Numerical Integration

BLG 202E

Week 12

26.04.2016

Numerical Integration (Quadrature)

$$\int_a^b f(x)\,dx = ?$$

Let $f(x)$ be a continuous real-valued fn. defined in $[a,b]$

Recall: $f'(x) = ?$

$f(x) \approx p_n(x)$

Differentiation: $f'(x) \approx p_n'(x)$

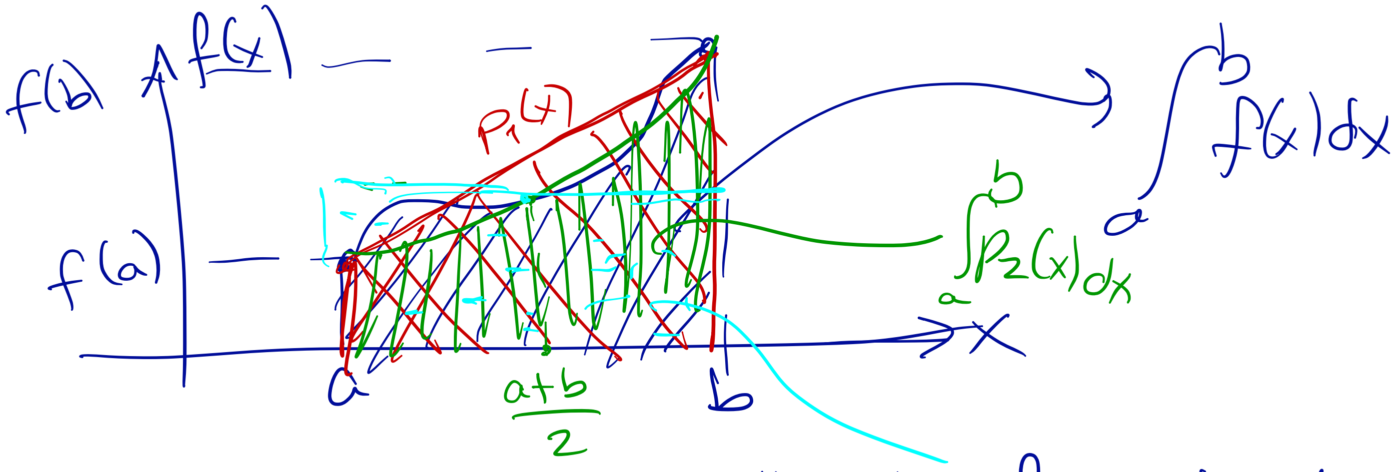
Integration: $\displaystyle\int_a^b f(x)\,dx \approx \int_a^b p_n(x)\,dx$

eg. $\displaystyle\int_a^b \frac{x^2 e^x}{\sqrt{1+x}}\,dx = ?$

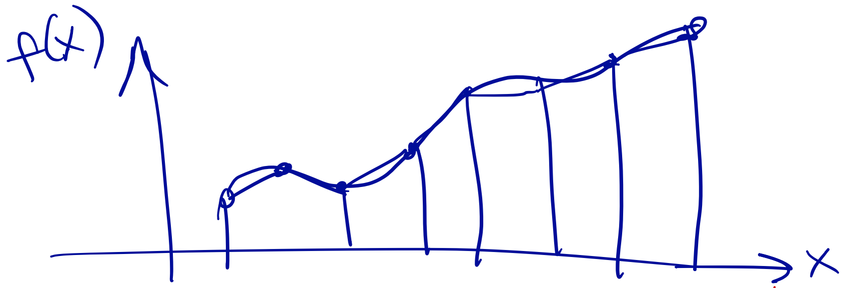
Quadrature: = approximate evaluation of a definite integral.

* We'll make use of the additive prop of integration

$a < c \leq b$: $\displaystyle\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx.$



We'll later subdivide the interval, and integrate.



Deriving Basic Quadrature Rules:

— Want to approximate definite integrals

$$\int_a^b f(x)\,dx \approx \int_a^b p_n(x)\,dx$$

$$f(x) \approx p_n(x)$$

— Given a fn. $f(x)$ on a <u>short</u> interval $[a,b]$, choose a set of nodes $x_0, x_1, \ldots, x_n \in [a,b]$, construct a polynomial interpolant:

$$p_n(x) = \sum_{j=0}^{n} f(x_j)\, L_j(x)$$

$$L_j(x) = \prod_{\substack{k=0 \\ k\neq j}}^{n} \frac{(x-x_k)}{(x_j-x_k)}$$

$$\int_a^b f(x)\,dx \approx \int_a^b p_n(x)\,dx = \int_a^b \sum_{j=0}^{n} f(x_j)L_j(x)\,dx$$

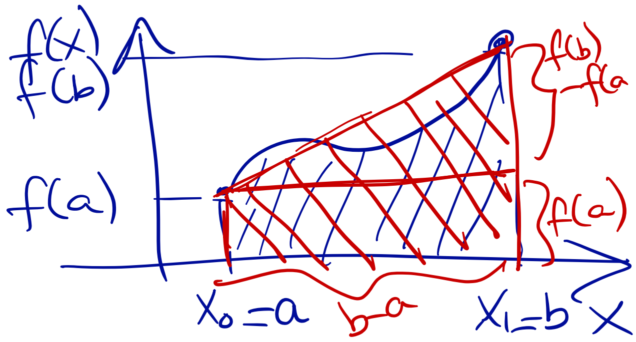
$$= \sum_{j=0}^{n} f(x_j) \boxed{\int_a^b L_j(x)\,dx}$$

set $a_j \triangleq \int_a^b L_j(x)\,dx$

quadrature weights

$$\boxed{\int_a^b f(x)\,dx \approx \sum_{j=0}^{n} f(x_j)\,a_j}$$

* Set $n=1$, interpolate at the ends $x_0=a$, $x_1=b$
(Linear polynomial)



$$L_0(x) = \frac{(x-b)}{(a-b)},$$

$$L_1(x) = \frac{(x-a)}{b-a}$$

To calculate the weights : $a_0 = \int_a^b L_0(x)\,dx = \int_a^b \frac{(x-b)}{a-b}\,dx = (b-a)/2$

$$a_1 = \int_a^b L_1(x)\,dx = \int_a^b \frac{(x-a)}{b-a}\,dx = \frac{b-a}{2}$$

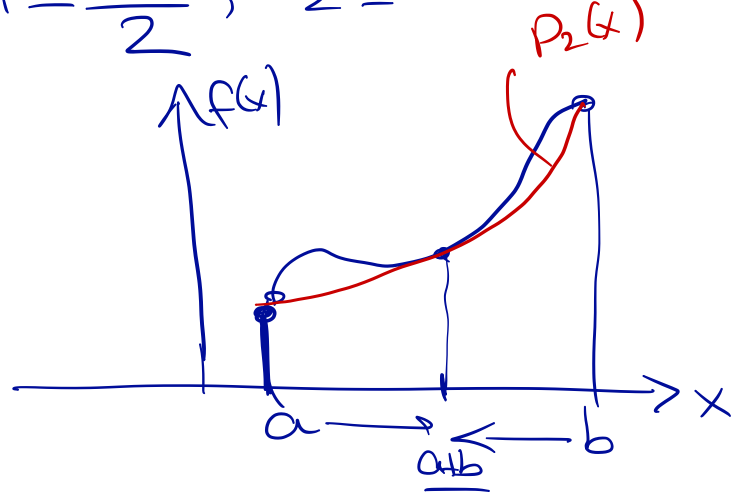
Result is the TRAPEZOIDAL rule :

$$I = \int_a^b f(x)\,dx \approx I_{trap} = a_0 f(x_0) + a_1 f(x_1)$$

$$\Longrightarrow \boxed{I_{trap} = \frac{b-a}{2}\left[f(a)+f(b)\right]}$$

★ Now, set $n=2$, use a quadratic interpolating polynomial, by adding a node at the middle point:

$$n=2, \quad x_0=a, \quad x_1=\frac{a+b}{2}, \quad x_2=b$$



$$L_0(x)=\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}$$

$$L_0(x)=\frac{\left(x-\left(\frac{a+b}{2}\right)\right)(x-b)}{\left(\frac{a-b}{2}\right)(a-b)}$$

$$L_1(x)=\frac{(x-a)(x-b)}{\left(\frac{b-a}{2}\right)^2} \quad ; \quad L_2(x)=\frac{(x-a)\left(x-\left(\frac{a+b}{2}\right)\right)}{(b-a)\left(\frac{b-a}{2}\right)}$$

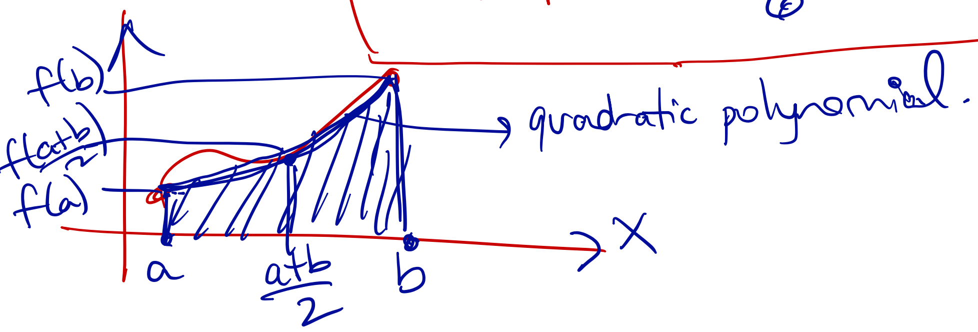
$$a_0=\int_a^b L_0(x)\,dx=\int_a^b \frac{\left(x-\left(\frac{a+b}{2}\right)\right)(x-b)}{(a-b)^2/2}\,dx$$

$$=\int_a^b \frac{\left[x^2-bx-\left(\frac{a+b}{2}\right)x+\left(\frac{a+b}{2}\right)b\right]}{(a-b)^2/2}\,dx \ldots$$

$$a_0=\frac{1}{6}(b-a) \quad ; \text{ similarly } \quad a_2=\frac{b-a}{6} \quad ; \quad a_1=(b-a)\frac{4}{6}$$

$$I \approx I_{simpson}=a_0 f(a)+a_1 f\left(\frac{a+b}{2}\right)+a_2 f(b)$$

$$\boxed{I_{simpson}=\frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]}$$



* (1) Trapezoid $(n=1)$ & (2) Simpson $(n=2)$ rules are instances of Newton–Cotes formules. → Uses Lagrange polyn. interpolation at equidistant abcissae to execute numerical integration.

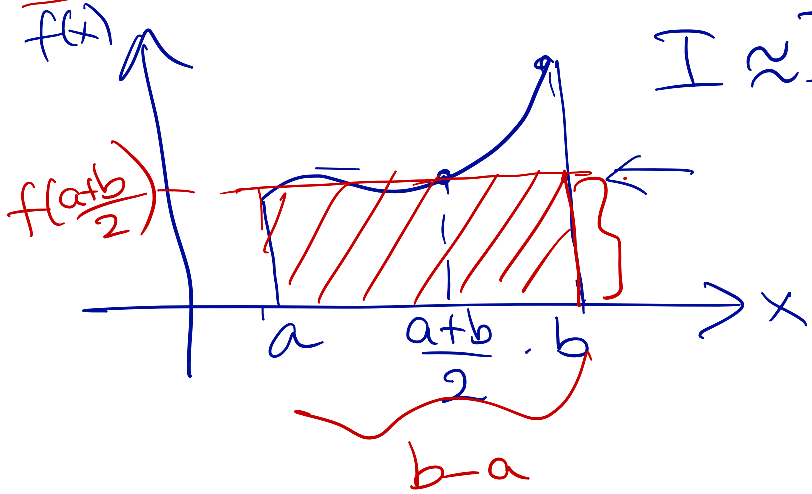
* The endpoints are included in trapezoid & Simpson methods.

$(x_0, x_1, \dots x_n)$

→ called Closed methods.

→ endpoints not included.

* (3) Midpoint Rule : Open formula.



$$I \approx I_{mid} = (b-a) f\left(\frac{a+b}{2}\right)$$

Uses a constant $(n=0)$ interpolant at the middle of the interval.

Basic Quadrature Error:

Recall: polynomial approx. error:

$$\text{error} = f(x) - p_n(x) = \underbrace{f[x_0, x_1, \dots x_n, x]}_{\text{divided diff.}} \prod_{i=0}^{n} (x - x_i)$$

Last time: $f'(x) - p_n'(x) = \frac{d}{dx}\big(\quad\big)$

Now, the quadrature error is the integral of this interpolation error:

$$\int (f(x) - p_n(x))\,dx = \int f[\quad] \prod_{i=0}^{n} (x - x_i)\,dx \Rightarrow$$

$$\Rightarrow E[f] = \int_a^b f(x)\,dx - \int_a^b p_n(x)\,dx = \int_a^b f(x)dx - \sum_{j=0}^{n} a_j f(x_j)$$

$$a_j = \int_a^b L_j(x)dx$$

— We won't derive the error functions.

$\Rightarrow$ Table (summary) (page 445) summarizes the error formulas for the 3 methods

Ex: (15.2) Let $f(x) = e^x$;

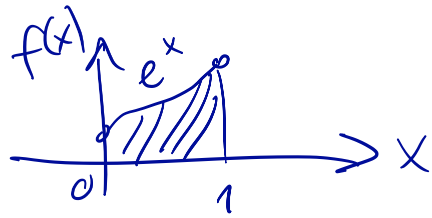
(i) $\underbrace{a=0,\ b=1}_{b-a=1}$: $I = \int_0^1 e^x dx = e-1 = 1.7183\ldots$

$$I_{trap} = \frac{b-a}{2}\left(f(a)+f(b)\right) = \frac{1}{2}\left(e^0+e^1\right) = 1.8591$$

$$I_{simp} = \frac{(b-a)}{6}\left(f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right) = \frac{1}{6}\left(1+4e^{0.5}+e^1\right)$$

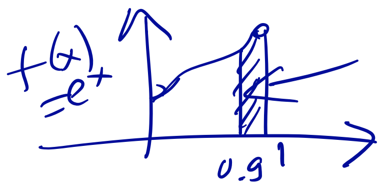
$$= 1.7189\ldots$$

$$I_{mid} = e^{1/2} = 1.6487$$



(ii) $\underbrace{a=0.9\ ,\ b=1}_{b-a=0.1}$

$$I = \int_{0.9}^1 e^x dx = e - e^{0.9} = 0.258678$$



$$I - I_{trap} = I - \frac{0.1}{2}\left(e^{0.9}+e\right) = -2.2 \cdot 10^{-4}$$

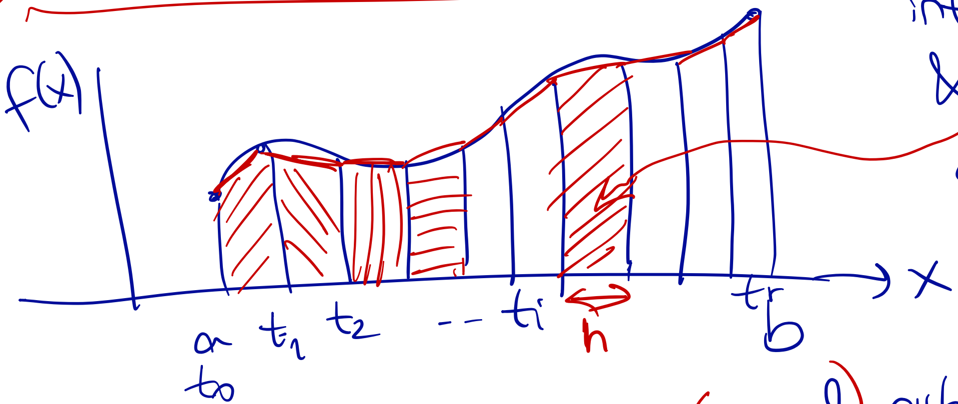
$$I - I_{simp} = I - \frac{0.1}{6}\left(e^{0.9}+4e^{0.95}+e\right) = -9 \cdot 10^{-9} \rightarrow \text{the best}$$

$$I - I_{mid} = I - 0.1\,e^{0.95} = 1.1 \cdot 10^{-4}$$

All 3 rules are quite accurate $\Leftarrow$ $(b-a) = 0.1$

⟹ This simple example indicates that basic quadrature rules can be adequate on sufficiently short intervals of integration.

⟹ COMPOSITE METHODS: Idea: partition $[a,b]$ interval into subintervals & apply the basic quadrature rule to each subinterval.



Divide $[a,b]$ into r (equal) subintervals of length $h = \frac{b-a}{r}$. $\underbrace{a+ih}_{t_i}$

$$\int_a^b f(x)\,dx = \sum_{i=1}^{r} \int_{\underbrace{a+(i-1)h}_{t_{i-1}}}^{\overbrace{a+ih}^{t_i}} f(x)\,dx = \sum_{i=1}^{r} \int_{t_{i-1}}^{t_i} f(x)\,dx$$

Say the error in the basic rule is $\tilde{K}(b-a)^{q+1}$ some +ve integer

then sum up the error in all subintervals, $i=1,\dots,r$

$$E(f) = \sum_{i=1}^{r} K h^{q+1} =$$

K_i replaced by some constant K

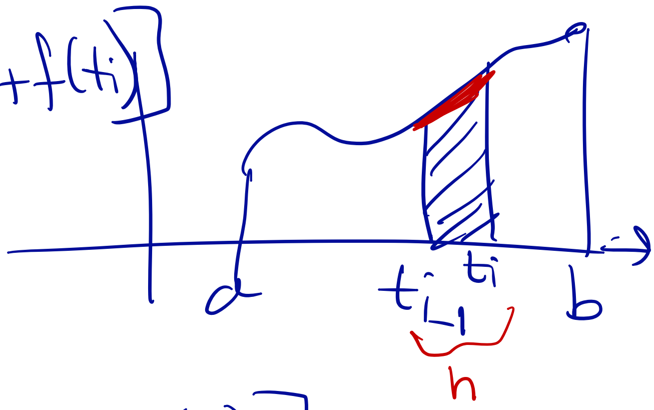
$$= \sum_{i=1}^{r} K h^q h = K h^q \sum_{i=1}^{r} h \;=\; (b-a)$$

error in composite methods ⟹ $\boxed{E(f) = K h^q (b-a)}$

1) Composite Trapezoidal Rule:

Apply the trapezoid rule to each subinterval $[t_{i-1}, t_i]$:

$$\int_{t_{i-1}}^{t_i} f(x)\,dx \simeq \frac{h}{2}\left[f(t_{i-1})+f(t_i)\right]$$



The composite method:

$$\int_a^b f(x)\,dx \simeq \frac{h}{2}\sum_{i=1}^{r}\left[f(t_{i-1})+f(t_i)\right]$$

$$= \frac{h}{2}\left[f(t_0)+2f(t_1)+2f(t_2)+\dots+2f(t_{r-1})+f(t_r)\right]$$

$$\boxed{I_{comp,trap} = \frac{h}{2}\left[f(a)+2f(t_1)+\dots+2f(t_{r-1})+f(b)\right]}$$

The associated error:

$$E(f) = \sum_{i=1}^{r}\left(-\frac{f''(\xi_i)}{12}h^3\right) = \underbrace{-\frac{f''(\xi)}{12}}_{K}(b-a)h^2$$

$$(t_{i-1}\le \xi_i \le t_i,\ a\le \xi \le b)$$

$$= K(b-a)h^2 \Longrightarrow O(h^2)$$

Composite Trapezoid method is 2^{nd} order accurate.

Composite Simpson Method: One of the most commonly used quadrature methods

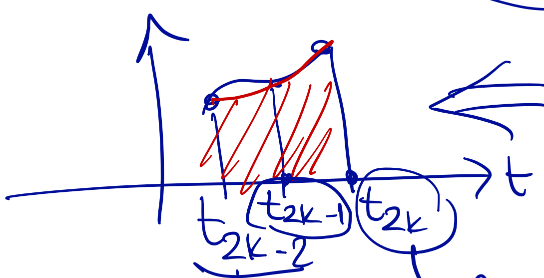
— Set $\boxed{r \text{ even}}$;
we consider subintervals in pairs, $\Rightarrow$ our subintervals are now of length $2h$:

$$[t_{2k-2}, t_{2k}], \quad k = 1, 2, \dots, \frac{r}{2}$$

— On each subinterval $[t_{2k-2}, t_{2k}]$, apply basic Simpson method, then sum them up:

$$\int_{t_{2k-2}}^{t_{2k}} f(x)\,dx \approx \frac{2h}{6}\left[f(t_{2k-2}) + 4f(t_{2k-1}) + f(t_{2k})\right]$$

$\rightarrow$ Sum these up



subinterval of length $2h$

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{r/2} \int_{t_{2k-2}}^{t_{2k}} f(x)\,dx$$

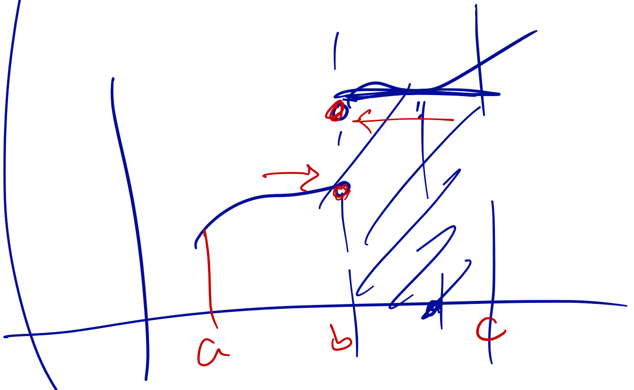
$$= \frac{h}{3} \sum_{k=1}^{r/2} \left(f(t_{2k-2}) + 4f(t_{2k-1}) + f(t_{2k})\right)$$

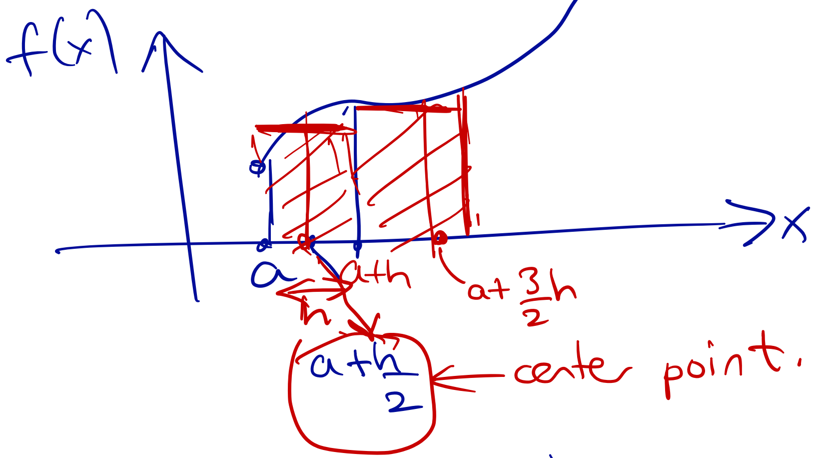
well-known Simpson's formula

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left[f(a) + 2\sum_{k=1}^{r/2-1} f(t_{2k}) + 4\sum_{k=1}^{r/2} f(t_{2k-1}) + f(b)\right]$$

Composite Midpoint Rule:

$$\boxed{I=\int_a^b f(x)\,dx \approx h\sum_{i=1}^{n} f\left(a+\left(i-\tfrac{1}{2}\right)h\right)}$$

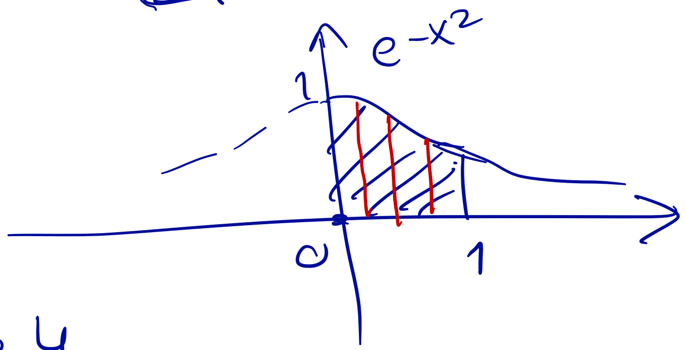




could be ~ ?

Good when the integrand $f(x)$ has jump (discontinuties) at the nodes.

Ex 15.3: $I=\int_0^1 e^{-x^2}dx \approx 0.746824133$



Divide $[0,1]$ interval into $n=4$ subintervals; $h=0.25$,

$t_i = i\cdot h$, $i=0,1,2,3,4$

$t_0=0$, $t_1=h$, $t_2=2h$, $t_3=3h$, $t_4=4h=1$

Composite rules:

$$I_{trap}=0.125\left[e^0+2e^{-h^2}+2e^{(-2h)^2}+2e^{(-3h)^2}+e^{(-4h)^2}\right]$$

$$=0.742984$$

$I_{simp} = \ldots\ldots = 0.746855$ $\longrightarrow$ Composite Simpson rule is more accurate.

exercise: calculate

Error in Composite Simpson Rule:

$$\left| \int_a^b f(x)\,dx - I_{simp} \right| = (b-a)\,h^4 \left| -\frac{f^{(4)}(\xi)}{180} \right|$$

$\Longrightarrow O(h^4)$ error

$a \leq \xi \leq b$

Error in Trapezoid Rule:

$$\left| \int_a^b f(x)\,dx - I_{trap} \right| = \frac{(b-a)h^2}{12} \left| f''(\xi) \right| , \quad \xi \in [a,b]$$

$\hookrightarrow O(h^2)$ error

Chapter 15: Numerical Integration

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Slides for the book
A First Course in Numerical Methods (published by SIAM, 2011)
http://www.ec-securehost.com/SIAM/CS07.html

Numerical integration (quadrature)

- The need to integrate arises very frequently in numerical computations. Instance: finite element methods for differential equations use basis functions in the spirit of Chapter 11, in combination with integrals computed over tiny pieces of the computational domain.
- The need to know how to integrate numerically can be more immediate than in the case of differentiation because we often do not know how to integrate even simple-looking functions.
- As opposed to differentiation, which is local in nature, integration is a *global* operation.
- Note that while the derivative of $f(x)$ is typically rougher than f, the integral of $f(x)$ is smoother. Consequently, no special roundoff error difficulties are expected here, unlike in Chapter 14.
- Many-dimensional integration often arises in statistical applications.

Basic rules

Consider only definite integrals; quadrature $\equiv$ numerical integration in one dimension. Seek approximation formulas of the form

$$I_f = \int_a^b f(x)dx \approx \sum_{j=0}^{n} a_j f(x_j).$$

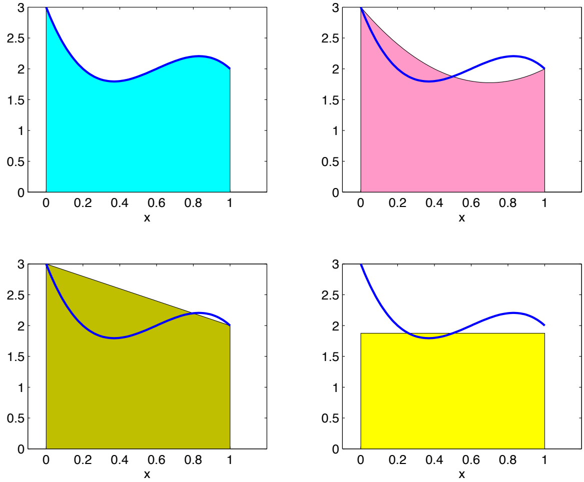
- Derive basic quadrature rules by interpolating the integrand $f(x)$ using Lagrange form and integrating the resulting polynomial.
- The *weights* a_j are then given by

$$a_j = \int_a^b L_j(x)dx, \quad L_j(x) = \prod_{\substack{k=0 \\ k\neq j}}^{n} \frac{(x-x_k)}{(x_j-x_k)}.$$

- These weights are independent of f and can be found in advance!

Basic trapezoidal, midpoint and Simpson rules

A picture is better than 2048 bytes. Upper left: exact; upper right: Simpson; lower left: trapezoidal; lower right: midpoint.



Error in basic rules

- The error satisfies

$$\begin{aligned} E(f) &= \int_a^b f(x)dx - \sum_{j=0}^{n} a_j f(x_j) \\ &= \int_a^b f[x_0, x_1, \ldots, x_n, x](x - x_0)(x - x_1)\cdots(x - x_n)dx. \end{aligned}$$

- To estimate this further can be delicate. Results:

Method	Formula	Error
Midpoint	$(b-a)f(\frac{a+b}{2})$	$\frac{f''(\xi_1)}{24}(b-a)^3$
Trapezoidal	$\frac{b-a}{2}[f(a)+f(b)]$	$-\frac{f''(\xi_2)}{12}(b-a)^3$
Simpson	$\frac{b-a}{6}[f(a)+4f(\frac{b+a}{2})+f(b)]$	$-\frac{f''''(\xi_3)}{90}(\frac{b-a}{2})^5$

- These are all Newton-Cotes formulas: Trapezoidal and Simpson are *closed*, midpoint is *open*.

Composite methods

- The basic rules are good for small intervals. So, use them on subintervals.
- Similar to piecewise polynomial interpolation, but easier because no need here to worry about global smoothness.
- $$\int_a^b f(x)dx = \sum_{i=1}^{r} \int_{t_{i-1}}^{t_i} f(x)dx, \quad \text{e.g. } t_i = a + ih.$$
- If error in basic rule is $E(f) = \tilde{K}(b-a)^{q+1}$ then error in composite method is

$$E(f) = K(b-a)h^q.$$

Composite trapezoidal method

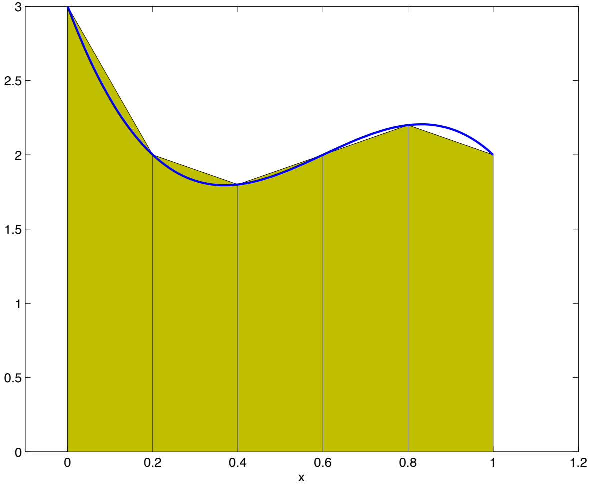
- Composite method

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(a) + 2f(t_1) + 2f(t_2) + \cdots + 2f(t_{r-1}) + f(b)].$$

- Error estimate

$$E(f) = \sum_{i=1}^{r} \left(-\frac{f''(\eta_i)}{12} h^3 \right) = -\frac{f''(\eta)}{12}(b-a)h^2.$$

Composite trapezoidal



Composite Simpson method

- Composite method (for convenience, pose basic rule on subinterval of length $2h$):

$$\int_{t_{2k-2}}^{t_{2k}} f(x)dx \approx \frac{2h}{6}[f(t_{2k-2}) + 4f(t_{2k-1}) + f(t_{2k})].$$

Then sum up contributions (using even r), obtaining the famous formula

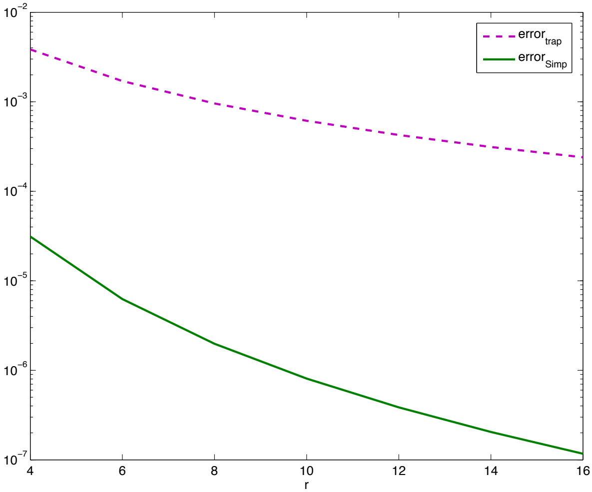
$$\int_a^b f(x)dx \quad \approx \quad \frac{h}{3}[f(a) + 2\sum_{k=1}^{r/2-1} f(t_{2k}) + 4\sum_{k=1}^{r/2} f(t_{2k-1}) + f(b)].$$

Error estimate

$$E(f) = -\frac{f''''(\zeta)}{180}(b-a)h^4.$$

Example: errors for trapezoidal and Simpson

Integrate $I = \int_0^1 e^{-x^2} dx$.
Plot errors for $h = 1/r$: evidently the 4th order Simpson is much more accurate.



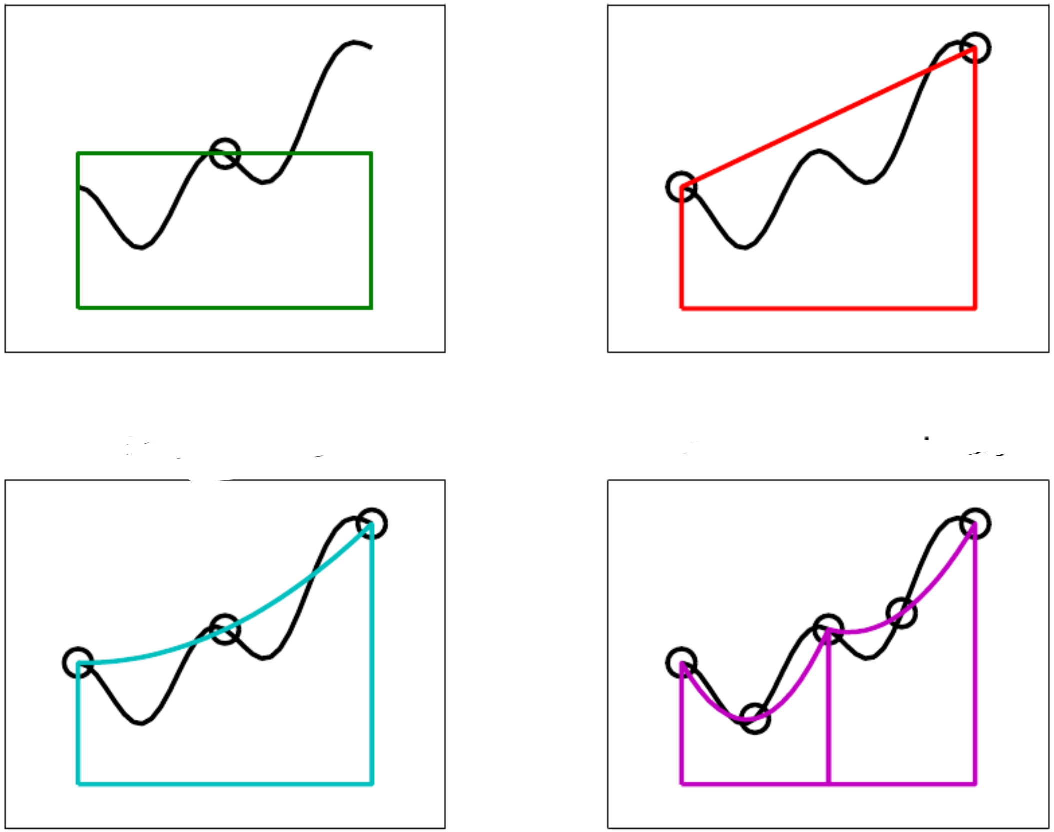
Composite trapezoidal, midpoint and Simpson methods

With $rh = b - a$, r a positive integer (must be even in the Simpson case), we have the **formulas**

$$\begin{aligned}\int_a^b f(x)dx &\approx \frac{h}{2}[f(a) + 2\sum_{i=1}^{r-1} f(a+ih) + f(b)], \quad \text{trapezoidal} \\ &\approx \frac{h}{3}[f(a) + 2\sum_{k=1}^{r/2-1} f(t_{2k}) + 4\sum_{k=1}^{r/2} f(t_{2k-1}) + f(b)], \quad \text{Simpson} \\ &\approx h\sum_{i=1}^{r} f(a+(i-1/2)h), \quad \text{midpoint.}\end{aligned}$$

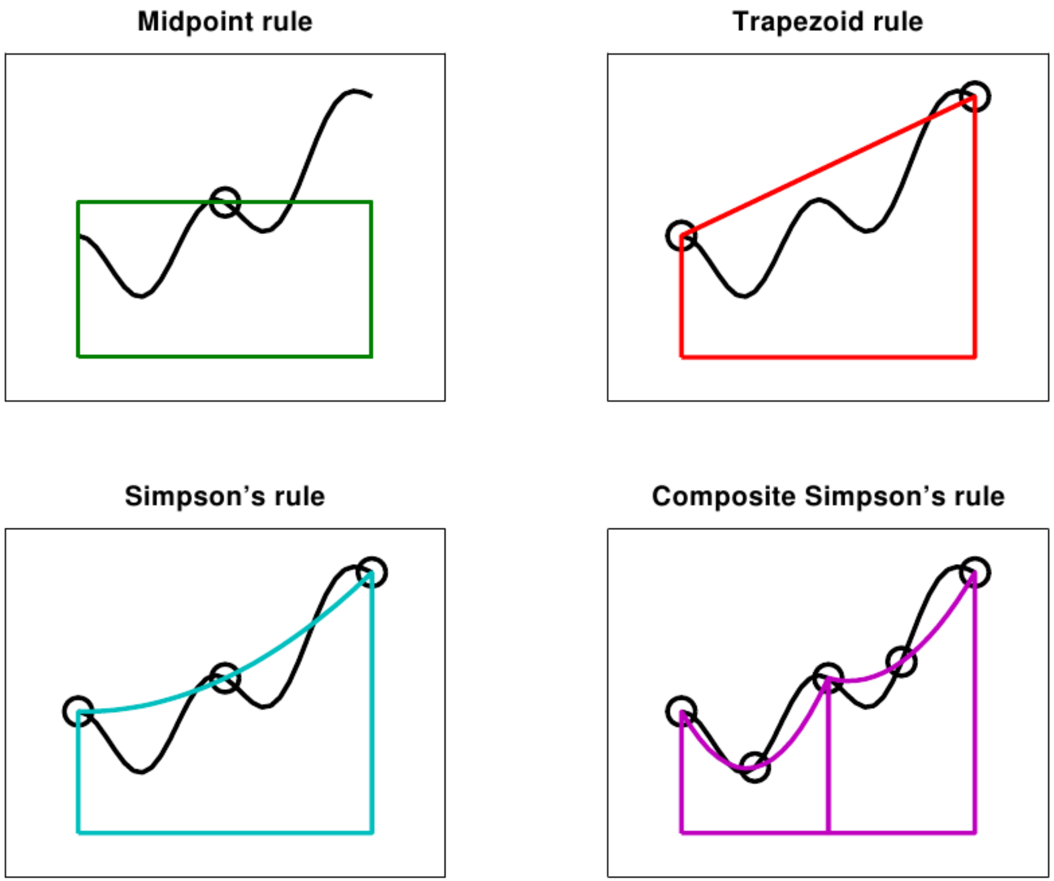
Composite Rules (cont.)

Which plot shows which method?



Picture from Moler: Numerical Computing with MATLAB.

Composite Rules (cont.)



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