计算物理

Lecture 10

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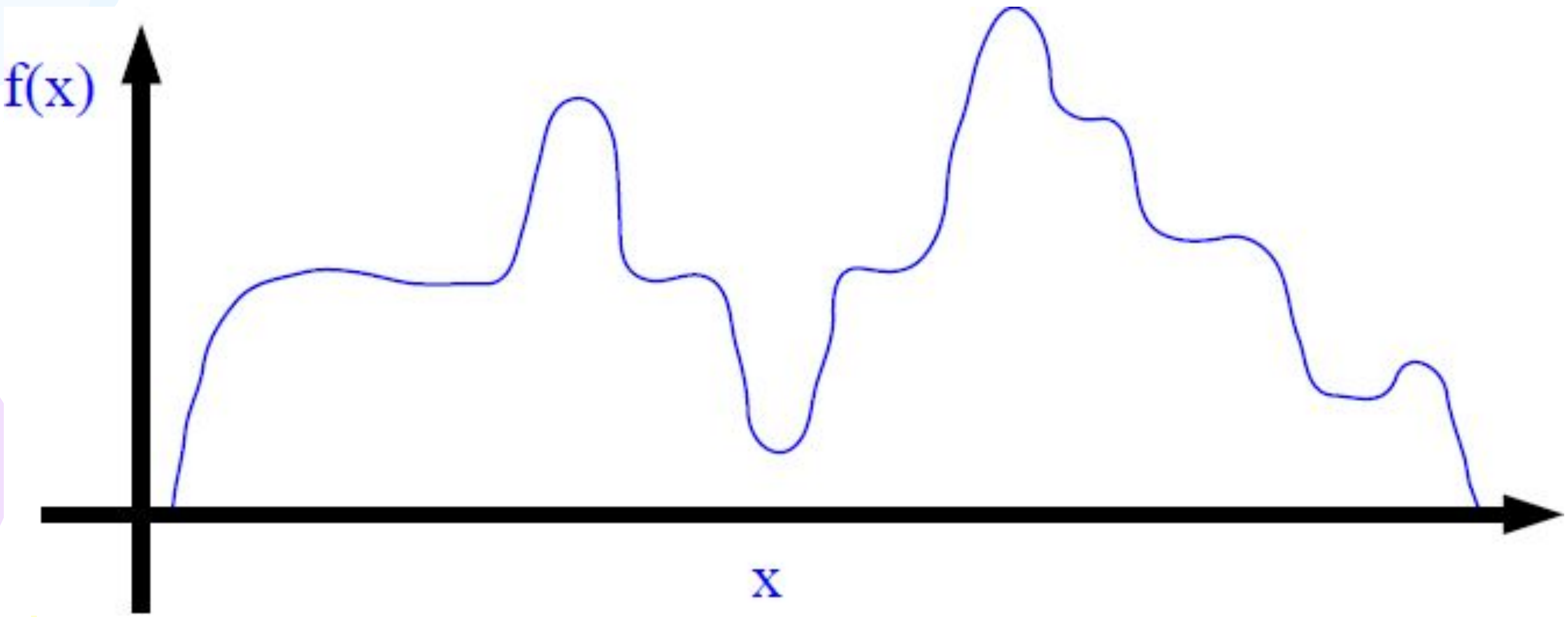
Today's Lecture

- Numerical integration
  - Simple rules
  - Romberg Integration
  - Gaussian quadrature
- References: Numerical Recipes has a pretty good discussion

Numerical Integration

For a given function f(x) the solution can exist in an exact analytical form but frequently an analytical solution does not exist and it is therefore necessary to solve the integral numerically



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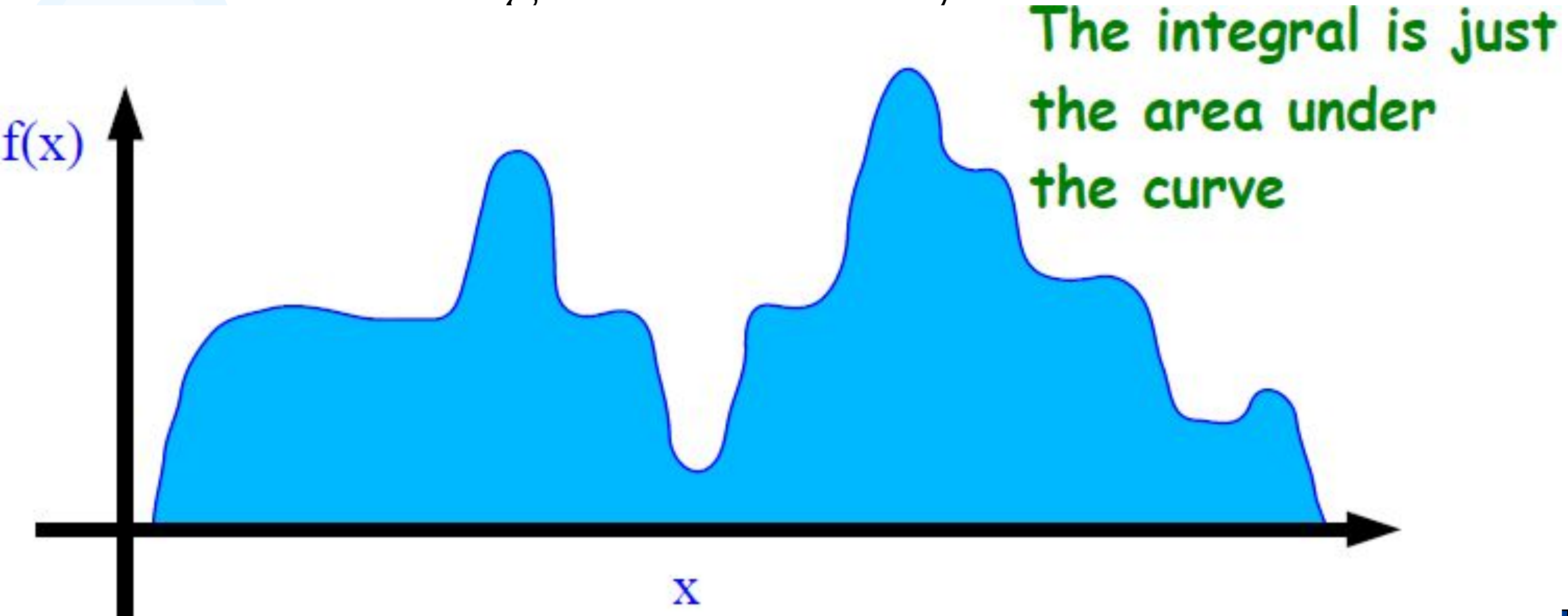
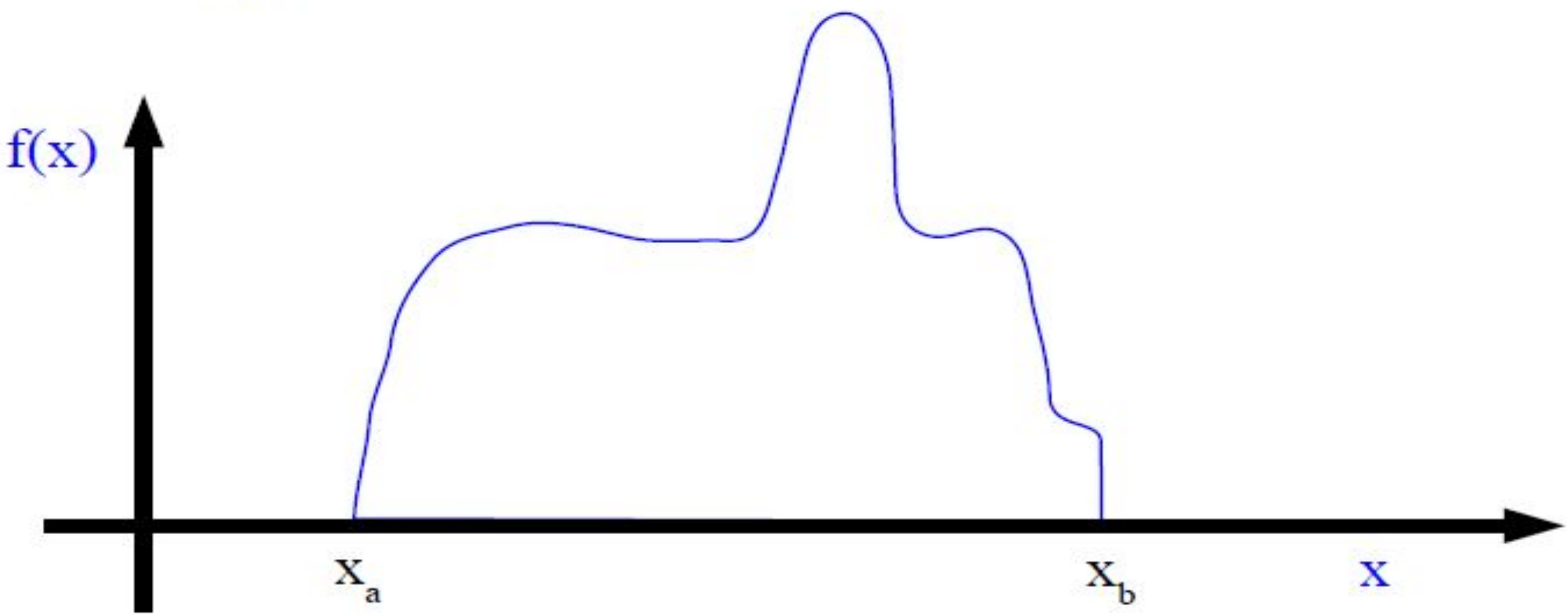


Calculate Area to Calculate Integral

Newton-Cotes Method of Order Zero [Rectangle Midpoint Rule]

- approximate f(x) as a constant
  - $f(x) \approx f(x=x_{midpoint})$
- area = $f(x_{mid})$ *w



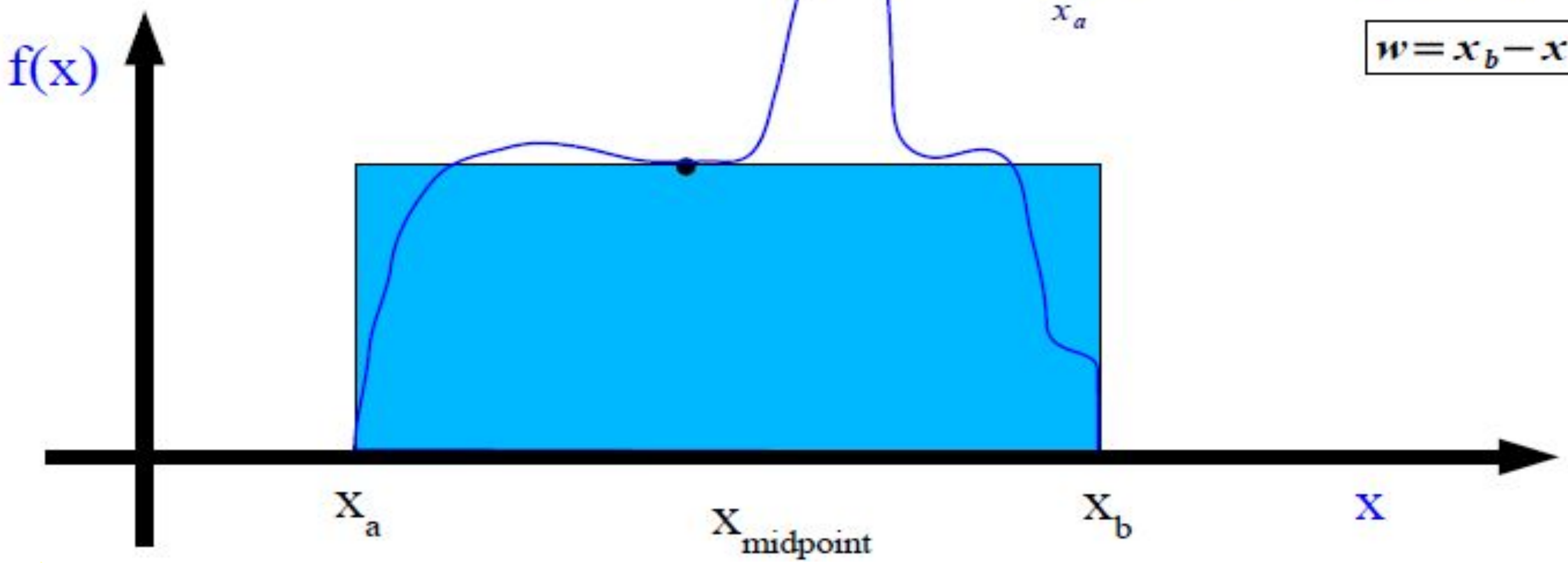
Calculate Area to Calculate Integral

Newton-Cotes Method of Order Zero [Rectangle Midpoint Rule]

- approximate f(x) as a constant
  - $f(x) \approx f(x = x_{midpoint})$
- area = $f(x_{mid}) * w$

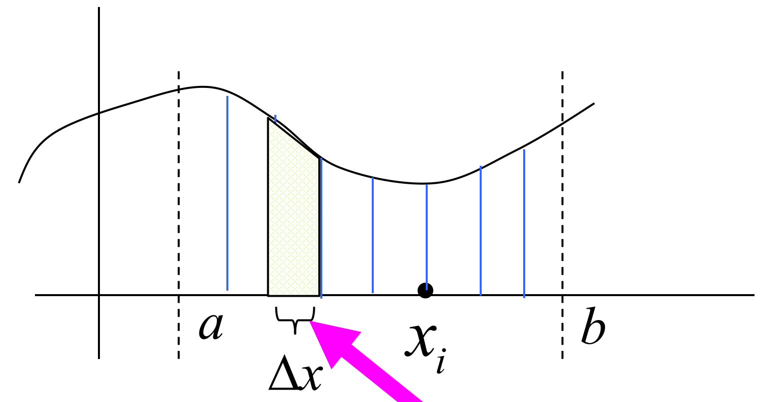
$$\int_{x_a}^{x_b} f(x)\,dx \approx f(x_m) * w$$

$$\boxed{w = x_b - x_a}$$



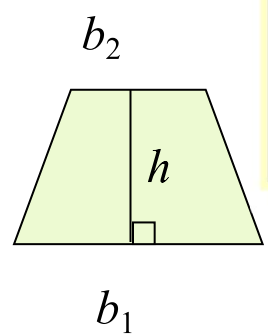
Trapezoidal Rule

- Instead of calculating approximation rectangles we will use trapezoids
  - More accuracy



- Area of a trapezoid

$$A=\frac{1}{2}\left(b_1+b_2\right)\cdot h$$

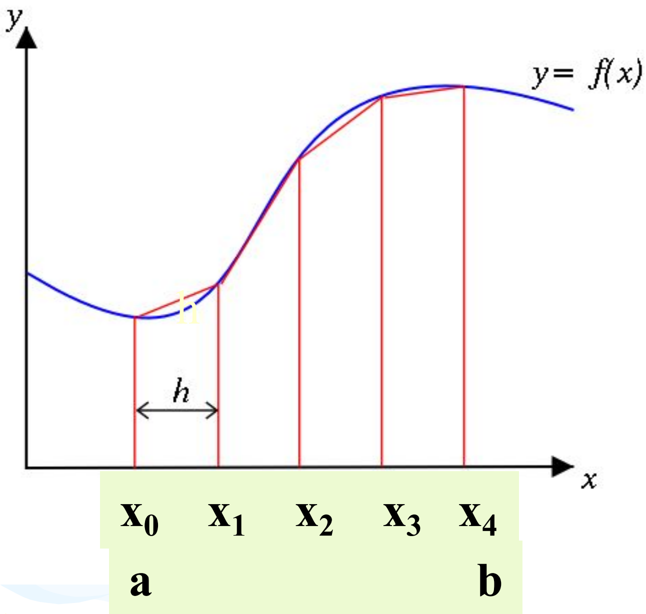


- Which dimension is the h?
- Which is the b_1 and the b_2

Quadrature & interpolation

- Quadrature has become a synonym for numerical integration
  - Primarily in 1d, higher dimensional evaluation is sometimes dubbed cubature
- All quadrature methods rely upon the interpolation of the integral function f using a class of functions
  - e.g. polynomials
  - Utilizing the known closed form integral of the interpolated function allows simple calculation of the weights
- Different functions will require different quadrature algorithms
  - Singular functions may require specialized Gaussian quadrature, or changes of variables
  - Oscillating functions require simpler methods, e.g. trapezoidal rule

Consider definite integration using trapezoids



Approximate integral using the areas of the trapezoids

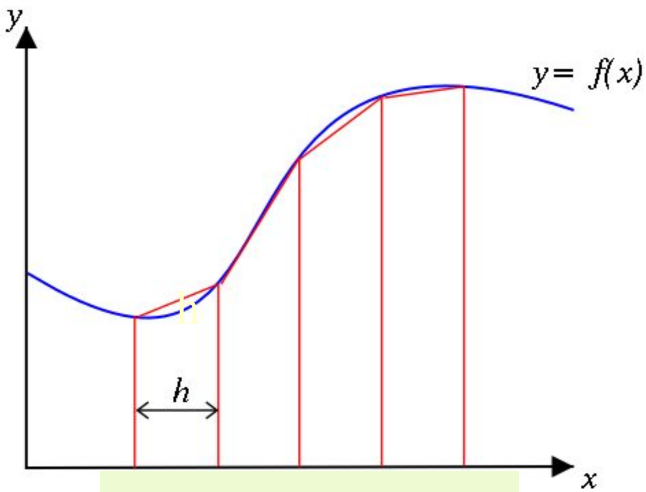
$$\int_a^b f(x)dx \cong \sum \text{area of trapezoids}$$

$$= h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + h\frac{f(x_2)+f(x_3)}{2} + h\frac{f(x_3)+f(x_4)}{2}$$

$$= \frac{h}{2}\left[f(x_0)+2f(x_1)+2f(x_2)+2f(x_3)+f(x_4)\right]$$

$$= \frac{h}{2}\left[f(x_0)+f(x_4)\right]+h\left[f(x_1)+f(x_2)+f(x_3)\right]$$

Consider definite integration using trapezoids



x_0 x_1 x_2 x_3 x_4

a b

- Approximate integral using the areas of the trapezoids

For *n* intervals general formula is

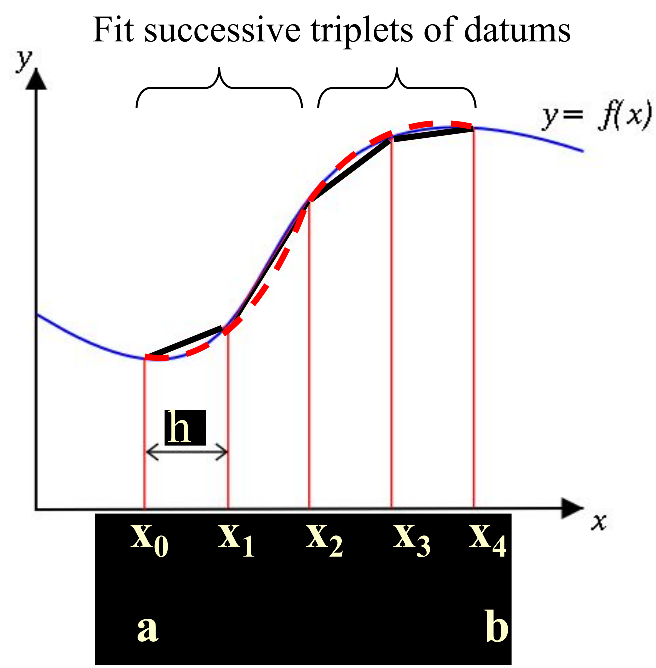
$$\int_a^b f(x)dx \cong \frac{h}{2}\left[f(a)+f(b)\right]+h\sum_{i=1}^{n-1} f(x_i) \qquad (1)$$

The *composite trapezoidal rule.*

Fitting multiple parabolas

- Using triplets of datums we can fit a parabola using the Lagrange interpolation polynomial

$$p_1(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)$$



- If the x_i, x_{i+1} are separated by h then

$$p_1(x) = \frac{(x-x_1)(x-x_2)}{2h^2} f(x_0) - \frac{(x-x_0)(x-x_2)}{h^2} f(x_1) + \frac{(x-x_0)(x-x_1)}{2h^2} f(x_2)$$

Need to integrate this expression to get area under the parabola

Compound Simpson's Rule

- After slightly lengthy but trivial algebra we get

$$\int_{x_0}^{x_2} p_1(x)dx = \frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)]$$

This is "Simpson's 3-point Rule"

- We can do the same on x_2, x_3, x_4 to get

$$\int_{x_2}^{x_4} p_1(x)dx = \frac{h}{3}[f(x_2)+4f(x_3)+f(x_4)]$$

- Hence on the entire region

$$\int_{x_0}^{x_4} f(x)dx \cong \frac{h}{3}[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+f(x_4)]$$

- In general for an even number of intervals n

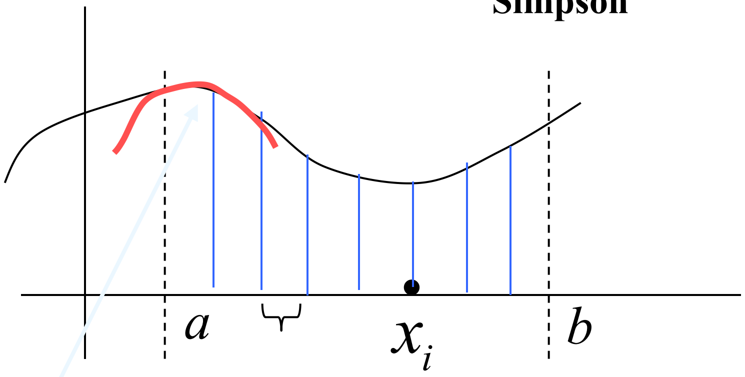
$$\int_a^b f(x)dx \cong \frac{h}{3}[f(a)+f(b)]+\frac{4h}{3}\sum_{i=1}^{\frac{n}{2}} f(x_{2i-1})+\frac{2h}{3}\sum_{i=1}^{\frac{n}{2}-1} f(x_{2i})$$

This is "Simpson's Composite Rule"

Simpson's Rule

Snidly Fizbane Simpson

- As before, we divide the interval into n parts
  - n must be even



- Instead of straight lines we draw parabolas through each group of three consecutive points
  - This approximates the original curve for finding definite integral – formula shown below

$$\int_a^b f(x)dx \approx \frac{dx}{3}[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+2f(x_4)$$

$$+\ldots+2f(x_{n-2})+4f(x_{n-1})+f(x_n)]$$

Higher order fits

- Can increase the order of the fit to cubic, quartic etc.
- For a cubic fit over x_0, x_1, x_2, x_3 we find

$$\int_{x_0}^{x_3} f(x)dx \cong \frac{3h}{8}\left[f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right]$$

Simpson's 3/8th Rule

- For a quartic fit over x_0, x_1, x_2, x_3, x_4

$$\int_{x_0}^{x_4} f(x)dx \cong \frac{2h}{45}\left[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)\right]$$

Boole's Rule

- In practice these higher order formulas are not that useful, we can devise better methods if we first consider the errors involved

Newton Cotes Formulae

- The trapezoid & Simpson's rule are examples of Newton-Cotes formulae ("Interpolatory quadrature rules")
  - Assume fixed $Dx=(b-a)/m$
  - Higher order formulae are given on mathworld.wolfram.com
    - Limit to value of higher order formulae, compound formulae with adaptive step sizes are usually better
- Lagrange interpolating polynomials are found to approximate a function given at $f(x_n)$
- The "degree" of the rule is defined as the order p of the polynomial that the quadrature rule integrates exactly
  - Trapezoid rule – $p=1$
  - Simpson's rule – $p=2$

Newton-Cotes Methods

- In Newton-Cote Methods, the function is approximated by a polynomial of order *n*
- Computing the integral of a polynomial is easy.

$$\int_a^b f(x)dx \approx \int_a^b \left(a_0 + a_1 x + \ldots + a_n x^n\right)dx$$

$$\int_a^b f(x)dx \approx a_0(b-a) + a_1 \frac{(b^2 - a^2)}{2} + \ldots + a_n \frac{(b^{n+1} - a^{n+1})}{n+1}$$

Newton-Cotes Methods

– Trapezoid Method (First Order Polynomial are used)

$$\int_a^b f(x)dx \approx \int_a^b \left(a_0 + a_1 x\right)dx$$

– Simpson 1/3 Rule (Second Order Polynomial are used),

$$\int_a^b f(x)dx \approx \int_a^b \left(a_0 + a_1 x + a_2 x^2\right)dx$$

Error in the Trapezoid Rule

- Consider a Taylor expansions of $f(x)$ about a

$$f(x) = f(a) + (x-a)f'(a) + \frac{(x-a)^2}{2!}f''(a) + \frac{(x-a)^3}{3!}f'''(a) + \ldots$$

- The integral of $f(x)$ written in this form is then

$$\int_a^b f(x)dx = \left[xf(a) + \frac{(x-a)^2}{2!}f'(a) + \frac{(x-a)^3}{3!}f''(a) + \frac{(x-a)^4}{4!}f'''(a) + \frac{(x-a)^5}{5!}f''''(a) + \ldots . \right]_a^b$$

$$= hf(a) + \frac{h^2}{2}f'(a) + \frac{h^3}{6}f''(a) + \frac{h^4}{24}f'''(a) + \ldots \qquad (1)$$

where $h=b-a$

Error in the Trapezoid Rule II

- Perform the same expansion about b

$$\int_a^b f(x)dx = hf(b) - \frac{h^2}{2} f'(b) + \frac{h^3}{6} f''(b) - \frac{h^4}{24} f'''(b) + \ldots \qquad (2)$$

- If we take an average of (1) and (2) then

$$\int_a^b f(x)dx = \frac{h}{2}[f(a) + f(b)] + \frac{h^2}{4}[f'(a) - f'(b)] + \frac{h^3}{12}[f''(a) + f''(b)]$$
$$+ \frac{h^4}{48}[f'''(a) - f'''(b)] + \frac{h^5}{240}\left[f^{iv}(a) + f^{iv}(b)\right] + \ldots \qquad (3)$$

- Notice that odd derivatives are differenced while even derivatives are added

Error in the Trapezoid Rule III

- We also make Taylor expansions of f' and f''' around both *a* & *b*, which allow us to substitute for terms in f'' and f^{iv} and to derive

$$\int_a^b f(x)dx = \frac{h}{2}[f(a)+f(b)] + \frac{h^2}{12}[f'(a)-f'(b)] + \frac{h^4}{720}[f'''(a)-f'''(b)] + \ldots \qquad (10)$$

- It takes *quite a bit of work* to get to this point, but the key issue is that we have now created correction terms which are all *differences*
- If we now use this formula in the composite trapezoid rule there will be a large number of cancellations

Error in the Composite Trapzoid

- We now sum over a series of trapezoids to get

$$
\begin{aligned}
\int_a^b f(x)dx &= \frac{h}{2}\left[\left(f(a)+f(x_1)\right)+\left(f(x_1)+f(x_2)\right)+\ldots+\left(f(x_{n-2})+f(x_{n-1})\right)+\left(f(x_{n-1})+f(b)\right)\right] \\
&+\frac{h^2}{12}\left[\left(f'(a)-f'(x_1)\right)+\left(f'(x_1)-f'(x_2)\right)+\ldots+\left(f'(x_{n-2})-f'(x_{n-1})\right)+\left(f'(x_{n-1})-f'(b)\right)\right] \\
&+\frac{h^4}{720}\left[\left(f'''(a)-f'''(x_1)\right)+\left(f'''(x_1)-f'''(x_2)\right)+\ldots+\left(f'''(x_{n-2})-f'''(x_{n-1})\right)+\left(f'''(x_{n-1})-f'''(b)\right)\right] \\
&+\ldots \\
&=\frac{h}{2}\left[f(a)+f(b)\right]+h\sum_{i=1}^{n-1}f(a+ih)+\frac{h^2}{12}\left[f'(a)-f'(b)\right]+\frac{h^4}{720}\left[f'''(a)-f'''(b)\right]+\ldots \qquad (11)
\end{aligned}
$$

- Note now $h=(b-a)/n$
- The expansion is in powers of h^{2i}

Error Estimation

- Trapezoidal error for *f* on [*a, b*]
  - Where M = max value of |f ''(x)| on [a, b]

$$\left|E_n\right| \le \frac{(b-a)^3}{12n^2} \cdot M$$

- Simpson's error for *f* on [*a, b*]
  - Where *K* = max value of $|f^{(4)}(x)|$ on [*a, b*]

$$\left|E_n\right| \le \frac{(b-a)^5}{180n^4} \cdot K$$

Example

$$\boxed{\int_0^{\pi} \sin(x)dx, \quad find\ h\ so\ that\ |\text{error}| \le \frac{1}{2}\times 10^{-5}}$$

$$|Error| \le \frac{b-a}{12} h^2 \max_{x\in[a,b]} |f''(x)|$$

$$b=\pi;\ a=0; \quad f'(x)=\cos(x); \quad f''(x)=-\sin(x)$$

$$|f''(x)| \le 1 \quad \Rightarrow |Error| \le \frac{\pi}{12}h^2 \le \frac{1}{2}\times 10^{-5}$$

$$\Rightarrow \qquad h^2 \le \frac{6}{\pi}\times 10^{-5}$$

Euler-Maclaurin Integration rule

- The formula (11) we just derived is called the Euler-Maclaurin integration rule. It has a number of uses:
  - If the integrand is easily differentiable the correction terms can be calculated precisely
  - We can use Richardson Extrapolation to remove the first error term and progressively produce a more accurate result
  - If the derivatives at **the end points** are zero then the formula immediately tells you that the simple Trapezoid Rule gives extremely accurate results!

Richardson Extrapolation: Review

- Idea is to improve results from numerical method from order $O(h^k)$ to $O(h^{k+1})$
- Suppose we have a quantity A that is represented by the expansion $A = A(h) + Kh^k + K'h^{k+1} + K''h^{k+2} + \ldots$
  - K, K', K'' are unknown and represent error terms, k is a known constant
- Write this expansion as $A = A(h) + Kh^k + O(h^{k+1})$ **(1)**
  - Note: If we drop the $O(h^{k+1})$ terms we have a linear equation in A & K
- By *reducing* the step size we get another equation for A

$$A = A(h/2) + K(h/2)^k + O(h^{k+1}) \qquad \textbf{(2)}$$

- Note the $O(h^{k+1})$ terms are different in each expansion

Eliminate the leading error

- So we have two equations in A again:

$$A = A(h) + Kh^k + O(h^{k+1}) \quad (1) \quad \text{and}$$

$$A = A(h/2) + K(h/2)^k + O(h^{k+1}) \quad (2)$$

$$= A(h/2) + \frac{Kh^k}{2^k} + O(h^{k+1})$$

- We can eliminate K, the leading order error:

$$2^k A - A = 2^\mathrm{k} \ (2) \ - \quad (1)$$

$$(2^k\text{-}1)A = 2^k A(h/2) + Kh^k + O(h^{k+1}) - A(h) - Kh^k - O(h^{k+1})$$

$$= 2^k A(h/2) - A(h) + O(h^{k+1})$$

$$\Rightarrow A = \frac{2^k A(h/2) - A(h)}{2^k - 1} + O(h^{k+1})$$

Define the higher order accurate estimate

- We have just eliminated K and found that

$$A = \frac{2^k A(h/2) - A(h)}{2^k - 1} + O(h^{k+1})$$

- Define $B(h)$ as follows: $$B(h) = \frac{2^k A(h/2) - A(h)}{2^k - 1}$$

- Then we have a new equation for A:

$$A = B(h) + O(h^{k+1})$$

- and $B(h)$ is accurate to higher order than our previous $A(h)$ $$A = A(h) + Kh^k + O(h^{k+1})$$

See Numerical Recipes, partially borrowed from A Ferri

Romberg Integration: preliminaries

- The starting point for Romberg integration is the composite trapezoid rule which we may write in the following form

$$I=\int_a^b f(x)\,dx=\frac{h}{2}\left[f(a)+f(b)+2\sum_{i=1}^{n-1}f(x_i)\right]+\frac{h^2}{12}[f'(a)-f'(b)]$$

- Can define a series of trapezoid integrations each with a successively larger *m* and thus more sub-divisions.
  - Let $n=2^{k-1}$: $k=1$ => 1 interval
  - The widths of the intervals are given by $h_k = (b-a)/2^{k-1}$

$$I=\int_a^b f(x)dx=\frac{h_k}{2}\left[f(a)+f(b)+2\sum_{i=1}^{2^{k-1}-1}f(a+ih_k)\right]+\frac{h_k^2}{12}[f'(a)-f'(b)]$$

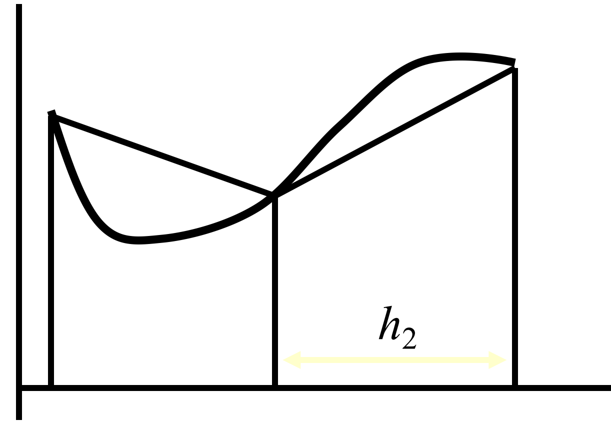
Define this as $R_{k,1}$ (it's just the comp. trap. rule)

Romberg Integration: preliminaries

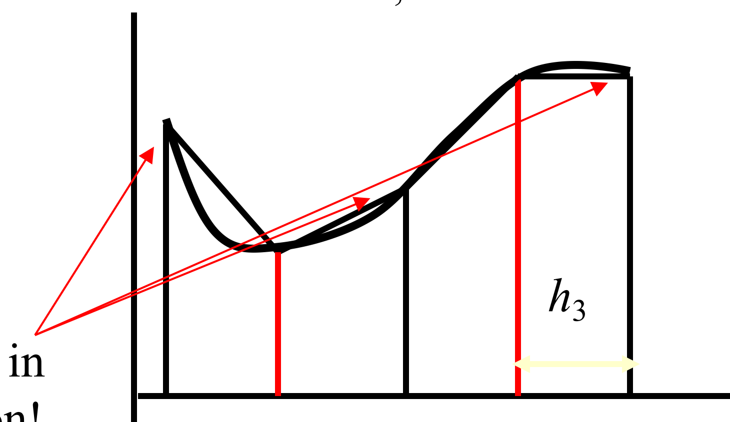
- The $R_{k,1}$ describes a family of progressively more accurate estimates
- Can show (see next slide) that there is a relationship between successive $R_{k,1}$

$$R_{k,1} = \frac{1}{2}\left\{R_{k-1,1} + h_{k-1}\sum_{i=1}^{2^{k-2}} f(a+(2i-1)h_k)\right\}$$

- Each new $R_{k,1}$ adds 2^{k-2} new interior points in the evaluation
- Series converges comparatively slow



$R_{2,1}$



$R_{3,1}$

Recurrence relationship

We defined $R_{k,1} \equiv \frac{h_k}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{2^{k-1}-1} f(a+ih_k) \right]$

Expand sum into odd & even parts and note $h_{k\text{-}1} = 2h_k$

$$R_{k,1} \equiv \frac{h_k}{2}[f(a)+f(b)] + h_k \sum_{i=1,3,5,..}^{2^{k-1}-1} f(a+ih_k) + h_k \sum_{i=2,4,6,..}^{2^{k-1}-1} f(a+ih_k)$$

$$= \frac{h_k}{2}[f(a)+f(b)] + h_k \sum_{i=1,3,5,..}^{2^{k-1}-1} f(a+ih_k) + h_k \sum_{j=1}^{2^{k-2}-1} f(a+2jh_k)$$

Even terms written as $2j$~i, sub for h_k

$$= \frac{h_k}{2}[f(a)+f(b)] + h_k \sum_{j=1}^{2^{k-2}-1} f(a+jh_{k-1}) + h_k \sum_{i=1,3,5,..}^{2^{k-1}-1} f(a+ih_k)$$

$$= \frac{1}{2}\left[\frac{h_{k-1}}{2}[f(a)+f(b)] + h_{k-1} \sum_{j=1}^{2^{k-2}-1} f(a+jh_{k-1}) \right] + h_k \sum_{i=1,3,5,..}^{2^{k-1}-1} f(a+ih_k)$$

$$= \frac{1}{2}\left[R_{k-1,1} + h_{k-1} \sum_{j=1}^{2^{k-2}} f(a+(2j-1)h_k) \right]$$

Odd terms written with $2j$-1~i

Consider $\int_0^{\pi} \sin x\, dx = 2$

$k=1$	$R_{1,1} = \frac{\pi}{2}[\sin(0) + \sin(\pi)] = 0$
$k=2$	$R_{2,1} = \frac{1}{2}[R_{1,1} + \pi \sin(\frac{\pi}{2})] = \frac{\pi}{2}$
$k=3$	$R_{3,1} = \frac{1}{2}[R_{2,1} + \frac{\pi}{2}[\sin(\frac{\pi}{4}) + \sin(\frac{3\pi}{4})]] = 1.8962$
$k=4$	$R_{4,1} = 1.9742$
$k=5$	$R_{5,1} = 1.9936$
$k=6$	$R_{6,1} = 1.9984$

Converges really fairly slowly…

Advantages of Recursive Trapezoid

Recursive Trapezoid:

- Gives the same answer as the standard Trapezoid method.
- Make use of the available information to reduce computation time.
- Useful if the number of iterations is not known in advance.

Motivation for Romberg Method

- Trapezoid formula with an interval h gives error of the order $O(h^2)$

- *We can combine two Trapezoid estimates with intervals $2h$ and h to get a better estimate.*

Romberg Integration

- Idea is to apply Richardson extrapolation to the series of approximations defined by $R_{k,1}$
  - Consider

$$\int_a^b f(x)\,dx = R_{k,1} + \sum_{i=1}^{\infty} K_i h_k^{2i} \Rightarrow \int_a^b f(x)dx - R_{k,1} = K_1 h_k^2 + \sum_{i=2}^{\infty} K_i h_k^{2i} \quad (1)$$

Powers of h_k^{2i} because of Euler-Maclaurin expansion

  - We also have the expansion for the h_{k+1}

$$\int_a^b f(x)\,dx = R_{k+1,1} + \sum_{i=1}^{\infty} K_i h_{k+1}^{2i}$$

$$= R_{k+1,1} + K_1 h_{k+1}^2 + \sum_{i=2}^{\infty} K_i h_{k+1}^{2i} \quad \text{but } h_{k+1} = h_k / 2$$

$$= R_{k+1,1} + \frac{K_1 h_k^2}{2^2} + \sum_{i=2}^{\infty} K_i \frac{h_k^{2i}}{2^{2i}} = R_{k+1,1} + \frac{K_1 h_k^2}{4} + \sum_{i=2}^{\infty} K_i \frac{h_k^{2i}}{4^i}$$

$$\Rightarrow \int_a^b f(x)dx - R_{k+1,1} = \frac{K_1 h_k^2}{4} + \sum_{i=2}^{\infty} K_i \frac{h_k^{2i}}{4^i} \quad (2)$$

Eliminate the leading error again

- So we now subtract ¼ of (1) from (2) to get

$$\frac{3}{4}\int_a^b f(x)\,dx - R_{k+1,1} + \frac{1}{4}R_{k,1} = \frac{K_1 h_k^2}{4} + \sum_{i=2}^{\infty} K_i \frac{h_k^{2i}}{4^i} - \frac{K_1 h_k^2}{4} - \frac{1}{4}\sum_{i=2}^{\infty} K_i h_k^{2i}$$

$$= \sum_{i=2}^{\infty} K_i h_k^{2i}\left(\frac{4-4^i}{4^{i+1}}\right)$$

$$\Rightarrow \int_a^b f(x)dx = \frac{4}{3}R_{k+1,1} + \frac{1}{3}R_{k,1} + \frac{1}{3}\sum_{i=2}^{\infty} K_i h_k^{2i}\left(\frac{1-4^{i-1}}{4^{i-1}}\right)$$

$$= \underbrace{R_{k+1,1} + \frac{\left(R_{k+1,1} - R_{k,1}\right)}{3}}_{\text{Define this as } R_{k,2}} + \frac{1}{3}\sum_{i=2}^{\infty} K_i h_k^{2i}\left(\frac{1-4^{i-1}}{4^{i-1}}\right)$$

Eliminating the error at stage j

- Almost the same as before except now

$$\int_a^b f(x)\,dx = R_{k,j-1} + \sum_{i=j-1}^{\infty} K_i h_k^{2i} \Rightarrow \int_a^b f(x)\,dx = R_{k,j-1} + K_{j-1} h_k^{2(j-1)} + \sum_{i=j}^{\infty} K_i h_k^{2i} \text{ (A)}$$

and $\int_a^b f(x)\,dx = R_{k-1,j-1} + \sum_{i=j-1}^{\infty} K_i h_{k-1}^{2i}$

substitute for $h_{k-1} = 2h_k \Rightarrow \int_a^b f(x)\,dx = R_{k-1,j-1} + 4^{j-1} K_{j-1} h_k^{2(j-1)} + \sum_{i=j}^{\infty} 4^i K_i h_k^{2i}$ (B)

Subtract (B) from $4^{j\text{-}1} \times$(A)to get :

$$(4^{j-1} - 1)\int_a^b f(x)\,dx = 4^{j-1} R_{k,j-1} - R_{k-1,j-1} + \text{terms order } h_k^{2j} \text{ \& higher}$$

$$\Rightarrow \int_a^b f(x)\,dx = \frac{4^{j-1} R_{k,j-1} - R_{k-1,j-1}}{(4^{j-1} - 1)} + \text{terms order } h_k^{2j} \text{ \& higher}$$

$$\therefore \int_a^b f(x)\,dx = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{(4^{j-1} - 1)} + \text{terms order } h_k^{2j} \text{ \& higher}$$

Define this as $R_{k,j}$

Generalize to get Romberg Table

Using our previous definition:

$$\boxed{R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}}$$

Error: $O(h_k^{2j})$

Construct Romberg Table

Obtain from a single composite trapezoidal integration

$$\begin{array}{cccccc}
R_{1,1} & & & & & \\
R_{2,1} & R_{2,2} & & & & \\
R_{3,1} & R_{3,2} & R_{3,3} & & & \\
R_{4,1} & R_{4,2} & R_{4,3} & R_{4,4} & & \\
\vdots & \vdots & \vdots & \vdots & & \\
R_{n,1} & R_{n,2} & R_{n,3} & R_{n,4} & \cdots & R_{n,n}
\end{array}$$

$\boxed{I=R_{n,n} + O(h_n^{2n})}$

$\boxed{I=R_{n,1} + O(h_n^{2})}$

Consider previous example

$$\int_0^{\pi} \sin x \, dx = 2$$

0.00000000					
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	1.99999999	
1.99839336	2.00000103	2.00000000	2.00000000	2.00000000	2.00000000

Error in $R_{6,6}$ is only 6.61026789e-011 – very rapid convergence

Accurate to $O(h_6^{12})$

What is numerical integration really calculating?

- Consider the definite integral

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

- The integral can be approximated by weighted sum

$$I \approx \sum_{i=1}^{n} \omega_i f(x_i)$$

- The w_i are weights, and the x_i are abscissas
- Assuming that f is finite and continuous on the interval $[a,b]$ numerical integration leads to a unique solution
- The goal of any numerical integration method is to choose abscissas and weights such that errors are minimized for the smallest n possible for a given function

NON EXAMINABLE

See Numerical Recipes for a lengthy discussion

Gaussian Quadrature

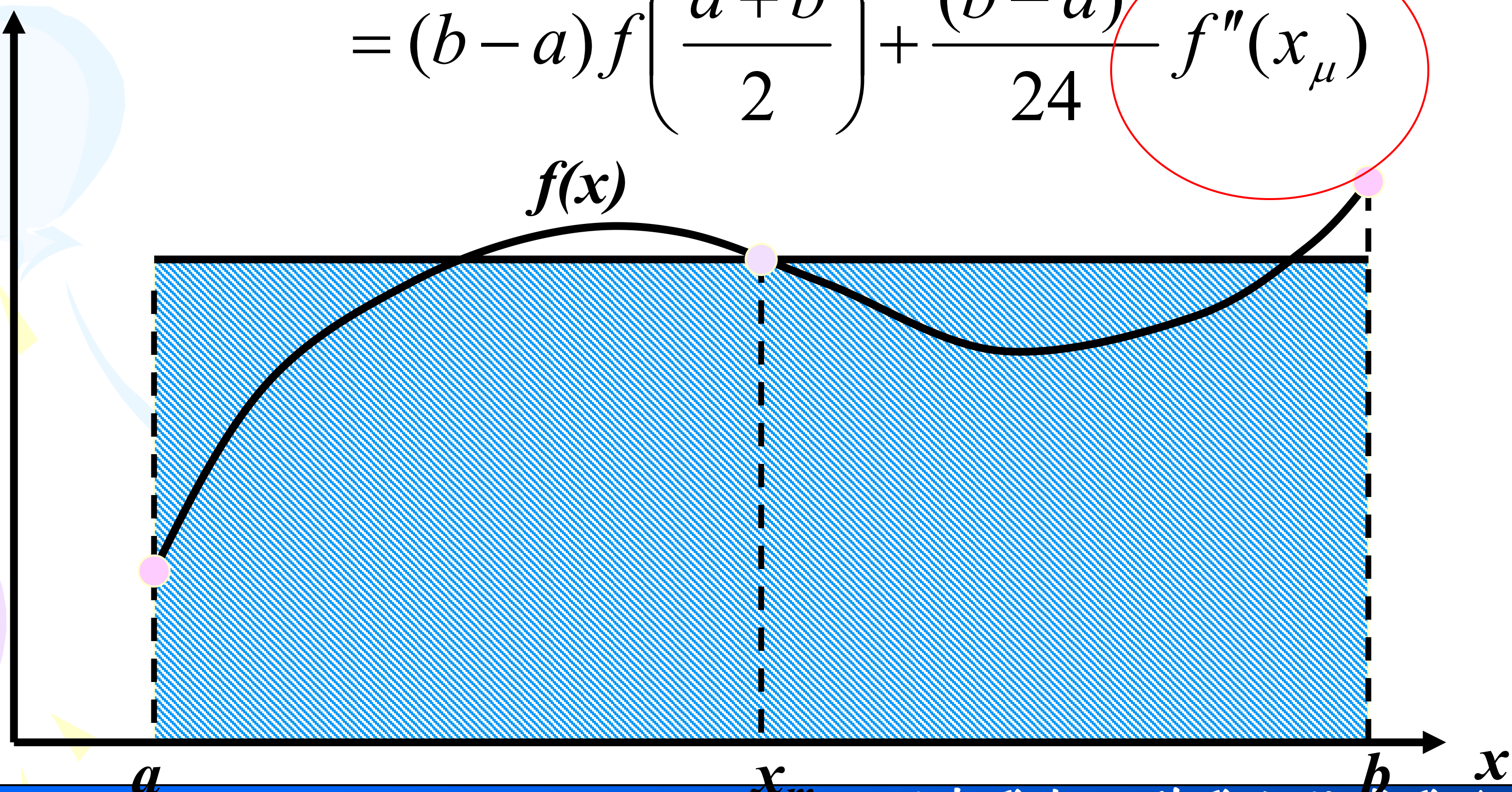
- Thus far we have considered regular spaced abscissas, although we have considered the possibility of adapting spacing
- We've also looked solely at closed interval formulas
- Gaussian quadrature achieves high accuracy and efficiency by optimally selecting the abscissas
- It is usual to apply a change of variables to make the integral map to [-1,1]
- There are also a number of different families of Gaussian quadrature, we'll look at Gauss-Legendre
- Let's look at a related example first

Midpoint Rule: better error properties than expected

$$\int_a^b f(x)dx \approx (b-a)f(x_{mid})$$

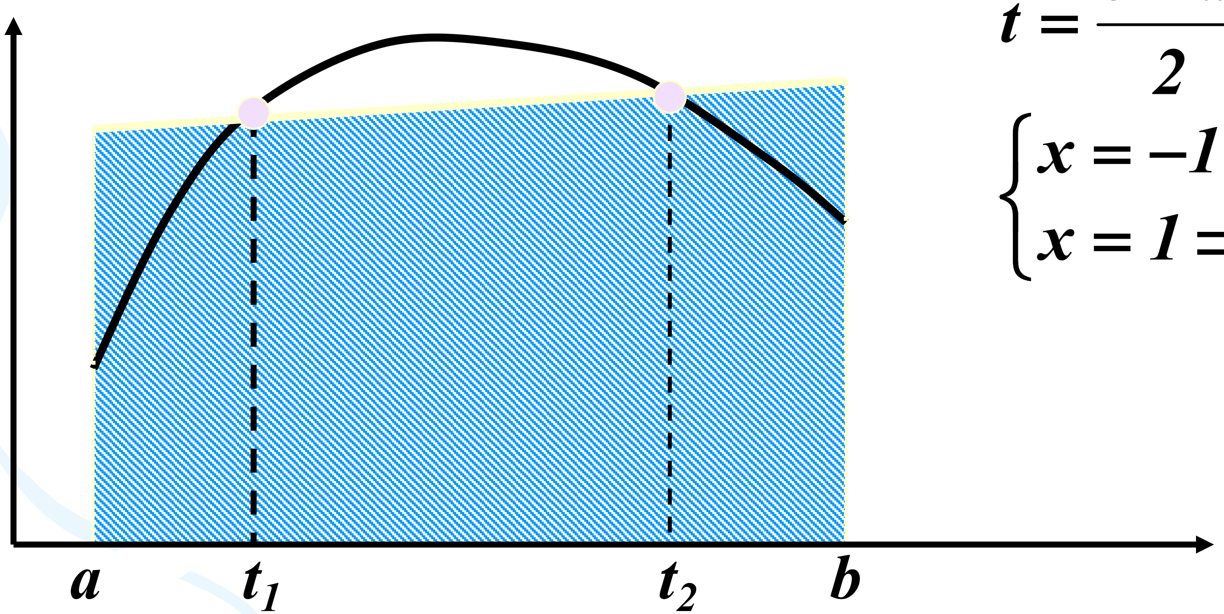
$$=(b-a)f\left(\frac{a+b}{2}\right)+\frac{(b-a)^3}{24}f''(x_\mu)$$

Despite fitting a single value error occurs in second derivative



Coordinate transformation on to [-1,1]

- The transformation is a simple linear mapping



$$t = \frac{b-a}{2}x + \frac{b+a}{2}$$

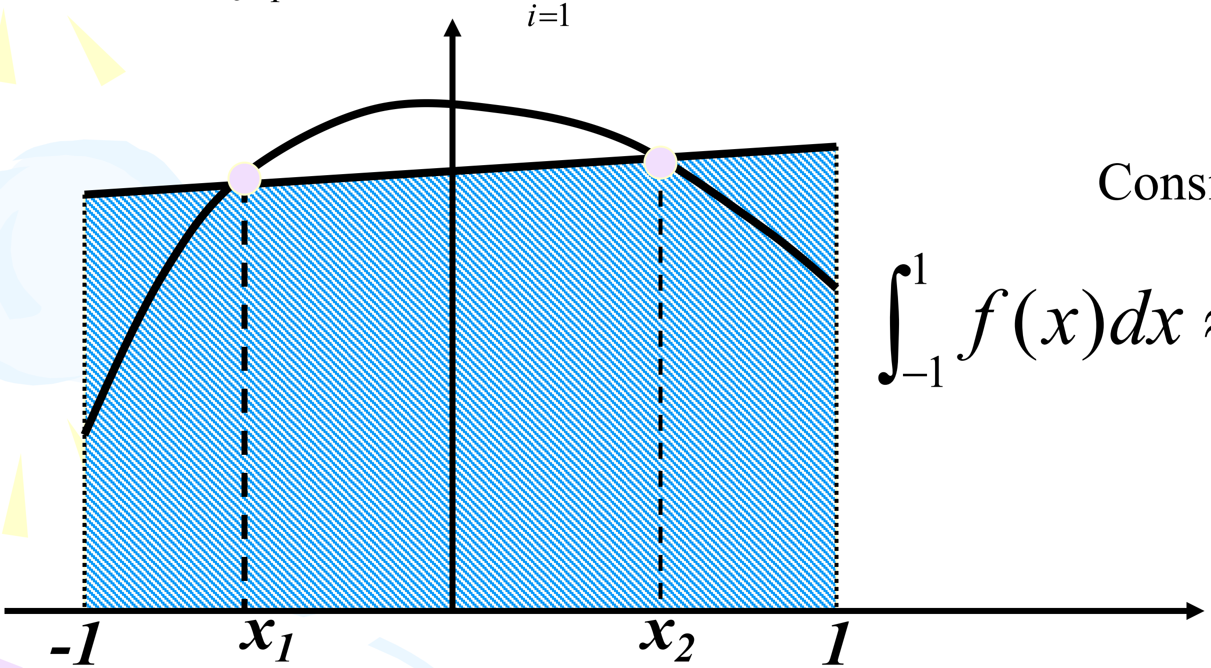
$$\begin{cases} x = -1 \Rightarrow t = a \\ x = 1 \Rightarrow \quad t = b \end{cases}$$

$$\int_a^b f(t)dt = \int_{-1}^{1} f(\frac{b-a}{2}x + \frac{b+a}{2})(\frac{b-a}{2})dx = \int_{-1}^{1} g(x)dx$$

Gaussian Quadrature on [-1, 1]

Recall the original series approximation

$$I=\int_{-1}^{1}f(x)dx\approx\sum_{i=1}^{n}c_i f(x_i)=c_1 f(x_1)+c_2 f(x_2)+\cdots+c_n f(x_n)$$



Consider, n=2, then we have

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

- We have 4 unknowns, c_1, c_2, x_1, x_2, so we can *choose* these values to yield *exact integrals* for $f(x)=x^0, x, x^2, x^3$

Gaussian Quadrature on [-1, 1]

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

Evaluate the integrals for $f = x^0, x^1, x^2, x^3$

– Yields four equations for the four unknowns

$$\begin{cases} f = 1 \Rightarrow \int_{-1}^{1} 1dx = 2 = c_1 + c_2 \\ f = x \Rightarrow \int_{-1}^{1} xdx = 0 = c_1 x_1 + c_2 x_2 \\ f = x^2 \Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 \\ f = x^3 \Rightarrow \int_{-1}^{1} x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3 \end{cases} \Rightarrow \begin{cases} c_1 = 1 \\ c_2 = 1 \\ x_1 = \frac{-1}{\sqrt{3}} \\ x_2 = \frac{1}{\sqrt{3}} \end{cases}$$

$$\boxed{I = \int_{-1}^{1} f(x)dx \cong f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)}$$

Higher order strategies

- Method generalizes in a straightforward way to higher numbers of abscissas
  - Exact integrals increase to always provide *n* integral equations for the *n* unknowns
  - Note the midpoint rule is the n=1 formula
- Example, for n=3
- Need to find $(c_1, c_2, c_3, x_1, x_2, x_3)$ given functions $f(x) = x^0, x^1, x^2, x^3, x^4, x^5$
  - Gives

$$I = \int_{-1}^{1} f(x)dx \cong \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$$

Alternative Gauss-based strategies

- The abscissas are the roots of a polynomial belonging to a class of orthogonal polynomials – in this case Legendre polynomials
- Thus far we considered integrals only of a function f (where f was a polynomial)
- Can extend this to $$\int_a^b W(x) f(x) dx \approx \sum_{i=1}^{m} \omega_i f(x_i)$$
  - Example:

$$I = \int_{-1}^{1} \frac{\exp(-\cos^2 x)}{\sqrt{1-x^2}} dx$$

  - We may also need to change the interval to (-1,1) to allow for singularities
- Why would we do this?
  - To hide integrable singularities in $f(x)$
- The orthogonal polynomials will also change depending on $W(x)$ (can be Chebyshev, Hermite,…)

Summary

- Low order Newton-Cotes formulae have comparatively slow convergence properties
  - Higher order methods have better convergence properties but can suffer from numerical instabilities
  - High order $\neq$ high accuracy
- Applying Richardson Extrapolation to the compound trapezoid rule gives Romberg Integration
  - Very good convergence properties for a simple method
- Gaussian quadrature, and related methods, show good stability and are computationally efficient
  - Implemented in many numerical libraries

Next lecture

- Numerical integration problems
  - Using changes of variable
  - Dealing with singularities
- Multidimensional integration

Homework 10: 05/15/2019

Problem 1. Heat capacity of a solid:

Debye's theory of solids gives the heat capacity of a solid at temperature T to be where V is the volume of the solid, ρ is the number density of atoms, k_B is Boltzmann's constant, and θ_D is the so called Debye temperature, a property of solids that depends on their density and speed of sound.

$$C_V = 9V\rho k_B \left(\frac{T}{\theta_D}\right)^3 \int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x dx}{(e^x - 1)^2} dx$$

a) Write a function $C_v(T)$ that calculates C_V for a given value of the temperature, for a sample consisting of 1000 cubic centimeters of solid aluminum, which has a number density of ρ=6.022 × 1028 m−3 and a Debye temperature of θ_D = 428 K. Use Simpson's rule to evaluate the integral, with N = 50 sample points.

b) Use your function to make a graph of the heat capacity as a function of temperature from T = 5 K to T = 500 K.

Problem 2. Adaptive integration:

(a) Write a program that uses the adaptive trapezoidal rule method to calculate the value of the integral I to an approximate accuracy of $\varepsilon = 10^{-10}$ (i.e., correct to ten digits after the decimal point). Start with one single integration slice and work up from there to two, four, eight, and so forth. Have your program print out the number of slices, its estimate of the integral, and its estimate of the error on the integral, for each value of the number of slices starting with N=2, until the target accuracy is reached. (**Hint**: you should find the result is around I = 0.45.)

$$I = \int_0^1 \sin^2(\sqrt{100x})dx$$

(b) Now modify your program to add the evaluation of the same integral using the Simpson's rule integration, again to an approximate accuracy of $\varepsilon = 10^{-10}$. Using the formula provided in the lecture notes, starting with one integration slice, and working up from there, print out the results as in part (a) until the required accuracy is reached. You should find you reach the accuracy for a significantly smaller number of slices than with the trapezoidal rule calculation of part (a). Does this agree with expectations? Explain.

Problem 3: Write a code to integrate

$$I = \int_0^1 \frac{dx}{1+x^2} = \frac{\pi}{4}$$

to an approximate accuracy of $\varepsilon = 10^{-2}$. 10^{-3}. 10^{-4}. 10^{-5}. 10^{-6}. 10^{-7}. 10^{-8}. 10^{-9}, 10^{-10}, 10^{-11}, 10^{-12}, etc

a) trapezoids

b) Simpson's Rule

c) Romberg Integration

For each of the above methods, please test the error relationship?

(**hints**: fit to the h)

PS: If the error relationships are not satisfied, please give an interpretation?

We will begin with the special case with the value of c being zero. We begin by integrating the 2nd degree polynomial $p(t)=c_2t^2+c_1t+c_0$. We will simplify it some after integrating it.

x	y
$-h$	$y_0=f(-h)$
0	$y_1=f(0)$
h	$y_2=f(h)$

$$\int_{-h}^{h} c_2t^2+c_1t+c_0\,dt$$

$$=\tfrac{c_2}{3}t^3+\tfrac{c_1}{2}t^2+c_0t\Big|_{-h}^{h}$$

$$=\tfrac{c_2}{3}h^3+\tfrac{c_1}{2}h^2+c_0h-\left(-\tfrac{c_2}{3}h^3+\tfrac{c_1}{2}h^2-c_0h\right)$$

$$=\tfrac{2}{3}c_2h^3+2c_0h$$

$$y_0=c_2h^2-c_1h+c_0$$

$$y_1=c_0$$

$$y_2=c_2h^2+c_1h+c_0$$

$$y_0+y_2=2c_2h^2+2c_0$$

$$c_2=\frac{y_0-2y_1+y_2}{2h^2}$$

$$=\frac{2}{3}\left(\frac{y_0-2y_1+y_2}{2h^2}\right)h^3+2y_1h$$

Substitute c_0 and c_2 values.

$$=\tfrac{h}{3}\left(y_0-2y_1+y_2+6y_1\right)$$

$$=\tfrac{h}{3}\left(y_0+4y_1+y_2\right)$$