CS 3200
Introduction to Scientific Computing

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Topic: Quadrature Numerical Integration

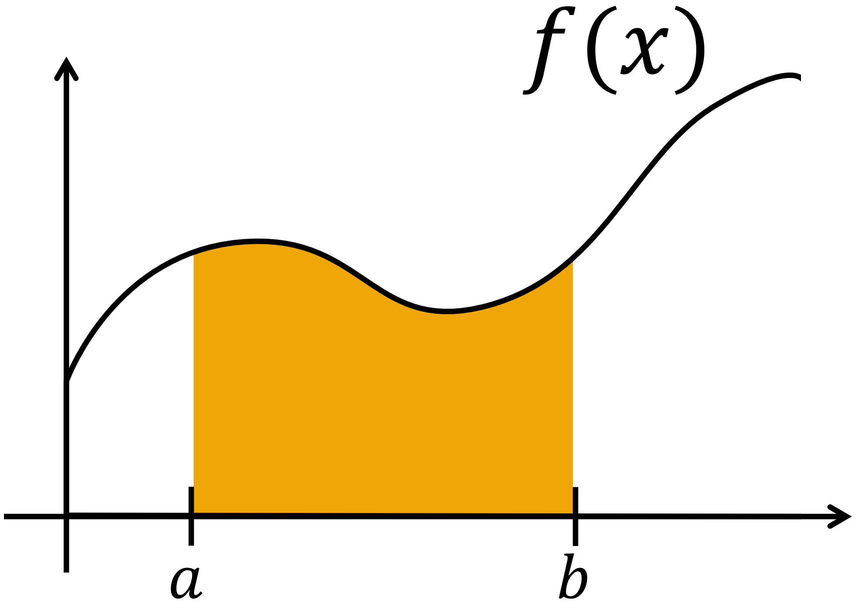
Application of polynomial theory

Numerical Integration

- Goal: find the area under the curve

$$\int_a^b f(x)dx$$

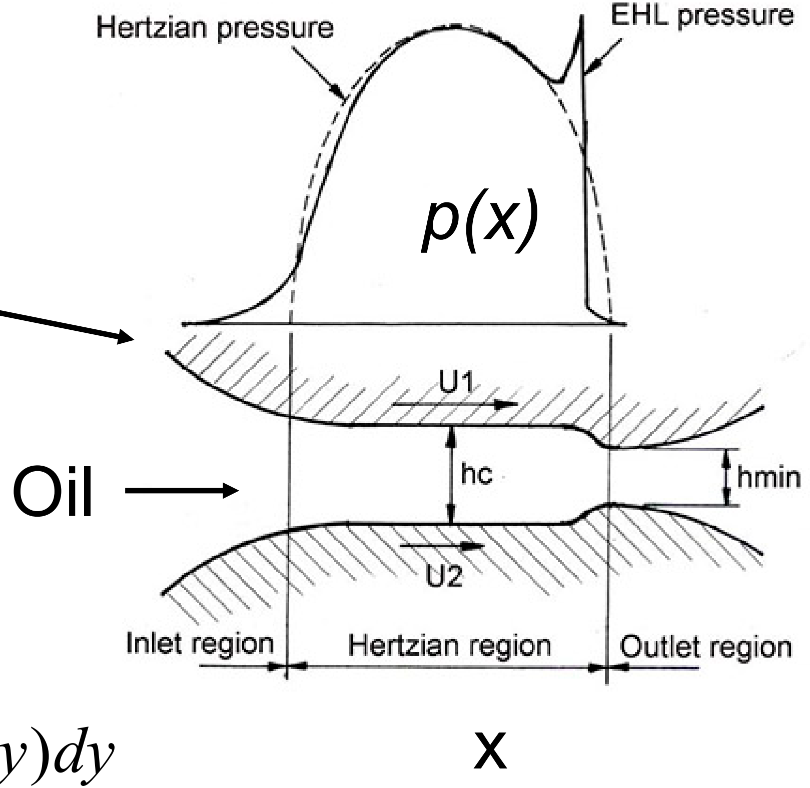
Approximate f(x) by using a polynomial or a polynomial spline, as above and integrate that polynomial



Example from Engineering

- When oil is used in lubricating a car engine the pressures are sufficiently high that the steel deforms from the original semi-circular shape to
- The relationship between the pressure *p(x)* and the thickness of the oil film *h(x)* is given by the integral. Note this is part of a much larger problem.

$$h(x) = h_{00} + \frac{x^2}{2R_x} - \frac{4}{\pi E}\int_{-\infty}^{\infty} \ln\left|\frac{x-y}{x_0}\right| p(y)\,dy$$

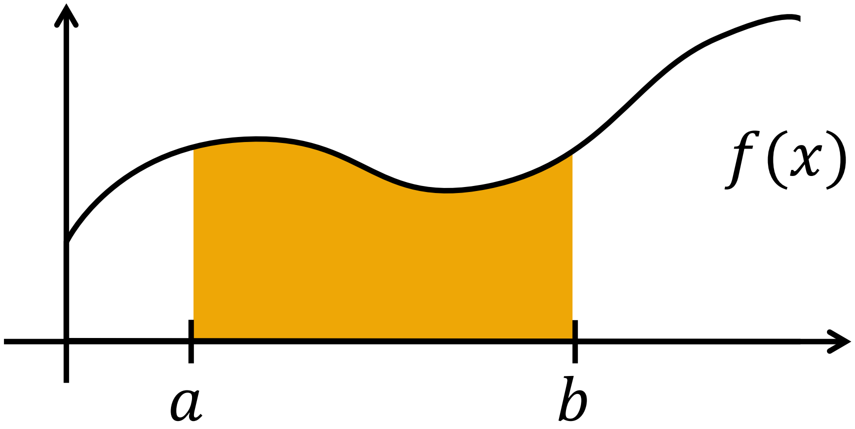


Numerical Integration

- How: the weighted sum of the function sampled N-times

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} w_i f(x_i)$$

- With each –
  - w_i: sampling weight
  - x_i: sampling location



Calculation of $\{w_i, x_i\}$ pairs known as:

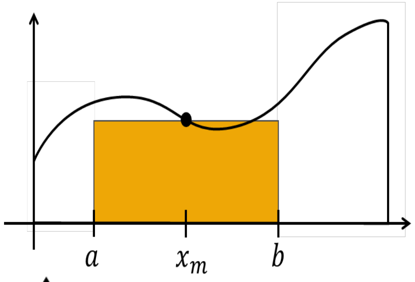
QUADRATURE SCHEMES

Main ideas

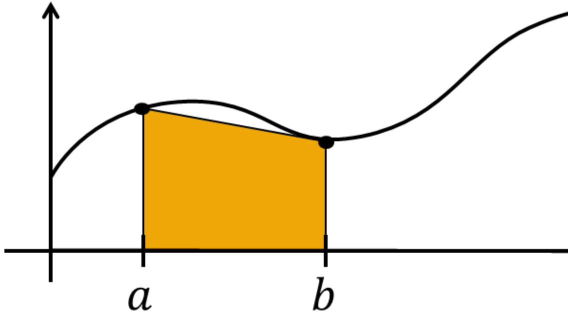
- Approximate f(x) by a polynomial using the data points on a mesh of size h
- Integrate the polynomial to approximate the integral.
- Repeat the process with h/2 to get a second solution
- Use a combination of the solution to estimate the error

Polynomial Approximations

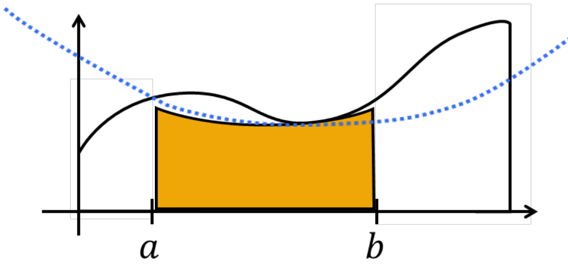
Midpoint Rule
piecewise constant approximation



Trapezoidal Rule
Piecewise linear approximation



Simpson’s rule
Piecewise quadratic approximation

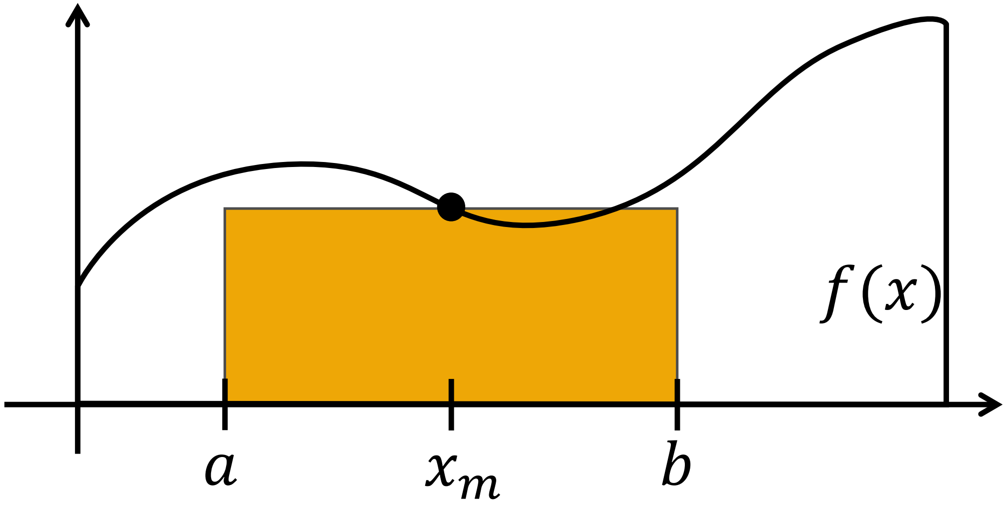


Midpoint Rule

Approximate the integral by a rectangle defined by the midpoint between a and b

$$:\int_a^b f(x)dx \approx (b-a)f(x_m)$$

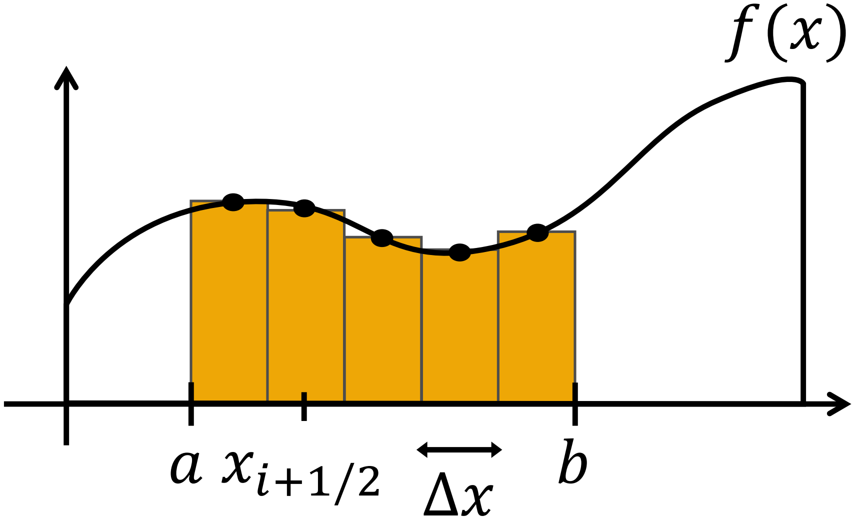
$$x_m = \frac{a+b}{2}$$



Composite Midpoint Rule

- Approximate the integral by N applications of the midpoint rule between a and b:

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} w_i f(x_i)$$



- Given $\Delta x = \frac{b-a}{N}$,

$$x_{i+1/2} = a + (i - .5)\Delta x$$

$$w_i = \Delta x$$

Estimating the error using Taylors Series

General idea:

(i) Expand the function being integrated about the points used in the numerical method (here the midpoint) using Taylors series

(ii) Evaluate the expression for the error by looking carefully at which terms cancel

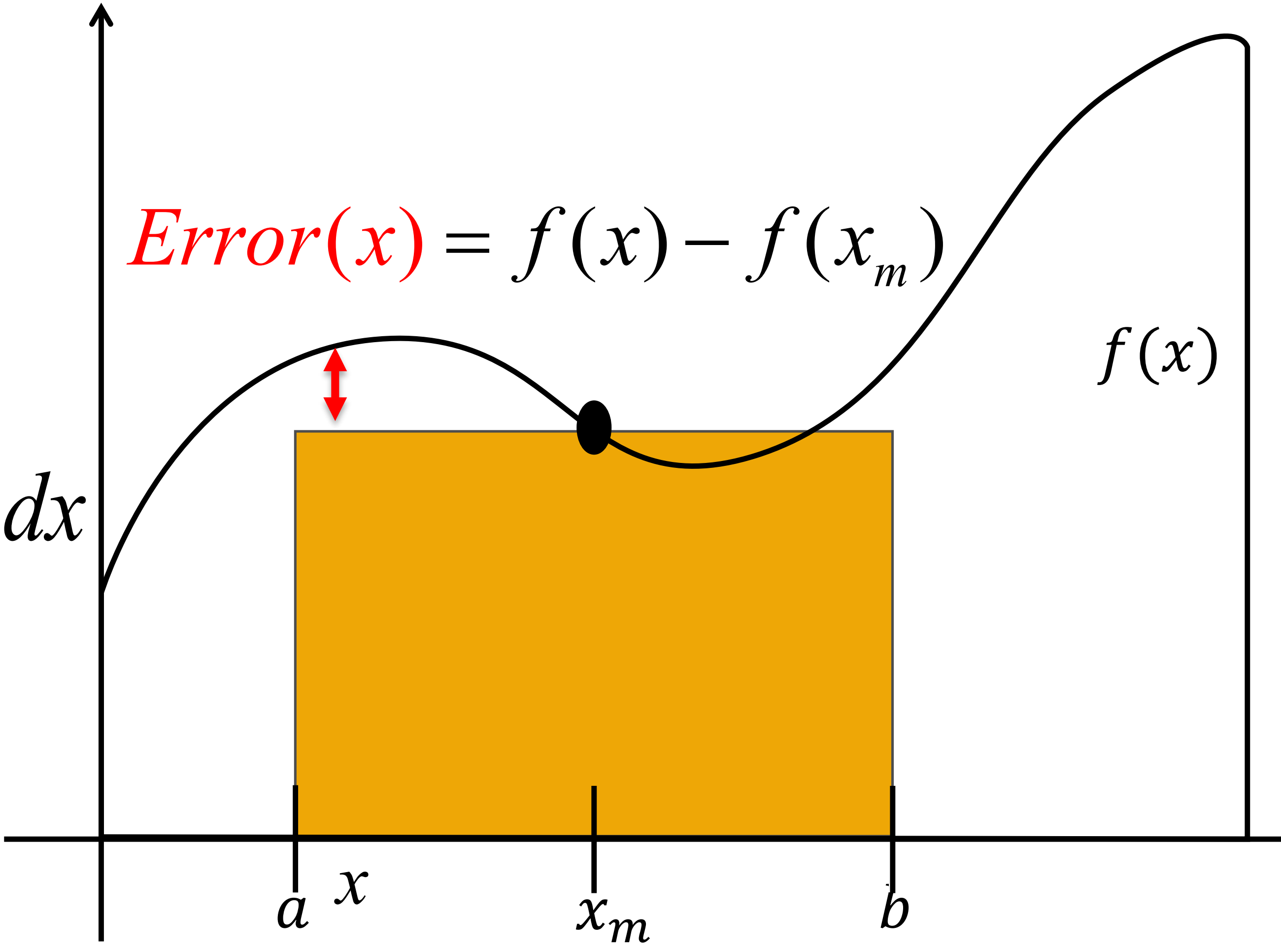
(iii) Obtain an expression involving h or Δx the step width or mesh spacing of the numerical method.

Midpoint Rule Quadrature Error

$$Error(x) = f(x) - f(x_m)$$

$$E_{ab} = \int_a^b Error(x)dx$$

$$x_m = \frac{a+b}{2}$$



Estimating the error using Taylors Series

Expand the function being integrated about the midpoint

Error

$$f(x) = f\left(\frac{a+b}{2}\right) + \left(x - \frac{a+b}{2}\right)\frac{df}{dx}\left(\frac{a+b}{2}\right) + \left(x - \frac{(a+b)}{2}\right)^2 \frac{d^2 f}{dx^2}(\xi_i),$$

where $\xi \in (x_i, x_{i+1})$

Estimating the error using Taylors Series

Expand the function being integrated about the midpoint

$$Error(x) = f(x) - f(\frac{a+b}{2})$$

$$Error(x) = (x - \frac{a+b}{2})\frac{df}{dx}(\frac{a+b}{2}) + 0.5(x - \frac{(a+b)}{2})^2 \frac{d^2 f}{dx^2}(\xi_i), \quad \xi \in (x_i, x_{i+1})$$

Estimating the error using Taylors Series

Let I_h be the integral $\mathrm{I} = \int_a^b f(x)dx$ estimated with one interval

Let $\mathrm{I}_{h/2}$ be the integral estimated with two interval

Expand the function being integrated about the midpoint

$$\mathrm{I}\text{-}\mathrm{I}_h = \int_a^b f(x) - f\left(\frac{a+b}{2}\right)dx$$

$$I - I_h = \int_a^b \left(x - \frac{(a+b)}{2}\right)\frac{df}{dx}\left(\frac{(a+b)}{2}\right) + 0.5\left(x - \frac{(a+b)}{2}\right)^2 \frac{d^2 f}{dx^2}(\xi_i)dx$$

Estimating the error using Taylors Series

Expand the function being integrated about the midpoint

$$\mathrm{I} - \mathrm{I}_h = \int_a^b f(x) - f\left(\frac{a+b}{2}\right) dx$$

$$I - I_h = \int_a^b \underbrace{\left(x - \frac{(a+b)}{2}\right)\frac{df}{dx}\left(\frac{(a+b)}{2}\right)}_{=0} + \underbrace{0.5\left(x - \frac{(a+b)}{2}\right)^2 \frac{d^2 f}{dx^2}(\xi_i) dx}$$

Estimating the error using Taylors Series

Expand the function being integrated about the midpoint

$$\text{I-I}_h = \int_a^b f(x) - f(\frac{a+b}{2})dx$$

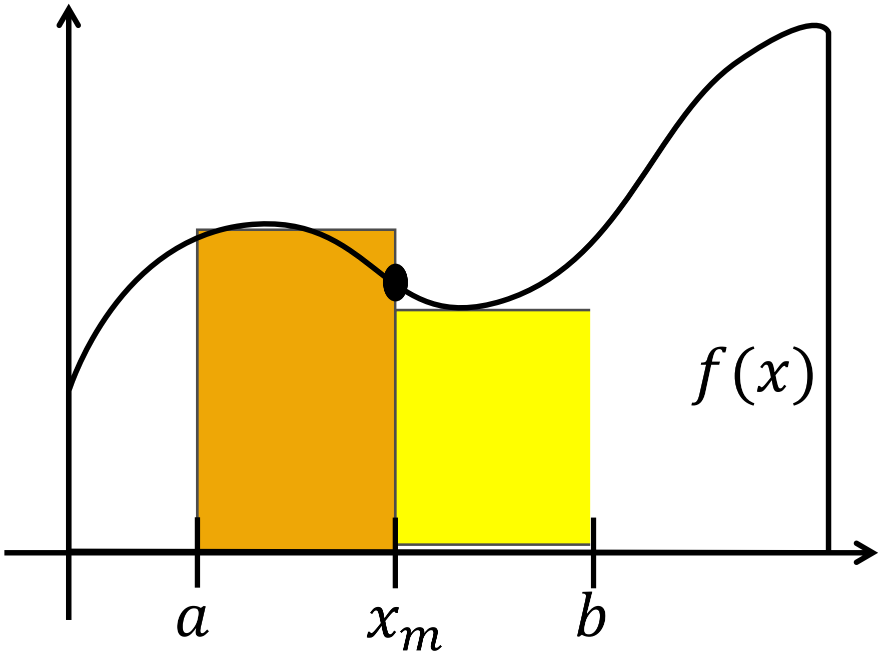
$$I - I_h = \int_a^b \underbrace{(x - \frac{(a+b)}{2})\frac{df}{dx}(\frac{(a+b)}{2})}_{=\,0} + \underbrace{0.5(x - \frac{(a+b)}{2})^2 \frac{d^2 f}{dx^2}(\xi_i)}dx$$

$$= \left[\frac{0.5}{3}(x - \frac{(a+b)}{2})^3 \frac{d^2 f}{dx^2}(\xi_i)\right]_a^b$$

$$= \frac{1}{24}\frac{d^2 f}{dx^2}(\xi_i)(b-a)^3$$

Apply Midpoint Rule Twice

$$I - I_{h/2} = \int_{a}^{x_m} \textcolor{red}{Error(x)}dx \quad + \quad \int_{x_m}^{b} \textcolor{red}{Error(x)}dx$$



$$x_m = \frac{a+b}{2}$$

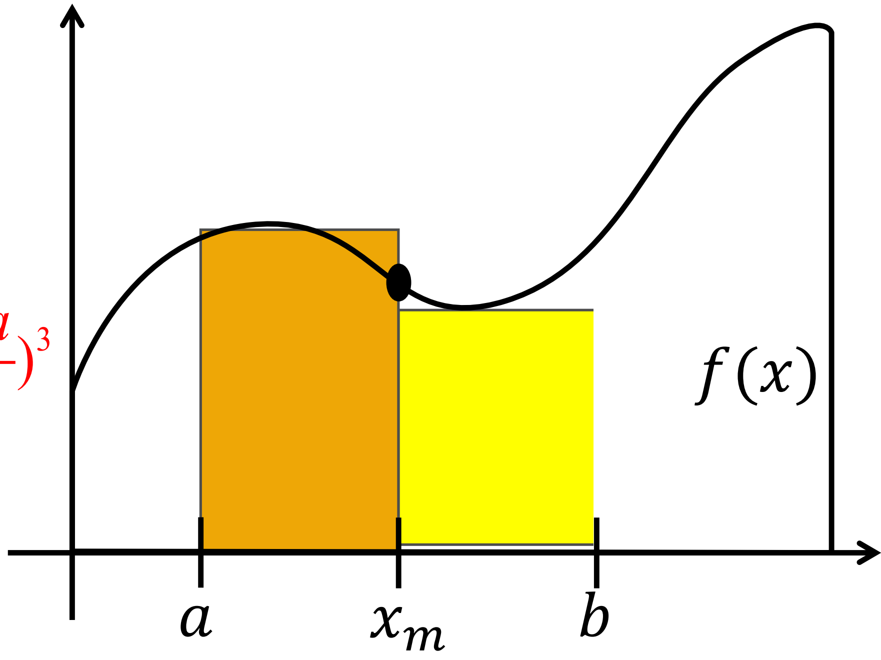
Apply Midpoint Rule Twice

$$I - I_{h/2} = \int_a^{x_m} Error(x)dx \quad + \quad \int_{x_m}^{b} Error(x)dx$$

$$= \frac{1}{24}\frac{d^2 f}{dx^2}(\xi_1)\left(\frac{b-a}{2}\right)^3 + \frac{1}{24}\frac{d^2 f}{dx^2}(\xi_2)\left(\frac{b-a}{2}\right)^3$$

$$= \frac{2}{24}\left(\frac{b-a}{2}\right)^3 \frac{1}{2}\left[\frac{d^2 f}{dx^2}(\xi_1) + \frac{d^2 f}{dx^2}(\xi_2)\right]$$

$$I - I_{h/2} = \frac{2}{24}\left(\frac{b-a}{2}\right)^3 \quad C_2$$



$$x_m = \frac{a+b}{2}$$

How do we actually estimate the error?

Let I_h be the integral estimated with one interval

Let $\mathrm{I}_{h/2}$ be the integral estimated with two interval

Assume that $C_0 = C_2$

Subtract the second equation from the first

$$I_{h/2} - I_h = \frac{3}{4}\frac{1}{24}(b-a)^3\ C_2$$

$$I - I_h = \int_a^b Error(x)dx$$

$$= \frac{1}{24}\frac{d^2 f}{dx^2}(\xi_0)(b-a)^3$$

$$\mathrm{I}\text{-}\mathrm{I}_h \quad = \frac{1}{24}(b-a)^3 C_0$$

$$I - I_{h/2} = \frac{2}{24}\left(\frac{b-a}{2}\right)^3\ C_2$$

We can now estimate the error in either integral

As $$I_{h/2} - I_h = \frac{3}{4}\frac{1}{24}(b-a)^3 \; C_2$$

Then $$\text{I-I}_h = \frac{1}{24}(b-a)^3 C_0 = \frac{4}{3}(I_{h/2} - I_h)$$

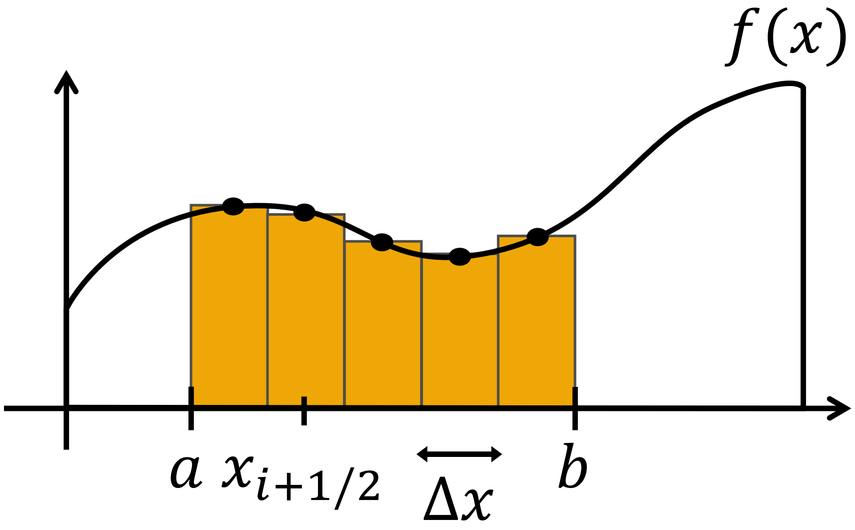
$$I - I_{h/2} = \frac{2}{24}\left(\frac{b-a}{2}\right)^3 \; C_2 = \frac{1}{3}(I_{h/2} - I_h)$$

Hence by doing the calculation twice we can estimate the error in each case!

Composite Midpoint Rule

- Approximate the integral by N applications of the midpoint rule between a and b:

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} w_i f(x_i)$$



- Given $\Delta x = \frac{b-a}{N}$,

$$x_{i+1/2} = a + (i - .5)\Delta x$$

$$w_i = \Delta x$$

Local and Global Errors

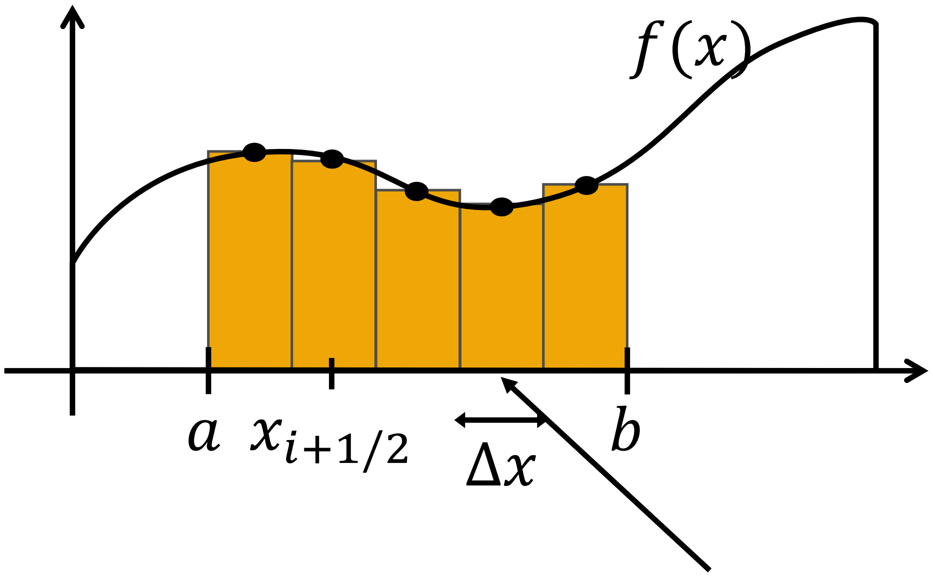
The global; or overall error is given by summing over the intervals:

$$\epsilon \le \frac{N\Delta x^3}{24} f''(\zeta)$$

As $N\Delta x = (b-a)$

$$= \frac{(b-a)\Delta x^2}{24} f''(\zeta)$$

$$= \mathcal{O}(\Delta x^2)$$



Local Error in each interval is $\mathcal{O}(\Delta x^3)$

The global error is one power of Δx less

Estimating the error using Taylors Series Across multiple intervals

Now $\quad a = x_i \quad$ and $\quad b = x_{i+1}$

Error on interval $[x_i, x_{i+1}]$

$$= f''(\xi^*)\frac{\Delta x^3}{24}, \text{ where } \Delta x = x_{i+1} - x_i$$

Error on range of integration $\quad [a,b]$

$$E_{ab} = \sum_{i=1}^{N} f''(\xi_i^*)\frac{\Delta x^3}{24}, \text{ where } \Delta x = x_{i+1} - x_i$$

Now a and b are fixed and b-a $= N\Delta x$

$$E_{ab} = \Delta x N\left[\frac{1}{N}\sum_{i=1}^{N} f''(\xi_i^*)\right]\frac{\Delta x^2}{24}, = (b-a) \;\; C \quad \frac{\Delta x^2}{24}$$

Composite Midpoint Rule

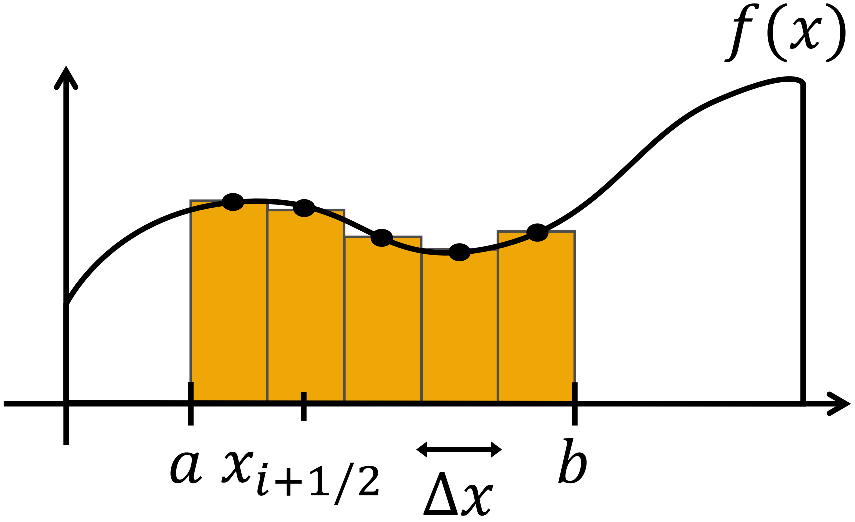
- This rule's error is given by summing over the intervals:

$$\epsilon \leq \frac{N\Delta x^3}{24} f''(\zeta)$$

As $N\Delta x = (b - a)$

$$= \frac{(b-a)\Delta x^2}{24} f''(\zeta)$$

$$= \mathcal{O}(\Delta x^2)$$



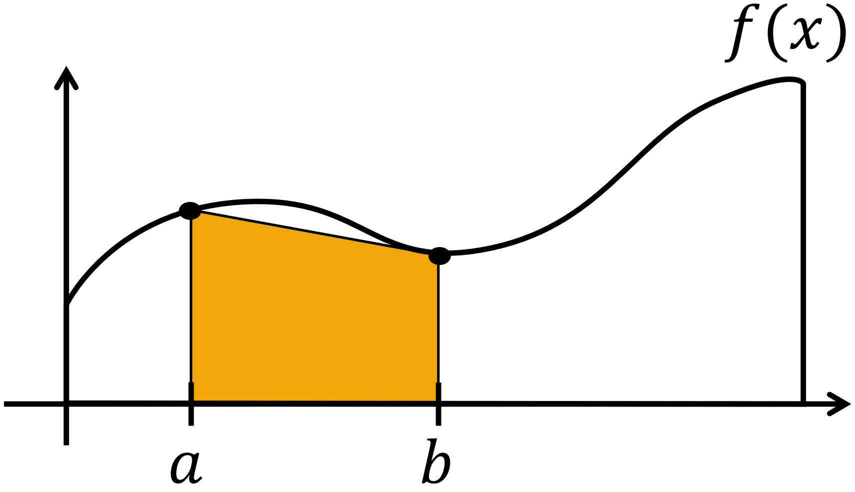
Trapezoidal Rule

- Approximate the integral by the area of a trapezoid with endpoints a and b:

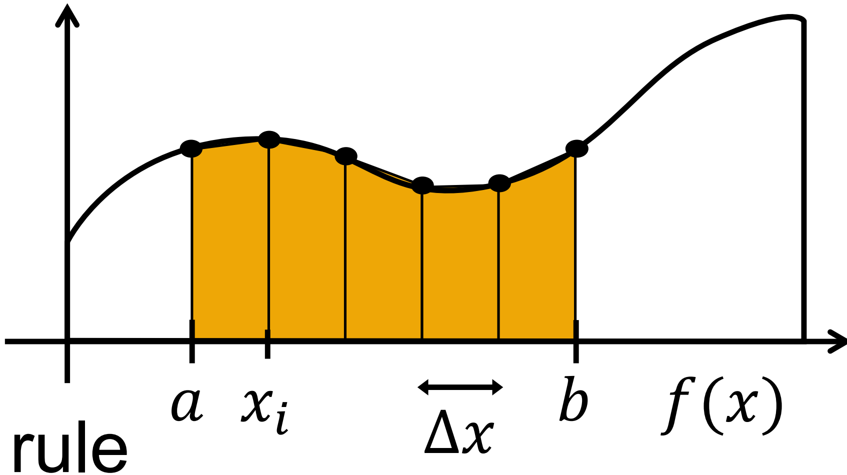
$$\int_a^b f(x)dx \approx \frac{1}{2}(b-a)(f(a)+f(b))$$

- The rule's error on one interval is given by:

$$\epsilon \leq \frac{(b-a)^3}{12} f''(\zeta) = \mathcal{O}((b-a)^3)$$



Composite Trapezoidal Rule



- Approximate the integral by $N-1$ applications of the trapezoidal rule

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N-1} \frac{1}{2}\frac{b-a}{N}[f(x_{\mathrm{i}}) + f(x_{i+1})]$$

where $x_i = a + \frac{(\mathrm{b}-\mathrm{a})}{\mathrm{N}}(\mathrm{i}-1)$

Composite Trapezoidal Rule

- Quadrature notation

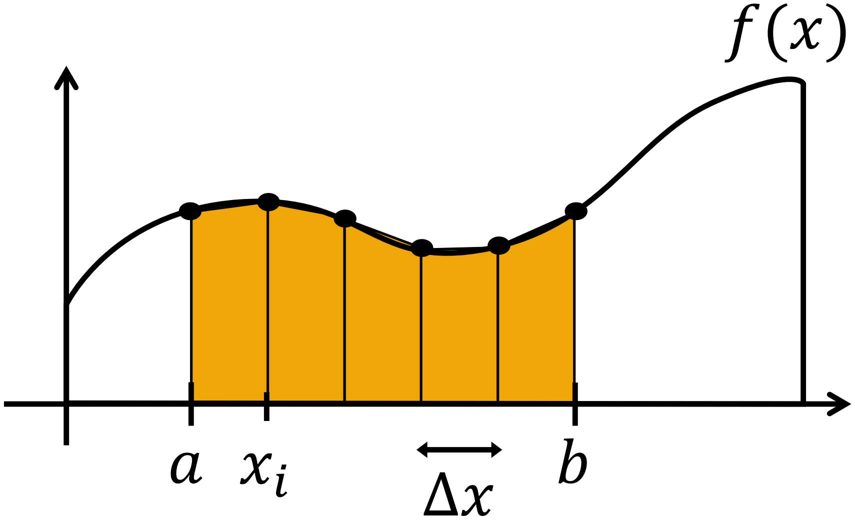
$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} w_i f(x_i)$$

- This can be written as

$$x_i = a + (i-1)\Delta x$$

$$w_i = \begin{cases} \frac{\Delta x}{2}, & i = 1, N \\ \Delta x, & i = 2, \dots, N-1 \end{cases}$$

where $\Delta x = \frac{b-a}{N-1}$



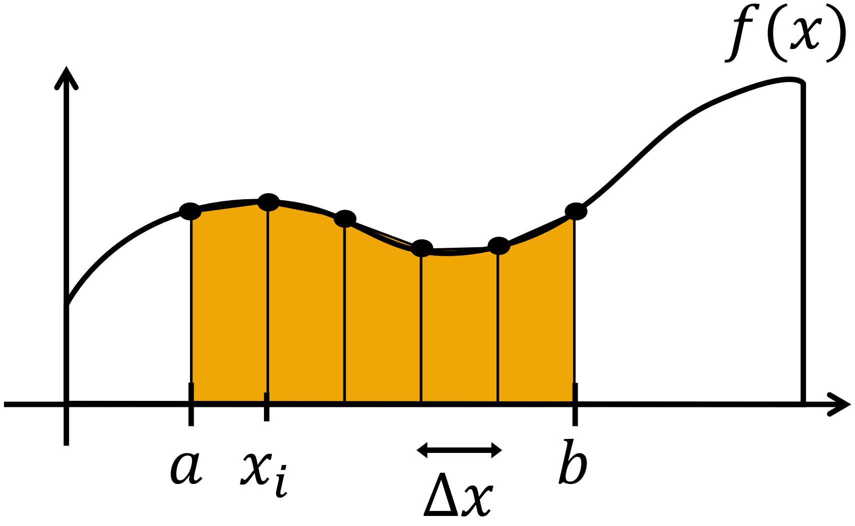
Composite Trapezoidal Rule

- The rule's error on N intervals is governed by:

$$\epsilon \le \frac{N\Delta x^3}{12} f''(\zeta)$$

$$= \frac{(b-a)\Delta x^2}{12} f''(\zeta)$$

$$= \mathcal{O}(\Delta x^2)$$

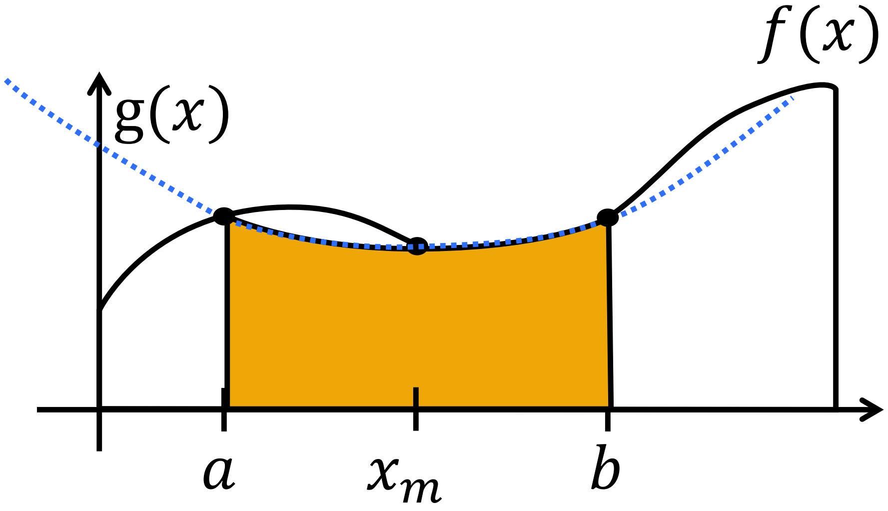


Simpson's Rule

- Evaluate the function at a, b, and the midpoint
- Find a quadratic polynomial with known integral that interpolates the three points
- Approximate the integral by the exact integral of the interpolating polynomial:

$$\int_a^b f(x)dx \approx \int_a^b g(x)dx$$

- We'll use a Quadratic Lagrange Polynomial



Lagrange Polynomial

Quadratic Lagrange Polynomial

- Given known a, x_m, b, and $f(x)$

- $g(x) = f(a)\frac{(x-x_m)(x-b)}{(a-x_m)(a-b)} + f(x_m)\frac{(x-a)(x-b)}{(x_m-a)(x_m-b)} + f(b)\frac{(x-a)(x-x_m)}{(b-a)(b-x_m)}$

- Integral of which is:

$$\int_a^b g(x)dx = \frac{1}{6}(b-a)[f(a) + 4f(x_m) + f(b)]$$

Simpson’s Rule

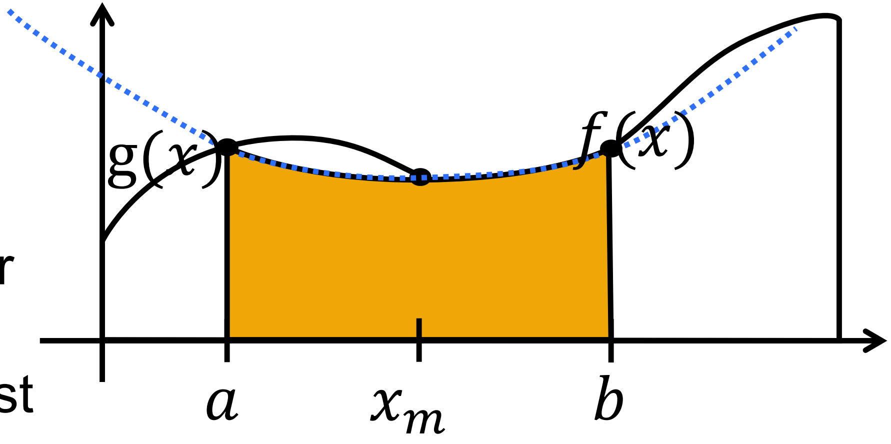
Thus Simpson’s Rule defines the integral by:

$$\int_a^b f(x)dx \approx \frac{1}{6}(b-a)[f(a)+4f(x_m)+f(b)]$$

The error is defined by

$$\epsilon \leq \frac{(b-a)^5}{2880} f^{(4)}(\varphi) = \mathcal{O}\left((b-a)^5\right)$$

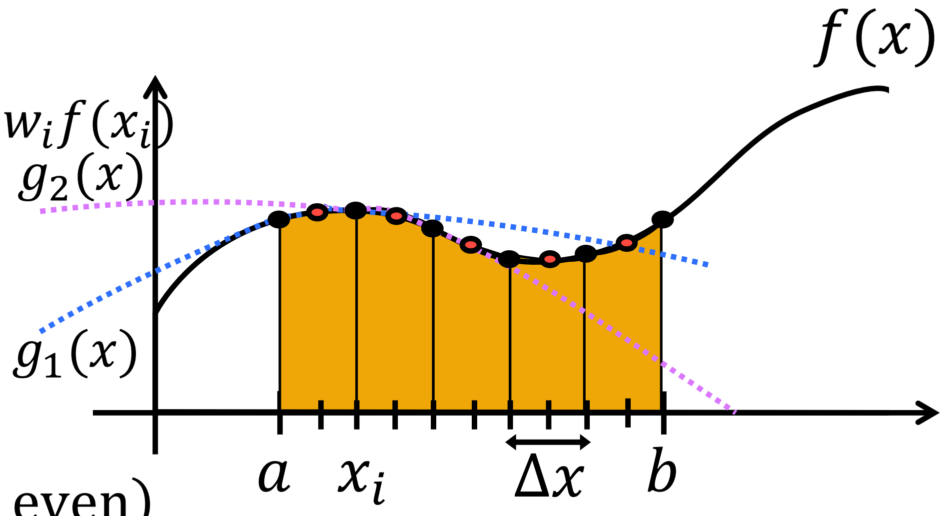
Note there is one extra power of (b-a) over what is expected from interpolating the polynomial error. This is because the lowest interpolation error term integrates to zero…



Composite Simpson's Rule

- In quadrature notation:

$$\int_a^b f(x)dx \approx \sum_{i=1}^{N} \int_a^b g(x)dx = \sum_{i=1}^{2N+1} w_i f(x_i)$$



- Simpson Quadrature:

$$w_i = \begin{cases} \frac{\Delta x}{3} & : \quad i = 1, 2N+1 \\ \frac{4\Delta x}{3} & : \quad i = 2, \ldots, 2N \quad (i \text{ even}) \\ \frac{2\Delta x}{3} & : \quad i = 3, \ldots, 2N-1 \quad (i \text{ odd}) \end{cases}$$

$$x_i = a + (i-1)\Delta x \qquad \text{where } \Delta x = \frac{b-a}{2N}$$

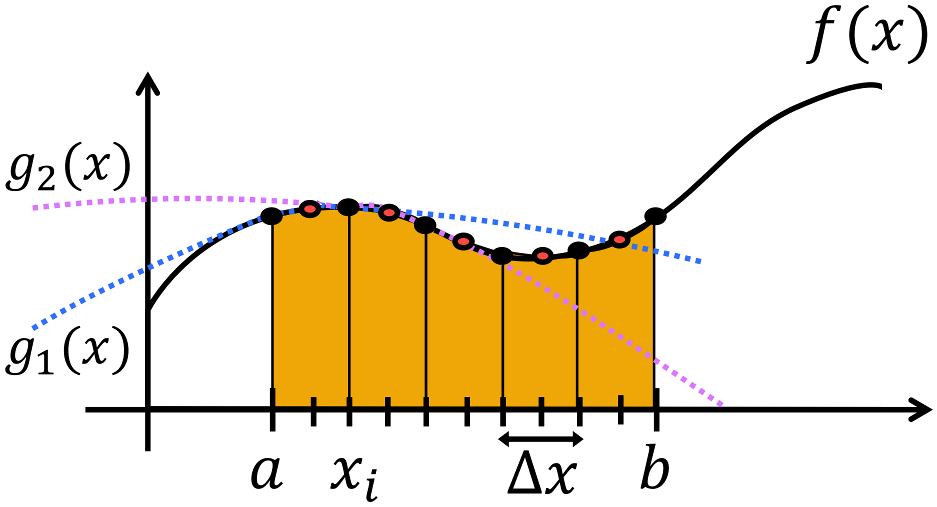
Composite Simpson's Rule

- The error in composite Simpson's rule is governed by:

$$\epsilon \leq \frac{N\Delta x^5}{2880} f^{(4)}(\varphi)$$

$$= \frac{(b-a)\Delta x^4}{2880} f^{(4)}(\varphi)$$

$$= \mathcal{O}(\Delta x^4)$$



Example

$$\int_0^{\pi} \sin(x)\, dx = 2.0$$

n	Trapez.	Simpson
2	1.570796	2.094395
4	1.896119	2.004560
8	1.974232	2.000269
16	1.993570	2.000017
32	1.998393	2.000001
64	1.999598	2.000000
128	1.999900	2.000000
256	1.999975	2.000000
512	1.999994	2.000000
1024	1.999998	2.000000
2048	2.000000	2.000000
4096	2.000000	2.000000
8192	2.000000	2.000000
16384	2.000000	2.000000
32768	2.000000	2.000000
65536	2.000000	2.000000

Example

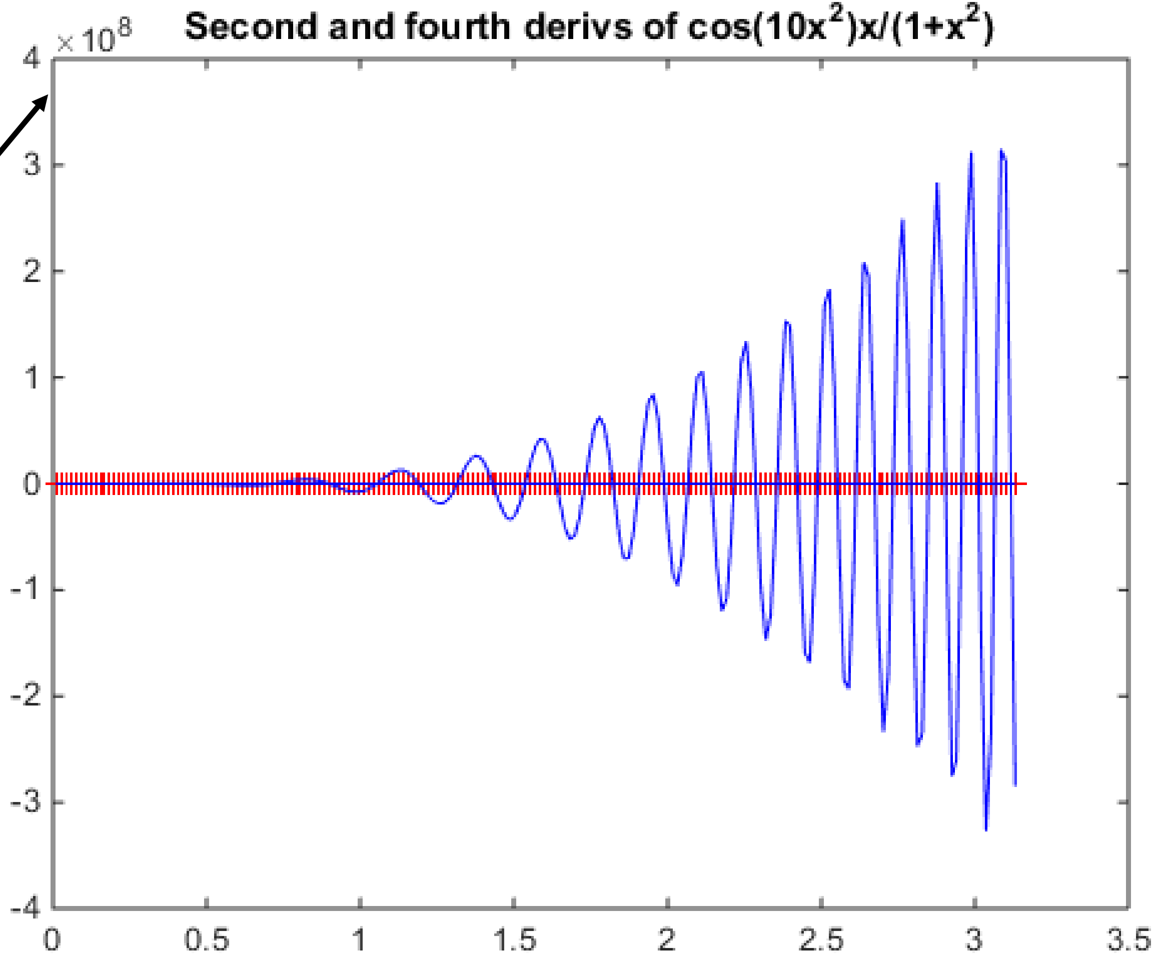
$$\int_0^{\pi} \frac{x}{x^2+1} \cos(10x^2)\, dx = 0.0003156$$

n	Trapez.	Simpson
64	0.004360	−0.013151
128	0.001183	−0.001110
256	0.000526	−0.000311
512	0.000368	0.000006
1024	0.000329	0.000161
2048	0.000319	0.000238
4096	0.000316	0.000277
8192	0.000316	0.000296
16384	0.000316	0.000306
32768	0.000316	0.000311
65536	0.000316	0.000313
131072	0.000316	0.000314
262144	0.000316	0.000315
524288	0.000316	0.000315
1048576	0.000316	0.000315
2097152	0.000316	0.000316
4194304	0.000316	0.000316

Why might trapezoidal be better than Simpson?

Comparison of Second and Fourth Derivatives

Note scale



Trapezoidal error involves second derivatives while Simpson's error involves fourth derivatives

Gaussian Quadrature

- Newton-Cotes formulae use regular spaced sample points.
- Not used with higher order generally as weights can be negative.
- Gaussian quadrature creates a polynomial with non-uniform sampling.
- By picking both the weights and sample points we can get much greater accuracy.

Gaussian Quadrature

- Gaussian quadrature is developed with the idea that we want to specify N points and N weights to integrate a polynomial of $2N-1$ degree polynomial
- For simplicity, Gaussian quadrature is specified over a fixed interval $[-1,1]$:

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{N} w_i f(x_i)$$

Gauss-Legendre Quadrature Table

- In practice, Gaussian quadrature points and weights are tabulated for small N

N	x_i	w_i
1	0	2
2	$\pm 1/\sqrt{3}$	1
3	0	$8/9$
	$\pm\sqrt{3/5}$	$5/9$
4	$\pm\sqrt{(3-2\sqrt{6/5})/7}$	$(18+\sqrt{30})/36$
	$\pm\sqrt{(3+2\sqrt{6/5})/7}$	$(18-\sqrt{30})/36$
5	0	$128/225$
	$\pm\frac{1}{3}\sqrt{5-2\sqrt{10/7}}$	$(322+13\sqrt{70})/900$
	$\pm\frac{1}{3}\sqrt{5+2\sqrt{10/7}}$	$(322-13\sqrt{70})/900$

Gaussian Quadrature - Transforming Intervals

- Substituting for Gaussian quadrature along the interval $[a, b]$ produces the following formula:

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\sum_{i=1}^{N} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

- This quadrature method's error is governed by the following relation:

$$\epsilon \leq \frac{(b-a)^{2N+1}(N!)^4}{(2N+1)\big((2N)!\big)^3} f^{(2N)}(\varphi) = \mathcal{O}\big((b-a)^{2N+1}\big)$$

Example

$$\int_a^b f(x)\,dx\,, \text{where } a = 1, b = 4, f(x) = 2x^2 + x + 1,$$

solution = 52.5

$$\int_a^b f(x)dx \approx \frac{b-a}{2}\sum_{i=1}^{N} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

x_i	w_i	N
0	$\frac{8}{9}$	3
$\pm\sqrt{\frac{3}{5}}$	$\frac{5}{9}$	

Example Continued

Transformed points are

$(a+b)//2 = 5/2$ and $(b-a)/2 = 3/2$

$5/2 - 3/2\sqrt{3/5}$

$5/2 + 3/2 \quad 0$

$5/2 + 3/2\sqrt{3/5}$

$$f\left(-\frac{3}{2}\sqrt{\frac{3}{5}} + \frac{5}{2}\right) = f(1.34) = 5.9$$

$$f\left(\frac{5}{2}\right) = 16$$

$$f\left(\frac{3}{2}\sqrt{\frac{3}{5}} + \frac{5}{2}\right) = f(3.66) = 31.5$$

$$\int_1^4 2x^2 + x + 1 dx \approx \frac{3}{2}\left(\frac{5}{9}5.9 + \frac{8}{9}16 + \frac{5}{9}31.5\right)$$

$$\approx 52.2$$

Gaussian Quadrature – Example

$$\int_0^1 (\mathrm{p}+1)\mathrm{x}\hat{}\mathrm{p}\,dx \approx \frac{1}{2}\sum_{i=1}^{5} w_i(p+1)\left(\frac{1}{2}x_i+\frac{1}{2}\right)\hat{}p$$

Exact value = 1 Matlab results for different values of p

P	2	3	4	5	6	7	8	9	10
Error	2e-16	2e-16	2e-16	4e1-6	4e-16	4e-16	4e-16	4e-16	2e-5

P	11	12	13	14	15	16	17	18	19
Error	9e-5	3e-4	8e-4	2e-3	3e-3	5e-3	8e-3	1e-2	2e-2

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% Gauss Quad Example 5 point formula.   applied to integral from 0 to 1 of (p+1)x^p dx
x(1) = -1/3*sqrt(5.0+2.0*sqrt(10./7.));   w(1)=(322-13.0*sqrt(70))/900.0;
x(2) = -1/3*sqrt(5.0-2.0*sqrt(10./7.));   w(2)=(322+13.0*sqrt(70))/900.0;
x(3) = 0.0;                               w(3)= 128.0/225.0;
x(4) = -x(2);                             w(4)= w(2);
x(5) = -x(1);                             w(5)=w(1);
for p = 2:20
   int = 0.0;
   for i = 1:5
       int = int + 0.5*w(i)*(p+1)*(0.5*x(i)+0.5)^p;     end
   error = abs(1.0-int);     disp(p);disp(error);
end
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Quadrature Summary

- A number of methods for integration of a function may be derived by using polynomial theory
- Methods based upon linear or quadratic polynomials work well for low accuracy
- Methods based based upon high order legendre (or other) polynomials work well at high accuracy if the function being integrated is smooth enough
- Error estimates typically depend on some derivative of the function being integrated and the stepsize used in the formula
- How do we estimate the error without, in many cases, knowing the function itself other than its value at the quadrature points?

Recommended Reading

- Additional Explanation of the:
  - Trapezoidal rule
  - Simpson's rule
  - Gaussian quadrature
- Error Analysis for Midpoint, Trapezoid, and Simpson Rules
  - http://pages.cs.wisc.edu/~amos/412/lecture-notes/lecture19.pdf