

Midterm Exam: Oct. 18, in class

- ▶ covers material up to and include §4.5 (six questions total)
 - ▶ one question each from chapters 1 and 4
 - ▶ two questions each from chapters 2 and 3

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- ▶ Sample exams will be provided, solutions will be available

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- ▶ Sample exams will be provided, solutions will be available
- ▶ one page cheat sheet on one side only
- ▶ You can skip the exam, but this is NOT encouraged
 - ▶ Final worth 50 (as opposed to 30) points if you do skip.
 - ▶ If you submit the exam, it WILL count.



Sample exam problem

- ▶ How many multiplications and additions are required to determine a sum of the form

$$S \stackrel{\text{def}}{=} \sum_{i=1}^n \sum_{j=1}^m \alpha_i \beta_j \quad (1)$$

- ▶ Modify the sum in part (1) to an equivalent form that reduces the number of computations.

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- ▶ Modify the sum in part (1) to an equivalent form that reduces the number of computations.

SOLUTION:

- ▶ it takes $m n$ multiplications and $m n$ additions in (1).
- ▶ Rewrite

$$S \stackrel{\text{def}}{=} \left(\sum_{i=1}^n \alpha_i \right) \left(\sum_{j=1}^m \beta_j \right)$$

it takes 1 multiplication and $m + n$ additions.

Sample exam problem

The following two methods are proposed to compute $7^{1/5}$.
Discuss their orders of convergence, assuming $p_0 = 1$.

1. $p_{n+1} = p_n - \frac{p_n^5 - 7}{5p_n^4}$

2. $p_{n+1} = p_n - \frac{p_n^5 - 7}{100}$

Sample exam problem

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2. $p_{n+1} = p_n - \frac{p_n^5 - 7}{100}$

SOLUTION:

1. Newton's method, quadratic convergence.
2. fixed point iteration, linear convergence.

Sample exam problem

A quadratic spline interpolating function S defined with the nodes $x_0 < x_1 < x_2$ is such that S is a quadratic polynomial on each of the intervals $[x_0, x_1]$ and $[x_1, x_2]$, respectively. Assume that $S(x) \in C^2[x_0, x_2]$. Show that S must be a quadratic polynomial on the entire interval $[x_0, x_2]$.

Sample exam problem

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SOLUTION: Parameterize S as

$$S(x) = \begin{cases} a_0 + b_0 (x - x_1) + c_0 (x - x_1)^2, & \text{if } x \in [x_0, x_1], \\ a_1 + b_1 (x - x_1) + c_1 (x - x_1)^2, & \text{if } x \in [x_1, x_2]. \end{cases}$$

The condition that $S(x) \in C^2[x_0, x_2]$ implies that

$$S(x) \Big|_{x=x_1^-} = S(x) \Big|_{x=x_1^+}, \quad S(x)' \Big|_{x=x_1^-} = S(x)' \Big|_{x=x_1^+}, \quad S(x)'' \Big|_{x=x_1^-} = S(x)'' \Big|_{x=x_1^+}$$

This leads to

$$a_0 = a_1, \quad b_0 = b_1, \quad c_0 = c_1$$

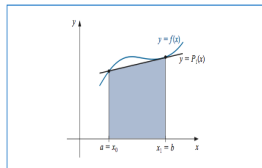
§4.3 The Trapezoidal Rule (Review) $n = 1, h = b - a$

$$\textbf{Quadrature} \quad \int_a^b f(x) dx = \frac{h}{2} (f(a) + f(b)).$$

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$$\text{Quadrature} \quad \int_a^b f(x) dx = \frac{h}{2} (f(a) + f(b)).$$

$$\begin{aligned} \text{error} &= \int_a^b \frac{1}{2} f''(\xi(x)) (x-a)(x-b) dx \\ &= \frac{f''(\xi)}{2} \int_a^b (x-a)(x-b) dx \\ &= -\frac{f''(\xi)}{12} (b-a)^3 \end{aligned}$$



Simpson's Rule: $n = 2$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

► **Quadratic Interpolation:**

$$P_2(x_j) = f(x_j), \quad j = 0, 1, 2.$$

$$\begin{aligned} P_2(x) = & \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_1)(x - x_0)}{(x_2 - x_1)(x_2 - x_0)} f(x_2) \\ & + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) \end{aligned}$$

$$f(x) = P_2(x) + \frac{1}{3!} f^{(4)}(\xi(x))(x - x_0)(x - x_1)(x - x_2)$$

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► **Simpson's Rule:**

$$\int_a^b f(x) dx = \int_a^b P_2(x) dx + \int_a^b \left(\frac{1}{3!} f^{(4)}(\xi(x))(x - x_0)(x - x_1)(x - x_2) \right) dx$$

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Requires special error analysis

Simpson's Rule: $n = 3$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

► **Cubic Interpolation** with double node in x_1 :

$$P_3(x_j) = f(x_j), \quad j = 0, 1, 2; \quad P'_3(x_1) = f'(x_1).$$

$$\begin{aligned} P_3(x) = & \frac{(x - x_1)^2(x - x_2)}{(x_0 - x_1)^2(x_0 - x_2)} f(x_0) + \frac{(x - x_1)^2(x - x_0)}{(x_2 - x_1)^2(x_2 - x_0)} f(x_2) \\ & + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \left(1 - \frac{(x - x_1)(2x_1 - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} \right) f(x_1) \\ & + \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f'(x_1). \end{aligned}$$

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► **Interpolation error:**

$$f(x) = P_3(x) + \frac{1}{4!} f^{(4)}(\xi(x))(x - x_0)(x - x_1)^2(x - x_2)$$

Simpson's Rule: $n = 3$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

► **Quadrature Rule**

$$\begin{aligned}\int_a^b P_3(x) dx &= f(x_0) \int_a^b \frac{(x-x_1)^2(x-x_2)}{(x_0-x_1)^2(x_0-x_2)} dx + f(x_2) \int_a^b \frac{(x-x_1)^2(x-x_0)}{(x_2-x_1)^2(x_2-x_0)} dx \\ &\quad + f(x_1) \int_a^b \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \left(1 - \frac{(x-x_1)(2x_1-x_0-x_2)}{(x_1-x_0)(x_1-x_2)} \right) dx \\ &\quad + f'(x_1) \int_a^b \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_1-x_0)(x_1-x_2)} dx\end{aligned}$$

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Stroke of luck: $f'(x_1)$ does not end up in quadrature

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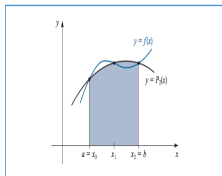
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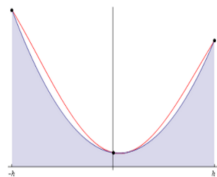
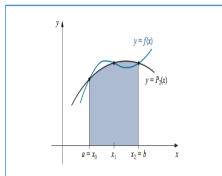
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Book wrong (middle): $f'(x_1) \neq P'(x_1)$

Correct plot (right): $f'(x_1) = P'(x_1)$

Example: approximate $\int_0^2 f(x)dx$: Simpson wins

	(a)	(b)	(c)	(d)	(e)	(f)
$f(x)$	x^2	x^4	$(x+1)^{-1}$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

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DoP = 1 for Trapezoidal Rule, **DoP** = 3 for Simpson.

§4.4 Simpson's Rule

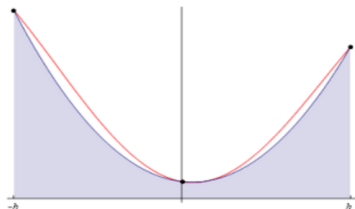
$$\int_a^b f(x) dx = \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2)) - \frac{f^{(4)}(\xi)}{90} h^5.$$



DoP = 3: $f^{(4)}(\xi) = 0$ for $f(x) = 1, x, x^2, x^3$

§4.4 Simpson's Rule

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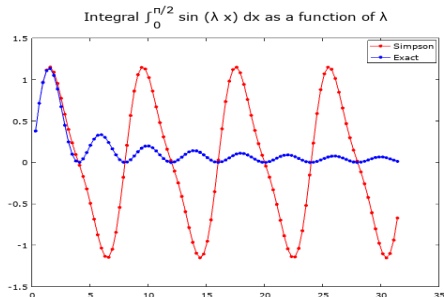
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► Example:

$$\begin{aligned} \int_0^{\pi/2} \sin \lambda x \, dx &= -\frac{1}{\lambda} \int_0^{\pi/2} d \cos \lambda x \\ &= \frac{1}{\lambda} (1 - \cos \lambda \pi/2) \end{aligned}$$

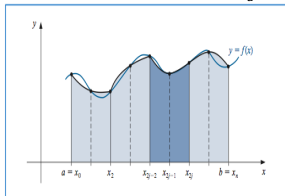
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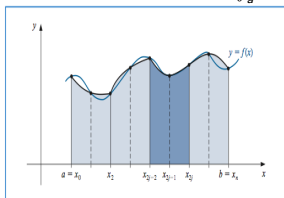


Composite Simpson's Rule ($n = 2m, x_j = a + jh, h = \frac{b-a}{n}, 0 \leq j \leq n$)

$$\int_a^b f(x) dx = \sum_{j=1}^m \int_{x_{2(j-1)}}^{x_{2j}} f(x) dx$$



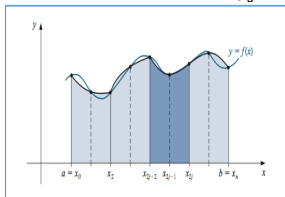
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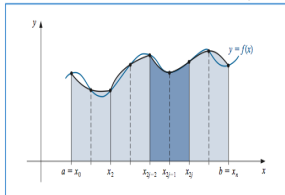
$$= \sum_{j=1}^m \left(\frac{h}{3} \left(f(x_{2(j-1)}) + 4f(x_{2j-1}) + f(x_{2j}) \right) - \frac{f^{(4)}(\xi_j)}{90} h^5 \right)$$

Composite Simpson's Rule ($n = 2m, x_j = a + jh, h = \frac{b-a}{n}, 0 \leq j \leq n$)



$$\begin{aligned}
 \int_a^b f(x) dx &= \sum_{j=1}^m \int_{x_{2(j-1)}}^{x_{2j}} f(x) dx \\
 &= \sum_{j=1}^m \left(\frac{h}{3} (f(x_{2(j-1)}) + 4f(x_{2j-1}) + f(x_{2j})) - \frac{f^{(4)}(\xi_j)}{90} h^5 \right) \\
 &= \frac{h}{3} \left(f(a) + 2 \sum_{j=1}^{m-1} f(x_{2j}) + 4 \sum_{j=1}^m f(x_{2j-1}) + f(b) \right) - \frac{h^5}{90} \sum_{j=1}^m f^{(4)}(\xi_j)
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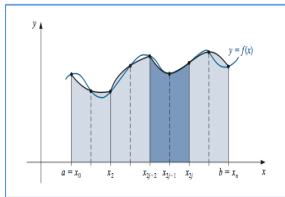
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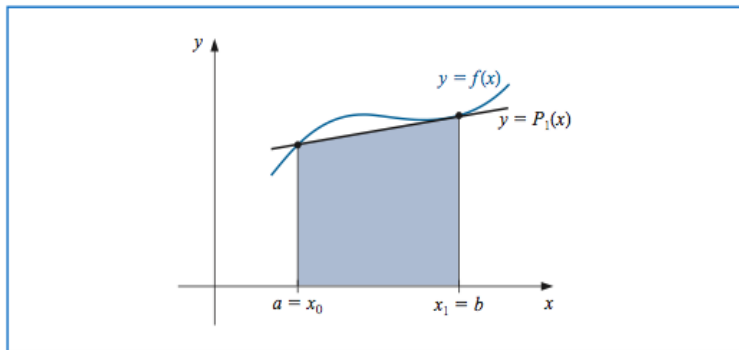
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 \end{aligned}$$

Trapezoidal Rule: $n = 1$, $x_0 = a$, $x_1 = b$, $h = b - a$.

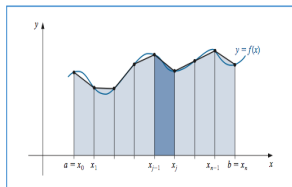
$$\int_a^b f(x) dx = \frac{h}{2} (f(x_0) + f(x_1)) - \frac{f''(\xi)}{12} h^3.$$



Degree of precision = 1: $f''(\xi) = 0$ for $f(x) = 1, x$

Composite Trapezoidal Rule ($x_j = a + j h, h = \frac{b-a}{n}, 0 \leq j \leq n$)

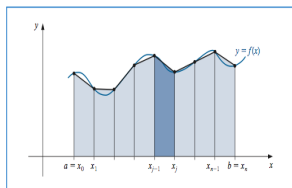
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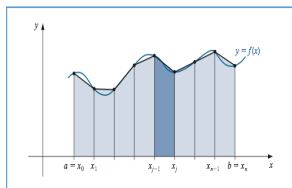
$$= \sum_{j=1}^n \left(\frac{h}{2} (f(x_{j-1}) + f(x_j)) - \frac{f''(\xi_j)}{12} h^3 \right)$$



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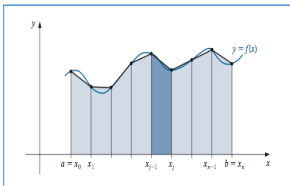
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FOR THE SAME WORK, COMPOSITE SIMPSON YIELDS
TWICE AS MANY CORRECT DIGITS.

Composite Simpson's Rule, example

Determine values of h for an approximation error $\leq \epsilon = 10^{-5}$ when approximating $\int_0^\pi \sin(x) dx$ with Composite Simpson.

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Choosing

$$\frac{\pi^5}{180n^4} \leq \epsilon, \quad \text{leading to} \quad n \geq \pi \left(\frac{\pi}{180\epsilon} \right)^{\frac{1}{4}} \approx 20.3.$$

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$$\begin{aligned} 2 &= \int_0^\pi \sin(x) dx \approx \frac{\pi}{3 \times 22} \left(2 \sum_{j=1}^{10} \sin\left(\frac{j\pi}{11}\right) + 4 \sum_{j=1}^{11} \sin\left(\frac{(2j-1)\pi}{22}\right) \right) \\ &\approx 2.0000046. \end{aligned}$$

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$$\left(\text{Trapezoidal: } \int_0^\pi \sin(x) dx \approx \frac{\pi}{2 \times 22} \left(2 \sum_{j=1}^{21} \sin\left(\frac{j\pi}{22}\right) \right) \approx 1.9966 \right)$$

Composite Simpson's Rule: Round-Off Error Stability

$(n = 2m, x_j = a + j h, h = \frac{b-a}{n}, 0 \leq j \leq n)$

$$\int_a^b f(x) dx \approx \frac{h}{3} \left(f(a) + 2 \sum_{j=1}^{m-1} f(x_{2j}) + 4 \sum_{j=1}^m f(x_{2j-1}) + f(b) \right)$$
$$\stackrel{\text{def}}{=} \mathcal{I}(f).$$

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Assume round-off error model:

$$f(x_i) = \widehat{f}(x_i) + e_i, \quad |e_i| \leq \epsilon, \quad i = 0, 1, \dots, n.$$

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Assume round-off error model:

$$f(x_i) = \hat{f}(x_i) + e_i, \quad |e_i| \leq \epsilon, \quad i = 0, 1, \dots, n.$$

$$\mathcal{I}(f) = \mathcal{I}(\hat{f}) + \frac{h}{3} \left(e_0 + 2 \sum_{j=1}^{m-1} e_{2j} + 4 \sum_{j=1}^m e_{2j-1} + e_n \right).$$

$$|\mathcal{I}(f) - \mathcal{I}(\hat{f})| \leq \frac{h}{3} \left(|e_0| + 2 \sum_{j=1}^{m-1} |e_{2j}| + 4 \sum_{j=1}^m |e_{2j-1}| + |e_n| \right) \\ \leq h n \epsilon = (b-a) \epsilon \quad (\text{numerically stable!!!})$$

§4.5 Recursive Composite Trapezoidal: with

$$n = 2^k, h_j = \frac{b-a}{2^j}.$$

$$\int_a^b f(x) dx = \frac{h_k}{2} \left(f(a) + 2 \sum_{j=1}^{n-1} f(x_j) + f(b) \right) - \frac{(b-a)h_k^2}{12} f''(\mu)$$

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$$\begin{aligned} \int_a^b f(x) dx &= \frac{h_k}{2} \left(f(a) + 2 \sum_{j=1}^{n-1} f(x_j) + f(b) \right) - \frac{(b-a)h_k^2}{12} f''(\mu) \\ &\stackrel{\text{book}}{=} \frac{h_k}{2} \left(f(a) + 2 \sum_{j=1}^{n-1} f(x_j) + f(b) \right) + \sum_{j=1}^{\infty} K_j h_k^{2j}. \\ &\stackrel{\text{def}}{=} \mathbf{R}_{k,1} + \sum_{j=1}^{\infty} K_j h_k^{2j}. \end{aligned}$$

Recursive Composite Trapezoidal: with $n = 2^k$, $h_j = \frac{b-a}{2^j}$.

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$$\mathbf{R}_{1,1} = \frac{h_0}{2} (f(a) + f(b)) = \frac{b-a}{2} (f(a) + f(b)) \quad \left(\stackrel{\text{def}}{=} \mathcal{N}_1(h_0) \right),$$

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\vdots

$$\mathbf{R}_{k,1} = \frac{1}{2} \left(\mathbf{R}_{k-1,1} + h_{k-2} \sum_{j=1}^{2^{k-2}} f(a + (2j-1)h_{k-1}) \right)$$

Recursive Composite Trapezoidal: with $n = 2^k$, $h_j = \frac{b-a}{2^j}$.

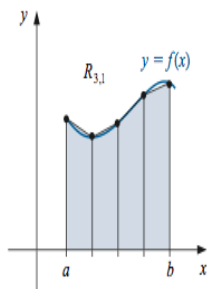
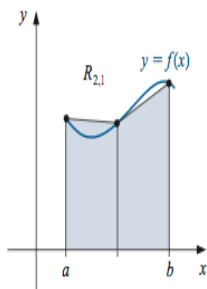
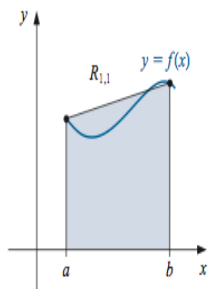
$$\int_a^b f(x) dx = \mathbf{R}_{k,1} + \sum_{j=1}^{\infty} K_j h_k^{2j}, \quad | \quad \mathbf{R}_{k,1} \stackrel{\text{def}}{=} \frac{h_k}{2} \left(f(a) + 2 \sum_{j=1}^{n-1} f(x_j) + f(b) \right).$$

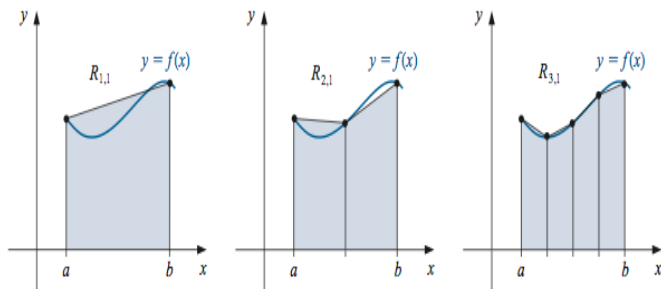
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Romberg Extrapolation (= even term Richardson Extrapolation)

$O(h_k^2)$	$O(h_k^4)$	$O(h_k^6)$	$O(h_k^8)$
$R_{1,1} \searrow$			
\rightarrow			
$R_{2,1} \searrow$	$R_{2,2} \searrow$		
\rightarrow	\rightarrow		
$R_{3,1} \searrow$	$R_{3,2} \searrow$	$R_{3,3} \searrow$	
\rightarrow	\rightarrow	\rightarrow	
$R_{4,1} \rightarrow$	$R_{4,2} \rightarrow$	$R_{4,3} \rightarrow$	$R_{4,4}$

Romberg Extrapolation for

$$\int_0^\pi \sin(x) dx, \quad n = 1, 2, 2^2, 2^3, 2^4, 2^5.$$

$$R_{1,1} = \frac{\pi}{2} (\sin(0) + \sin(\pi)) = 0,$$

$$R_{2,1} = \frac{1}{2} \left(R_{1,1} + \pi \sin\left(\frac{\pi}{2}\right) \right) = 1.57079633,$$

$$R_{3,1} = \frac{1}{2} \left(R_{2,1} + \frac{\pi}{2} \sum_{j=1}^2 \sin\left(\frac{(2j-1)\pi}{4}\right) \right) = 1.89611890,$$

$$R_{4,1} = \frac{1}{2} \left(R_{3,1} + \frac{\pi}{4} \sum_{j=1}^4 \sin\left(\frac{(2j-1)\pi}{8}\right) \right) = 1.97423160,$$

$$R_{5,1} = \frac{1}{2} \left(R_{4,1} + \frac{\pi}{8} \sum_{j=1}^8 \sin\left(\frac{(2j-1)\pi}{16}\right) \right) = 1.99357034,$$

$$R_{6,1} = \frac{1}{2} \left(R_{5,1} + \frac{\pi}{16} \sum_{j=1}^{2^4} \sin\left(\frac{(2j-1)\pi}{32}\right) \right) = 1.99839336.$$

Romberg Extrapolation, $\int_0^\pi \sin(x) dx = 2$

0						
1.57079633	2.09439511					
1.89611890	2.00455976	1.99857073				
1.97423160	2.00026917	1.99998313	2.00000555			
1.99357034	2.00001659	1.99999975	2.00000001	1.9999999		
1.99839336	2.00000103	2.00000000	2.00000000	2.0000000	2.0000000	

33 FUNCTION EVALUATIONS USED IN THE TABLE.

Recursive Composite Simpson:

$$\int_a^b f(x) dx \approx \frac{h}{3} \left(f(a) + 2 \sum_{j=1}^{m-1} f(x_{2j}) + 4 \sum_{j=1}^m f(x_{2j-1}) + f(b) \right) - \frac{(b-a)h^4}{12} f^{(4)}(\mu)$$

Recursive Composite Simpson:

$$\begin{aligned}\int_a^b f(x) dx &\approx \frac{h}{3} \left(f(a) + 2 \sum_{j=1}^{m-1} f(x_{2j}) + 4 \sum_{j=1}^m f(x_{2j-1}) + f(b) \right) \\ &\quad - \frac{(b-a)h^4}{12} f^{(4)}(\mu) \\ &\stackrel{\text{exists}}{=} \frac{h}{3} \left(f(a) + 2 \sum_{j=1}^{m-1} f(x_{2j}) + 4 \sum_{j=1}^m f(x_{2j-1}) + f(b) \right) \\ &\quad + \sum_{j=\boxed{2}}^{\infty} K_j h^{2j}. \\ &\stackrel{\text{def}}{=} \mathbf{R}_{k,1} + \sum_{j=2}^{\infty} K_j h^{2j}, \text{ for } n = 2^k.\end{aligned}$$

Recursive Composite Simpson: with $h_k = (b - a)/2^{k-1}$.

$$\int_a^b f(x) dx \approx \mathbf{R}_{k,1} + \sum_{j=2}^{\infty} K_j h^{2j}, \text{ for } n = 2^k.$$

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$$\mathbf{R}_{1,1} = \frac{b-a}{6} (f(a) + 4\mathbf{S}_1 + f(b)), \quad \mathbf{S}_1 = f((a+b)/2),$$

Recursive Composite Simpson: with $h_k = (b - a)/2^{k-1}$.

$$\int_a^b f(x) dx \approx \mathbf{R}_{k,1} + \sum_{j=2}^{\infty} K_j h^{2j}, \text{ for } n = 2^k.$$

$$\mathbf{R}_{1,1} = \frac{b-a}{6} (f(a) + 4\mathbf{S}_1 + f(b)), \quad \mathbf{S}_1 = f((a+b)/2),$$

$$\vdots \quad \quad \quad \vdots$$

$$\mathbf{T}_k = \sum_{j=1}^{2^{k-1}} f(a + (2j-1)h_k),$$

$$\mathbf{R}_{k,1} = \frac{h_k}{3} (f(a) + 2\mathbf{S}_{k-1} + 4\mathbf{T}_k + f(b)),$$

$$\mathbf{S}_k = \mathbf{S}_{k-1} + \mathbf{T}_k, \quad k = 2, \dots, \log_2 n.$$

Romberg Extrapolation Table for Simpson Rule

$O(h_k^4)$	$O(h_k^6)$	$O(h_k^8)$	$O(h_k^{10})$
$R_{1,1}$			
$R_{2,1}$	$R_{2,2}$		
$R_{3,1}$	$R_{3,2}$	$R_{3,3}$	
$R_{4,1}$	$R_{4,2}$	$R_{4,3}$	$R_{4,4}$

Special even term Richardson Extrapolation

Tricks of the Trade for $\int_a^b f(x)dx$

- ▶ Composite Simpson/Trapezoidal rules:
 - ▶ Adding more EQUI-SPACED points.

Tricks of the Trade for $\int_a^b f(x)dx$

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 - ▶ Adding more points ONLY WHEN NECESSARY.

quad function of matlab: combines all three tricks.

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Crying baby Principle

in adaptive algorithms

ADD MORE POINTS IN REGIONS
OF INADEQUATE ACCURACY

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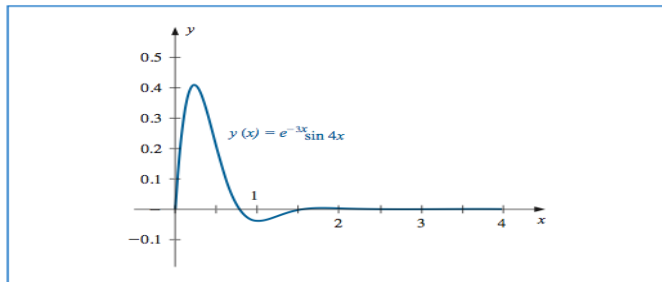
crying babies get more candies

presumed innocence: accuracy adequate unless detected otherwise

§4.6 Adaptive Quadrature Methods: step-size matters

$$y(x) = e^{-3x} \sin 4x.$$

- ▶ Oscillation for small x ; nearly 0 for larger x .
 - ▶ Mechanical engineering
(spring and shock absorber systems)
 - ▶ Electrical engineering
(circuit simulations)



- ▶ $y(x)$ behaves differently for small x than for large x .

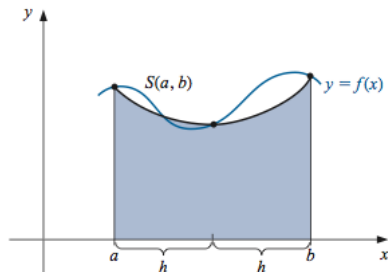
Adaptive Quadrature (I)



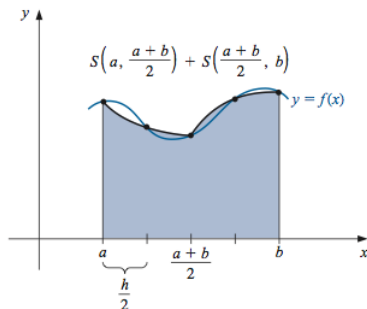
$$\int_a^b f(x)dx = S(a, b) - \frac{h^5}{90}f^{(4)}(\xi), \quad \xi \in (a, b),$$

where $S(a, b) = \frac{h}{3} (f(a) + 4f(a + h) + f(b))$, $h = \frac{b - a}{2}$.

Simpson on $[a, b]$



Composite Simpson



Adaptive Quadrature (II)



$$\int_a^b f(x)dx = S(a, b) - \frac{h^5}{90} f^{(4)}(\xi), \quad \xi \in (a, b)$$



$$\begin{aligned} \int_a^b f(x)dx &= \int_a^{\frac{a+b}{2}} f(x)dx + \int_{\frac{a+b}{2}}^b f(x)dx \\ &= S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b) \\ &\quad - \frac{(h/2)^5}{90} f^{(4)}(\xi_1) - \frac{(h/2)^5}{90} f^{(4)}(\xi_2) \\ &= S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b) - \frac{1}{16} \left(\frac{h^5}{90} \right) f^{(4)}(\hat{\xi}), \end{aligned}$$

where

$$\xi_1 \in (a, \frac{a+b}{2}), \quad \xi_2 \in (\frac{a+b}{2}, b), \quad \hat{\xi} \in (a, b).$$

Adaptive Quadrature (II)



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$$\frac{h^5}{90} f^{(4)}(\xi) \quad \overset{\text{hopefully}}{\approx} \quad \frac{h^5}{90} f^{(4)}(\hat{\xi}).$$

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$$\int_a^b f(x)dx = S(a, b) - \frac{h^5}{90} f^{(4)}(\xi), \quad \xi \in (a, b)$$



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$$\begin{aligned} \left| \int_a^b f(x)dx - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b) \right| &= \left| \frac{1}{16} \left(\frac{h^5}{90} \right) f^{(4)}(\hat{\xi}) \right| \\ &\approx \frac{1}{15} \left| S(a, b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b) \right|. \end{aligned}$$

Adaptive Quadrature (III)

For a given tolerance τ ,



$$\text{if } \frac{1}{15} \left| S(a, b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b) \right| \leq \tau,$$

then $S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b)$ is sufficiently accurate approximation to $\int_a^b f(x)dx$;

- ▶ otherwise recursively develop quadratures on $(a, \frac{a+b}{2})$ and $(\frac{a+b}{2}, b)$, respectively.

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AdaptQuad($f, [a, b], \tau$) for computing $\int_a^b f(x) dx$

▶ **compute** $S(a, b), S(a, \frac{a+b}{2}), S(\frac{a+b}{2}, b)$,

▶ **if**

$$\frac{1}{15} \left| S(a, b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b) \right| \leq \tau,$$

return $S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b)$.

▶ **else return**

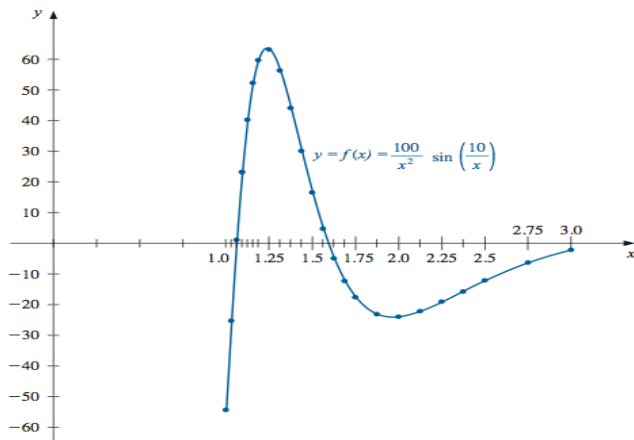
AdaptQuad($f, [a, \frac{a+b}{2}], \tau/2$) + **AdaptQuad**($f, [\frac{a+b}{2}, b], \tau/2$)

Adaptive Simpson, example

- ▶ Integral $\int_1^3 f(x) dx$,

$$f(x) = \frac{100}{x^2} \sin\left(\frac{10}{x}\right).$$

- ▶ Tolerance $\tau = 10^{-4}$.



function quad($f, [a, b], \tau$) **of** matlab

For a given tolerance τ ,

- ▶ **composite Simpson:** $S(a, b)$, $S(a, \frac{a+b}{2})$ and $S(\frac{a+b}{2}, b)$.
- ▶ **Romberg extrapolation:**

$$Q_1 = S(a, \frac{a+b}{2}) + S(\frac{a+b}{2}, b), \quad Q = Q_1 + \frac{1}{15} (Q_1 - S(a, b)).$$

- ▶ **if**

$$|Q - Q_1| \leq \tau,$$

return Q

function quad($f, [a, b], \tau$) **of** matlab

For a given tolerance τ ,

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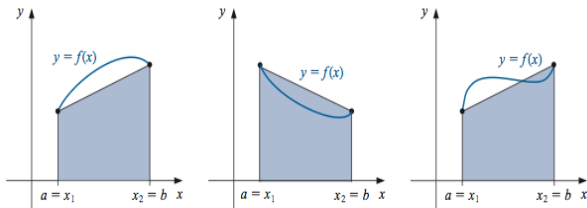
return Q (**Adaptive Simpson** returns Q_1)

► **else return**

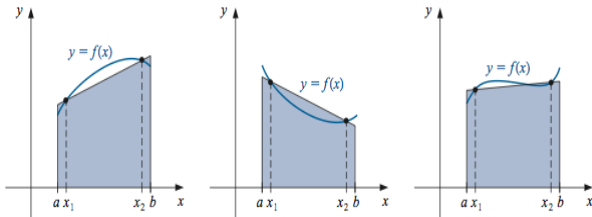
$$\text{quad}(f, [a, \frac{a+b}{2}], \tau/2) + \text{quad}(f, [\frac{a+b}{2}, b], \tau/2).$$

§4.7 Gaussian Quadrature (I)

- ▶ Trapezoidal nodes $x_1 = a, x_2 = b$ unlikely best choices.



- ▶ Likely better node choices.



Gaussian Quadrature (II)

- Given $n > 0$, choose both distinct nodes $x_1, \dots, x_n \in [-1, 1]$ and weights c_1, \dots, c_n , so quadrature

$$\int_{-1}^1 f(x) dx \approx \sum_{j=1}^n c_j f(x_j), \quad (1)$$

gives the greatest degree of precision (**DoP**).

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- ▶ $2n$ total number of parameters in quadrature, could choose $2n$ monomials in equation (1):

$$f(x) = 1, x, x^2, \dots, x^{2n-1} \quad (2)$$

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- ▶ directly solving equation (1) with all $f(x)$ in (2) very hard.

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**The world of quadratures is not a democratic society:
Efficiency more important than chaos
nodes matter, weights matter**

Gaussian Quadrature, $n = 2$ (I)

- Consider Gaussian quadrature

$$\int_{-1}^1 f(x) dx \approx c_1 f(x_1) + c_2 f(x_2).$$

Gaussian Quadrature, $n = 2$ (I)

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$$\int_{-1}^1 f(x) dx \approx c_1 f(x_1) + c_2 f(x_2).$$

- ▶ Choose parameters c_1, c_2 and $x_1 < x_2$ so that Gaussian quadrature is exact for $f(x) = 1, x, x^2, x^3$:

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

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- ▶ Choose parameters c_1, c_2 and $x_1 < x_2$ so that Gaussian quadrature is exact for $f(x) = 1, x, x^2, x^3$:

$$\int_{-1}^1 f(x) dx = c_1 f(x_1) + c_2 f(x_2), \quad \text{or}$$

$$\begin{aligned} 2 &= \int_{-1}^1 1 dx = c_1 + c_2, & 0 &= \int_{-1}^1 x dx = c_1 x_1 + c_2 x_2, \\ \frac{2}{3} &= \int_{-1}^1 x^2 dx = c_1 x_1^2 + c_2 x_2^2, & 0 &= \int_{-1}^1 x^3 dx = c_1 x_1^3 + c_2 x_2^3. \end{aligned}$$

Gaussian Quadrature, $n = 2$ (II)

► $x_1 < x_2$,

$$c_1 x_1 = -c_2 x_2, \quad c_1 x_1^3 = -c_2 x_2^3,$$

implying $x_1^2 = x_2^2$. Thus $x_1 = -x_2$ and $c_1 = c_2$.

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$$c_1 + c_2 = 2, \quad c_1 x_1^2 + c_2 x_2^2 = \frac{2}{3},$$

which implies $c_1 = c_2 = 1$, $x_2 = \frac{1}{\sqrt{3}}$.

- ▶ Gaussian quadrature for $n = 2$

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

- ▶ exact for $f(x) = 1, x, x^2, x^3$, but not for $f(x) = x^4$.

Gaussian Quadrature (III)

- ▶ Given $n > 0$, choose both distinct nodes $x_1, \dots, x_n \in [-1, 1]$ and weights c_1, \dots, c_n , so quadrature

$$\int_{-1}^1 f(x) dx \approx \sum_{j=1}^n c_j f(x_j), \quad (2)$$

gives the greatest degree of precision (**DoP**).

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- ▶ $2n$ parameters, allowing exact quadrature for $2n$ monomials

$$\int_{-1}^1 f(x) dx = \sum_{j=1}^n c_j f(x_j), \quad \text{for } f(x) = 1, x, x^2, \dots, x^{2n-1} \quad (3)$$

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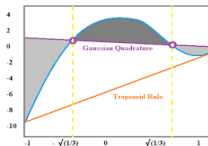
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- directly solving (2) can be very hard. But for $n = 2$,

$$\int_{-1}^1 f(x) dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \quad |$$

exact for $f(x) = 1, x, x^2, x^3$,

not for $f(x) = x^4$.



exact for cubic

Gaussian Quadrature by Legendre polynomials

Gaussian Quadrature by Legendre polynomials: $P_0(x) = 1$, $P_1(x) = x$,
 $(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$ for $n \geq 1$.

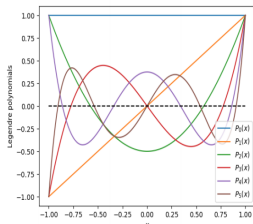
- ▶ $P_n(x)$ has degree n , always with n
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$$\int_{-1}^1 P_n(x) P_j(x) dx = 0, \quad \text{for } j < n$$

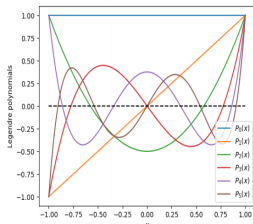


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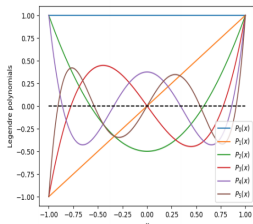
Thm: $\int_{-1}^1 P_n(x) Q(x) dx = 0$ for any $Q(x)$ with degree $< n$

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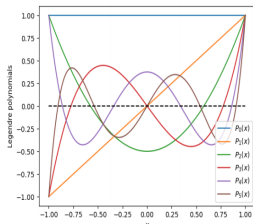
Gaussian quadrature: $\int_{-1}^1 f(x) dx \approx c_1 f(x_1) + c_2 f(x_2) + \dots + c_n f(x_n)$, $c_i \stackrel{\text{def}}{=} \int_{-1}^1 L_i(x) dx$

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Gaussian quadrature: $\int_{-1}^1 f(x) dx \approx c_1 f(x_1) + c_2 f(x_2) + \dots + c_n f(x_n)$, $c_i \stackrel{\text{def}}{=} \int_{-1}^1 L_i(x) dx$

quadrature exact for polynomial with degree $\leq n - 1$

Thm: Gaussian Quadrature **DoP** $= 2n - 1$

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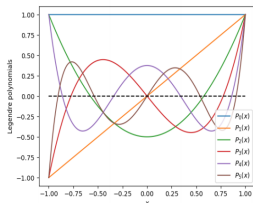
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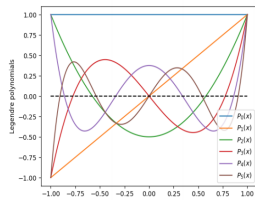
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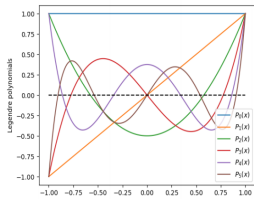


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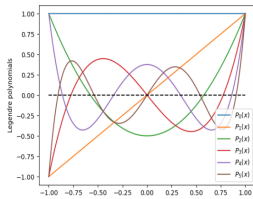
$$P(x) = P_n(x) Q(x) + R(x), \quad \text{deg of } Q(x), R(x) \leq n - 1 \quad (2)$$

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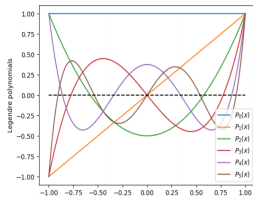
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- ▶ (recall) **Thm**: For each $x \in [a, b]$, there exists $\xi(x) \in (a, b)$,

$$f(x) = H(x) + R(x), \quad R(x) = \frac{f^{(2n)}(\xi(x))}{(2n)!} (x-x_1)^2 (x-x_2)^2 \cdots (x-x_n)^2.$$

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$$\int_{-1}^1 f(x) dx = \int_{-1}^1 H(x) dx + \int_{-1}^1 R(x) dx$$

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Gaussian Quadrature Error Estimate, matlab code

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Rapid convergence for smooth functions

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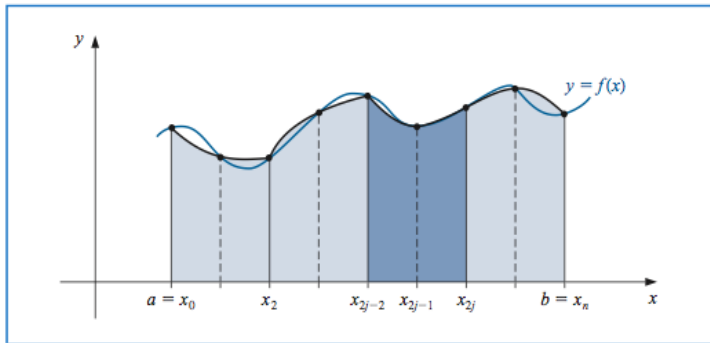
Rapid convergence for smooth functions

```
function [c,x] = Legendre(n)
%
b      = transpose((1:n-1));
b      = b./sqrt((2*b-1).*(2*b+1));
B      = diag(b,1)+diag(b,-1);
[Q,D]  = eig(B);
x      = diag(D);
x(abs(x)<1e-15) = 0;
c      = 2*transpose(Q(1,:).^2);
```

In contrast: Composite Simpson's Rule

$$(n = 2m, x_j = a + jh, h = \frac{b-a}{n}, 0 \leq j \leq n)$$

$$\int_a^b f(x) dx = \frac{h}{3} \left(f(a) + 2 \sum_{j=1}^{m-1} f(x_{2j}) + 4 \sum_{j=1}^m f(x_{2j-1}) + f(b) \right) - \frac{(b-a)h^4}{180} f^{(4)}(\mu)$$



Simpson/Trapezoidal vs. Gaussian Quadratures

Simpson/Trapezoidal:

- ▶ Composite rules:
 - ▶ Adding more EQUI-SPACED points.
- ▶ Romberg extrapolation:
 - ▶ Obtaining higher order rules from lower order rules.
- ▶ Adaptive quadratures:
 - ▶ Adding more points ONLY WHEN NECESSARY.

Gaussian Quadrature:

- ▶ points different for different n .

Gaussian Quadrature good for given n ,
Simpson good for given tolerance.