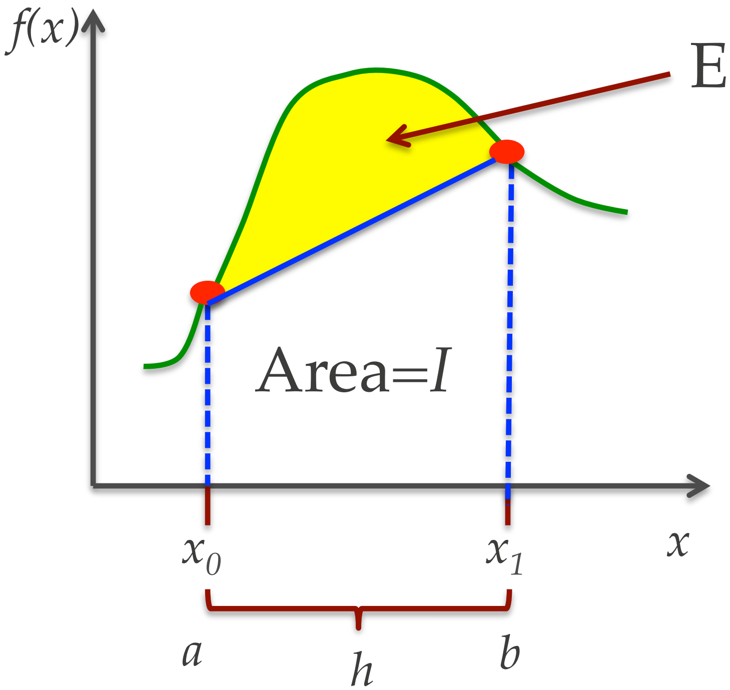
Trapezoidal Rule (n=1)



$$l_0(x) = \frac{(x - x_1)}{(x_0 - x_1)} = \frac{x - b}{-h} = \frac{-(x - b)}{h}$$

$$l_1(x) = \frac{(x - x_0)}{(x_1 - x_0)} = \frac{x - a}{h}$$

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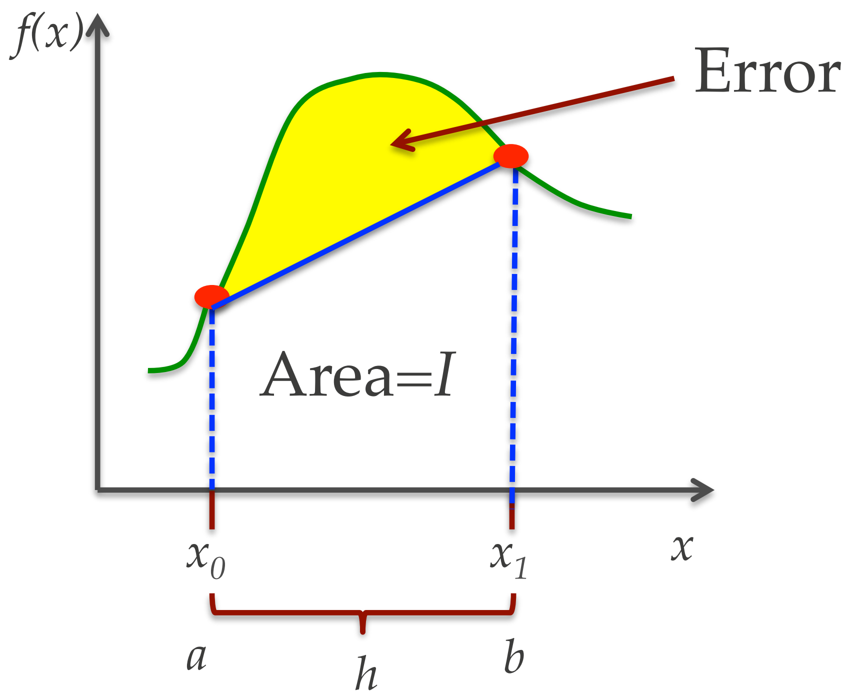
$$A_0 = \int_a^b l_0(x)dx = \frac{-1}{h}\int_a^b (x - b)dx = \frac{1}{2h}(b - a)^2 = \frac{h^2}{2h} = \frac{h}{2}.$$

Trapezoidal Rule (n=1)



$$A_1 = \int_a^b l_1(x)dx = \frac{1}{h}\int_a^b (x-a)dx$$

$$= \frac{1}{2h}(b-a)^2 = \frac{h^2}{2h} = \frac{h}{2}.$$

$$\text{So, } \quad I = \frac{h}{2}f(x_0) + \frac{h}{2}f(x_1)$$

$$= \frac{h}{2}\left[f(a) + f(b)\right].$$

What is the error for the TR?

Trapezoidal Rule (n=1)

- It can be shown that the error for the TR has the form:

$$E = \frac{-1}{12}(b-a)^3 f''(\xi) = \frac{-h^3}{12} f''(\xi),$$

where $\xi \in (a,b)$.

- So, in big-oh notation we would say ______________.

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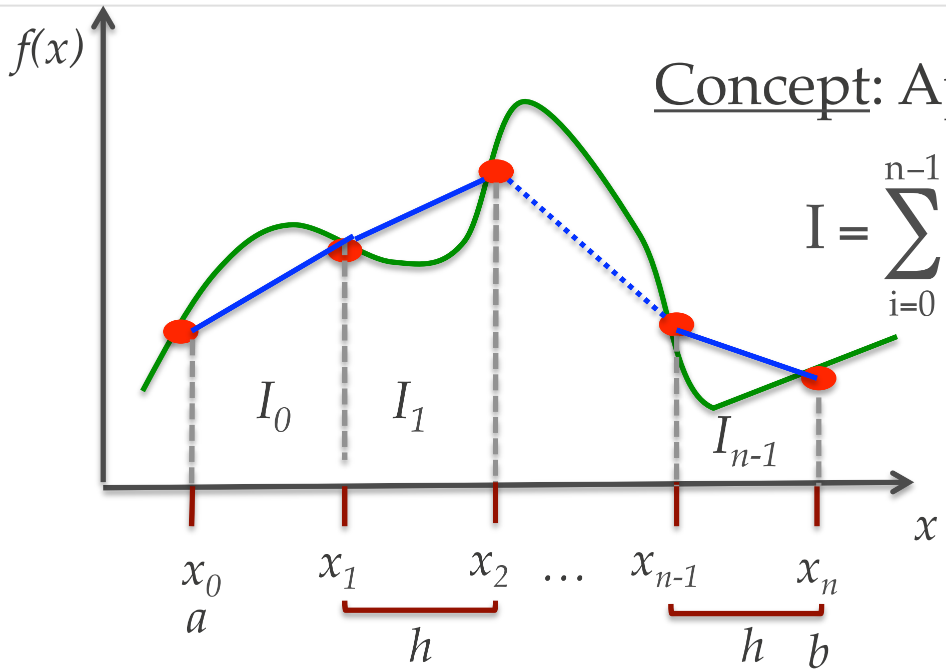
Composite Trapezoidal Rule



Concept: Apply TR in a piecewise fashion.

$$I = \sum_{i=0}^{n-1} I_i = \frac{h}{2}\begin{bmatrix} f(x_0) + 2f(x_1) + 2f(x_2) + \cdots \\ +2f(x_{n-1}) + f(x_n) \end{bmatrix}.$$

Overall error:

$$E = \frac{-(b-a)h^2}{12} f''(\xi),\ \xi \in (a,b).$$

Error in the *i*th panel: $E_i = \dfrac{-h^3}{12} f''(\xi_i),\ \xi_i \in (x_i, x_{i+1}).$

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Sample Problem

- **Problem #2**, Problem Set 6.1 (p. 212):
  Power P is supplied to the driving wheels of a car as a function of its speed v. If the mass of the car is m=2,000 kg, determine the time Δt it takes for the car to accelerate from 1m/s to 6m/s.
- Via Newton's Law $F = m\frac{dv}{dt}$ and the definition of power (P=Fv), we can define:

$$\Delta t = m\int_{1s}^{6s}\left(\frac{v}{p}\right)dv.$$

  Now we need data points to interpolate!

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Sample Problem

- Here is the recorded data for composite TR:

i	0	1	2	3	4	5	6
v_i (m/s)	1.0	1.8	2.4	3.5	4.4	5.1	6.0
p_i (kW)	4.7	12.2	19.0	31.8	40.1	43.8	43.2
$(v/p)_i$ kN^{-1}	0.2128	0.1475	0.1263	0.1101	0.1097	0.1164	0.1389

$$I = \int_1^6 (v/p)\,dv \approx \frac{1}{2}\sum_{i=0}^{5}\left[(v/p)_i + (v/p)_{i+1}\right](v_{i+1} - v_i)$$

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Recursive Trapezoidal Rule

- Let I_k be the integral approximation computed by the Composite Trapezoidal Rule (CRT) using 2^{k-1} panels. If k is incremented by 1, the number of panels is ____________; let $H=b-a$.

k (2^{k-1} panels)	I_k
1	$\left[f(a)+f(b)\right]\frac{H}{2}$
2	$\left[f(a)+2f\left(a+\frac{H}{2}\right)a+f(b)\right]\frac{H}{4}=\frac{1}{2}I_1+f\left(a+\frac{H}{2}\right)\frac{H}{2}$
3	$\frac{1}{2}I_2+\left[f\left(a+\frac{H}{4}\right)+f\left(a+\frac{3H}{4}\right)\right]\frac{H}{4}$
k	$\frac{1}{2}I_{k-1}+\frac{H}{2^{k-1}}\sum_{i=1}^{2^{k-2}}f\left[a+\frac{(2i-1)H}{2^{k-1}}\right], k=2,3,\ldots$

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Recursive Trapezoidal Rule

- The general form is $I(h) = \frac{1}{2} I(2h) + h \sum f(x_{new}), h = H/n$. ($h$ is the panel width)
- The advantage of this method is that you can monitor the convergence by comparing the difference in values obtained from I_{k-1} to I_k.
- See **`trapezoid.py`** on p. 203 of the textbook.

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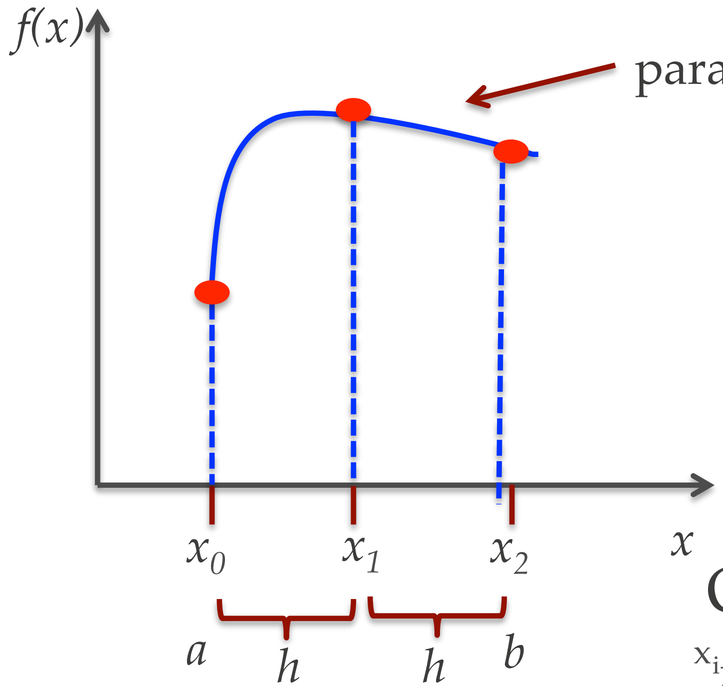
Simpson's Rule (n=2)



$$I = \left[f(a) + 4f\left((a+b)/2\right) + f(b)\right]\frac{h}{3}$$

For Composite Simpson's Rule, divide (a,b) into n panels, where n is even and h=(b-a)/n.

On adjacent panels, we would have:

$$\int_{x_i}^{x_{i+2}} f(x)\,dx \approx \left[f(x_i) + 4f(x_{i+1}) + f(x_{i+2})\right]\frac{h}{3}.$$

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Composite Simpson's Rule

- Integrating across the entire interval we would have:

$$\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx = \sum_{i=0,2,\ldots}^{n}\left[\int_{x_i}^{x_{i+2}} f(x)dx\right].$$

- So, applying Simpson's Rule on each pair of adjacent subintervals yields:

$$\int_a^b f(x)dx \approx I = \frac{h}{3}\left[\begin{array}{l} f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+\cdots \\ \cdots+2f(x_{n-2})+4f(x_{n-1})+f(x_n) \end{array}\right]$$

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Composite Simpson's Rule

- Composite Simpson's Rule:

$$\int_a^b f(x)\,dx \approx I = \frac{h}{3}\begin{bmatrix} f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+\cdots \\ \cdots+2f(x_{n-2})+4f(x_{n-1})+f(x_n) \end{bmatrix}$$

- Error: $E = \dfrac{(b-a)h^4}{180} f^{(iv)}(\xi).$

This means that the rule is exact if *f(x)* is a polynomial of degree ≤ ______.

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§6.4 Romberg Integration

- Combination of Trapezoidal Rule and Richardson extrapolation.
- Let $R_{i,1}=I_1$, where I_i approximates $\int_b^a f(x)dx$ using the Trapezoidal Rule with 2^{i-1} panels. The error in I_i is given by $E = c_1h^2 + c_2h^4 + \cdots$ for $h=(b-a)/2^{i-1}$ (panel width).
- We start with $R_{1,1}=I_1$ (1 panel) and $R_{2,1}=I_2$ (2 panels).

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Romberg Integration

- Then, we compute $R_{2,2}$ as defined below to eliminate the leading error term ($c_1 h^2$) via Richardson's extrapolation:

Error is $O(h^2)$

$$R_{2,2} = \frac{2^2 R_{2,1} - R_{1,1}}{2^2 - 1} = \frac{4}{3} R_{2,1} - \frac{1}{3} R_{1,1}.$$

Error is $O(h^4)$

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Romberg Integration

- Continuing with 4 panels we compute we compute $R_{3,1}=I_3$ and repeat Richardson's extrapolation:

$$R_{3,2} = \frac{4}{3}R_{3,1} - \frac{1}{3}R_{2,1}\,.$$

Array of results:

$$\begin{bmatrix} R_{1,1} & \\ R_{2,1} & R_{2,2} \\ R_{3,1} & R_{3,2} \end{bmatrix}$$

Results with error having c_2h^4 leading term

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Romberg Integration

- Applying Richardson's extrapolation with $R_{3,2}$ and $R_{2,2}$ we produce:

$$R_{3,3} = \frac{2^4 R_{3,2} - R_{2,2}}{2^4 - 1} = \frac{16}{15} R_{3,2} - \frac{1}{15} R_{2,2}.$$

So, the error in $R_{3,3}$ is now $O(h^6)$, and the array of results becomes:

$$\begin{bmatrix} R_{1,1} & & \\ R_{2,1} & R_{2,2} & \\ R_{3,1} & R_{3,2} & R_{3,3} \end{bmatrix}$$

Error: $O(h^2)$ $O(h^4)$ $O(h^6)$

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Romberg Integration

- Let's go another round of Richardson's extrapolation with $R_{4,3}$ and $R_{3,3}$ to produce:

$$R_{4,4} = \frac{2^6 R_{4,3} - R_{3,3}}{2^6 - 1} = \frac{64}{63} R_{4,3} - \frac{1}{63} R_{3,3}.$$

Error in $R_{4,4}$ is now $O(h^8)$!

Process is **terminated** when diff. between two successive diagonal terms is sufficiently small.

$$\begin{array}{cc}
 & \begin{bmatrix} R_{1,1} & & & \\ R_{2,1} & R_{2,2} & & \\ R_{3,1} & R_{3,2} & R_{3,3} & \\ R_{4,1} & R_{4,2} & R_{4,3} & R_{4,4} \end{bmatrix} \\
\text{Error:} & \begin{matrix} O(h^2) & O(h^4) & O(h^6) & O(h^8) \end{matrix}
\end{array}$$

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Romberg Integration

- General extrapolation formula:

$$R_{i,j} = \frac{4^{j-1} R_{i,j-1} - R_{i-1,j-1}}{4^{j-1} - 1}, i > 1, j = 2,3,\ldots,i.$$

- See `romberg.py` (pp. 209-210) for implementation and Example 6.7 (pp. 211-212) for an approximation to $\int_0^{\sqrt{\pi}} 2x^2 \cos x^2 \, dx.$

```
I,n=romberg(f,0,sqrt(pi))
def f(x):
   return 2.0*(x**2)*cos(x**2)
```

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§6.4 Gaussian Integration

- Good for estimating integrals of the form.

$$\int_b^a w(x)f(x)dx.$$

weighting function

- For $I = \sum_{i=0}^{n} A_i f(x_i),$

choose A_i's and x_i's so that the rule is exact for $f(x)$ a polynomial of degree $2n+1$ or less, i.e.,

$$\int_a^b w(x)P_m(x)dx = \sum_{i=0}^{n} A_i P_m(x_i), \ m \le 2n+1.$$

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Gaussian Integration

- How can we determine the A_i's and x_i's ?

$$\int_a^b w(x)P_m(x)dx = \sum_{i=0}^{n} A_i P_m(x_i),\ m \le 2n+1.$$

Suppose $P_0(x) = 1$ so that $\int_a^b w(x)x^j dx =$

$P_1(x) = x$

$$\sum_{i=0}^{n} A_i x_i^j,\ j = 0,1,2,\ldots,2n+1.$$

$P_2(x) = x^2$

$\vdots$

$P_{2n+1}(x) = x^{2n+1}$

Q: How many equations and how many unknowns?

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Gaussian Integration

- Example: $w(x)=e^{-x}$, $a=0$, $b=\infty$, and $n=1$.

$$1=\int_0^\infty e^{-x}\,dx = A_0 + A_1$$

$$1=\int_0^\infty e^{-x}x\,dx = A_0x_0 + A_1x_1$$

$$2=\int_0^\infty e^{-x}x^2\,dx = A_0x_0^2 + A_1x_1^2$$

$$6=\int_0^\infty e^{-x}x^3\,dx = A_0x_0^3 + A_1x_1^3$$

$$A_0x_0 + A_1x_1 = 1$$

$$A_0x_0 + A_1x_1 = 1$$

$$A_0x_0^2 + A_1x_1^2 = 2$$

$$A_0x_0^3 + A_1x_1^3 = 6$$

Solve nonlinear system for A_is and x_is.

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Gaussian Integration

- Example: $w(x)=e^{-x}$, $a=0$, $b=\infty$, and $n=1$.

$$x_0 = 2-\sqrt{2}$$

$$x_1 = 2+\sqrt{2}$$

$$A_0 = \frac{\sqrt{2}+1}{2\sqrt{2}}$$

$$A_1 = \frac{\sqrt{2-1}}{2\sqrt{2}}$$

So integration formula becomes…

$$\int_0^\infty e^{-x} f(x)\,dx \approx$$

$$\frac{1}{2\sqrt{2}}\left[(\sqrt{2}+1)f(2-\sqrt{2})+(\sqrt{2}-1)f(2+\sqrt{2})\right]$$

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Gaussian Integration

- Truncation error in Gaussian Quadrature:

$$E = \int_a^b w(x)f(x)\,dx - \sum_{i=0}^{n} A_i f(x_i)$$

$$= K(n) \cdot f^{(2n+2)}(c), \text{for } a < c < b.$$

This term depends on the quadrature rule.

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Gauss-Legendre Quadrature

- Rule:

$$\int_{-1}^{1} f(\xi)\,d\xi \approx \sum_{i=0}^{n} A_i f(\xi_i)$$

- Nodes are symmetric about $\xi = 0$.
- See Table of weights and abscissas on p. 217 (provided on next slide also).

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Gauss-Legendre Quadrature

- Nodes and Abscissas for G-L Quad. Rule:

$n = 1$

$$\xi_0 = 0.577350,\ A_0 = 1.0$$
$$\xi_1 = -0.577350,\ A_1 = 1.0$$

$n = 2$

$$\xi_0 = 0.0,\qquad A_0 = 0.888889$$
$$\xi_1 = 0.774597,\ A_1 = 0.555556$$
$$\xi_2 = -0.774597,\ A_2 = 0.555556$$

$n = 3$

$$\xi_0 = 0.339981,\ A_0 = 0.652145$$
$$\xi_1 = -0.339981,\ A_1 = 0.652145$$
$$\xi_2 = 0.861136,\ A_2 = 0.347855$$
$$\xi_3 = -0.861136,\ A_3 = 0.347855$$

(These values would be hardcoded in software.)

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Gauss-Legendre Quadrature

- How do you apply the GL rule below to $\int_a^b f(x)\,dx$?

$$\int_{-1}^{1} f(\xi)\,d\xi \approx \sum_{i=0}^{n} A_i f(\xi_i)$$

- Have to map (*a*,*b*) into (-*1*,*1*) first.
- Transformation: $x = \frac{b+a}{2} + \frac{b-a}{2}\xi$

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Gauss-Legendre Quadrature

- If $x = \frac{b+a}{2} + \frac{b-a}{2}\xi$, then $dx = d\xi\left(\frac{b-a}{2}\right)$,

  or, $d\xi = \left(\frac{2}{b-a}\right)dx.$

x

- Check mapping: $\xi = -1 \Rightarrow x = ?$

  $\xi = +1 \Rightarrow x = ?$

weights from G-L table

$$x_i = \frac{b+a}{2} + \frac{b-a}{2}\xi_i$$

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2}\sum_{i=0}^{n} A_i f(x_i)$$

Gaussian Integration

- Truncation error using G-L on $\int_a^b f(x)\,dx$:

$$E = \frac{(b-a)^{2n+3}[(n+1)!]^4}{(2n+3)[(2n+2)!]^3} f^{(2n+2)}(c), \text{for } a < c < b.$$

Recall desired accuracy of Gaussian Quadrature rules.

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Other GQ Rules

- Gauss-Chebyshev Quadrature:

$$\int_{-1}^{1}(1-x^2)^{-1/2} f(x)\,dx \approx \frac{\pi}{n+1}\sum_{i=0}^{n} A_i f(\xi_i),$$

$$A_i = \frac{\pi}{n+1}, \xi_i = \cos\left(\frac{(2i+1)\pi}{2n+2}\right).$$

- Truncation error:

$$E = \frac{2\pi}{2^{2n+2}(2n+2)!} f^{(2n+2)}(c), \text{for } -1 < c < 1.$$

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Other GQ Rules

- Gauss-Laguerre Quadrature: $$\int_0^\infty e^{-x} f(x)\,dx \approx \sum_{i=0}^{n} A_i f(\xi_i).$$

- See Table 6.4 (p. 223) for weights and abscissas.

- Truncation error: $$E = \frac{[(n+1)!]^2}{(2n+2)!} f^{(2n+2)}(c), \text{for } 0 < c < \infty.$$

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Other GQ Rules

- Gauss-Hermite Quadrature: $$\int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx \approx \sum_{i=0}^{n} A_i f(\xi_i).$$
- See Table 6.5 (p. 223) for weights and abscissas.
- Truncation error: $$E = \frac{\sqrt{\pi}(n+1)!}{2^2(2n+2)!} f^{(2n+2)}(c), \text{for} -\infty < c < \infty.$$

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Other GQ Rules

- Gauss Quadrature with Logarithmic Singularity: $$\int_0^1 \ln(x) f(x)\,dx \approx -\sum_{i=0}^{n} A_i f(\xi_i).$$
- See Table 6.6 (p. 224) for weights and abscissas.
- Truncation error: $$E = \frac{K(n)}{(2n+1)!} f^{(2n+1)}(c), \text{for } 0 < c < 1,$$ $$K(1) = 0.00285, K(2) = 0.00017, K(3) = 0.00001.$$

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GQ Examples

- Python function calls (see pp. 225-226):

```
x,A=gaussNodes(m,tol=1.E-9)
I=gaussQuad(f,a,b,m)
```

- Example 6.11 (pp. 228-229); determine how many nodes are required to evaluate $\int_0^{\pi} (\sin x / x)^2 dx$ with Gauss-Legendre quadrature to six decimal places? [Exact integral is 1.41815.]

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GQ Examples

- Problem 1 (Problem Set 6.2) on p. 230; evaluate $\int_1^{\pi} \frac{\ln x}{x^2 - 2x + 2} dx$ using Gauss-Legendre quadrature.

(a) Use 2 nodes

(b) Use 4 nodes

$$f(x) = \frac{\ln x}{x^2 - 2x + 2}, \; I = \int_1^{\pi} f(x)\,dx$$

$$x_i = \frac{b+a}{2} + \frac{b-a}{2}\xi_i, \; I \approx \frac{b-a}{2}\sum_{i=0}^{n} A_i f(x_i)$$

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GQ Examples

(a) Use 2 nodes:

$$x_0 = \frac{\pi+1}{2} + \frac{\pi-1}{2}(-0.577350) = 1.452572$$

$$x_1 = \frac{\pi+1}{2} + \frac{\pi-1}{2}(+0.577350) = 2.689021$$

$$A_0 = A_1 = 1$$

$$I \approx \frac{\pi-1}{2}(\underbrace{0.256743}_{f(x_o)} + \underbrace{0.309868}_{f(x_1)}) = 0.6067$$

GQ Examples

(b) Use 4 nodes:

$$x_0 = \frac{\pi+1}{2} + \frac{\pi-1}{2}(-0.861136) = 1.148695; A_0 = 0.347855$$

$$x_1 = \frac{\pi+1}{2} + \frac{\pi-1}{2}(-0.339981) = 1.706746; A_1 = 0.652145$$

$$x_2 = \frac{\pi+1}{2} + \frac{\pi-1}{2}(+0.339981) = 2.434847; A_2 = 0.652145$$

$$x3 = \frac{\pi+1}{2} + \frac{\pi-1}{2}(+0.861136) = 2.992898; A_3 = 0.347855$$

$$I \approx \frac{\pi-1}{2}(0.546107) = 0.5848$$

GQ Examples

- Problem 6 (Problem Set 6.2) on p. 230; evaluate $\int_0^1 \frac{2x+1}{\sqrt{x(1-x)}}dx$ using Gauss-Chebyshev quadrature.

$$x = \frac{(1+t)}{2},\ dx = \frac{dt}{2}, I = \int_{-1}^{1} \frac{2+t}{\sqrt{1-t^2}}dt.$$

Linear in *t* so GC will be exact for a single node!

$$\text{So, } I = \int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}}dt, f(t) = 2+t\,; I \approx \frac{\pi}{n+1}\sum_{i=0}^{n} f(t_i), t_i = \frac{\cos(2i+1)\pi}{2n+2}$$

$$I \approx \pi f(\cos(\pi/2)) = \pi(2+0) = 2\pi$$

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