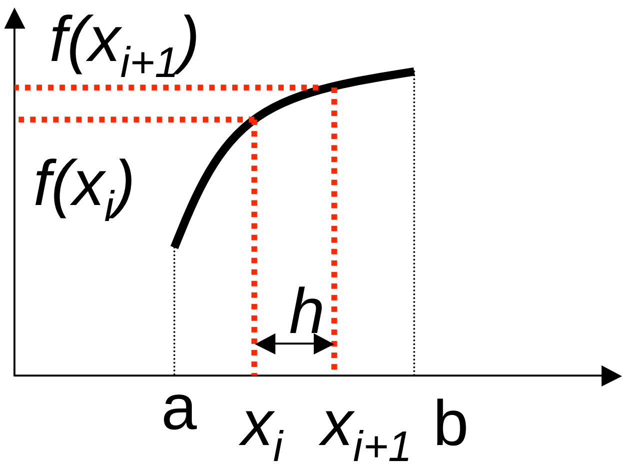
Numerical Integration

Numerical integration is used for definite integrals. Most techniques apply to low dimensional integration - we look at these today. Integration in many-dimensional space typically relies on Monte Carlo techniques (next semester).

We want to find a numerical approximation to

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



Newton-Cotes methods - use equidistant points:

$$x_i = a + ih \quad i = 0,\ldots,n \quad h = \frac{b-a}{n}$$

Lagrange Polynomials

For $n+1$ points (x_i,y_i), with

$$i = 0,1,\cdots,n \qquad\qquad x_i \neq x_{j\neq i}$$

there is a unique interpolating polynomial of degree n with

$$p(x_i) = y_i \qquad\qquad i = 0,1,\cdots,n$$

Can construct this polynomial using the Lagrange polynomials, defined as:

$$L_i(x) = \frac{(x-x_0)\cdots(x-x_{i-1})(x-x_{i+1})\cdots(x-x_n)}{(x_i-x_0)\cdots(x_i-x_{i-1})(x_i-x_{i+1})\cdots(x_i-x_n)}$$

Degree n (denominator is constant), and

$$L_i(x_k) = \delta_{i,k}$$

Lagrange Polynomials

The Lagrange Polynomials can be used to form the interpolating polynomial:

$$p(x) = \sum_{i=0}^{n} y_i L_i(x) = \sum_{i=0}^{n} y_i \prod_{k=0,k\neq i}^{n} \frac{x - x_k}{x_i - x_k}$$

In our application, $y_i = f(x_i)$

Integration of the polynomial yields:

$$\int_a^b p(x)\,dx = \sum_{i=0}^{n} f(x_i) \int_a^b \prod_{k=0,k\neq i}^{n} \frac{x - x_k}{x_i - x_k}\,dx = \sum_{i=0}^{n} f(x_i) \int_0^n \prod_{k=0,k\neq i}^{n} \frac{s-k}{i-k}\,h ds$$

where $x = a + sh$

Note that $\int_0^n \prod_{k=0,k\neq i}^{n} \frac{s-k}{i-k}\,h ds = \alpha_i h$

So α_i is just a number depending on *i,n*

Newton-Cotes Formulas

So, $$\int_a^b p(x)\,dx = h\sum_{i=0}^{n} f(x_i)\alpha_i$$

Look at some specific examples:

$n=1$ $$p(x) = f(x_0)\frac{x-x_1}{x_0-x_1} + f(x_1)\frac{x-x_0}{x_1-x_0}$$

$$\alpha_0 = \int_0^1 \prod_{k=0,k\neq i}^{1} \frac{s-k}{i-k}\,ds = \int_0^1 \frac{s-1}{0-1}\,ds = -\frac{1^2}{2}+1 = \frac{1}{2}$$

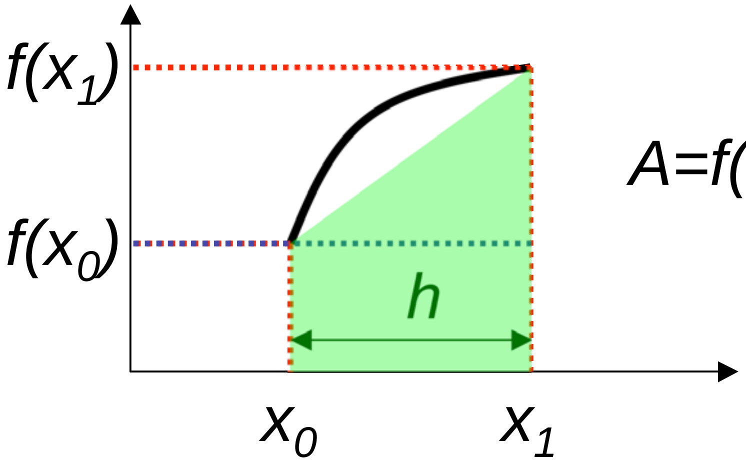
$$\alpha_1 = \int_0^1 \prod_{k=0,k\neq i}^{1} \frac{s-k}{i-k}\,ds = \int_0^1 \frac{s-0}{1-0}\,ds = \frac{1^2}{2} = \frac{1}{2}$$

$$\int_a^b p(x)\,dx = h\sum_{i=0}^{n} f(x_i)\alpha_i = hf(x_0)\frac{1}{2} + hf(x_1)\frac{1}{2} = \frac{h}{2}(f(x_0)+f(x_1))$$

Trapezoidal rule

Trapezoidal Rule

Graphically:



$A=f(x_0)h+1/2[f(x_1)-f(x_0)]h$

Of course, we can apply this to many subdivisions (composite trapezoidal rule) :

$$\int_a^b f(x)\,dx = \sum_{i=0}^{m}\int_{z_i}^{z_{i+1}} f(z)\,dz \quad \text{where } z_0 = a, \quad z_{m+1} = b$$

$$\int_a^b f(x)\,dx \approx h\left(\frac{f(x_0)}{2}+\frac{f(x_1)}{2}+\frac{f(x_1)}{2}+\frac{f(x_2)}{2}+\cdots+\frac{f(b-h)}{2}+\frac{f(b)}{2}\right)$$

$$\int_a^b f(x)\,dx \approx h\left(\frac{f(x_0)}{2}+f(x_1)+\cdots+f(b-h)+\frac{f(b)}{2}\right)$$

Error Order

To find the error order of a particular approximation, we consider a series approximation. For the numerical simulation of derivatives, we compared to a Taylor series. Here we compare to the Euler-Maclaurin summation formula:

$$\sum_{i=1}^{n-1} F(i) = \int_0^n F(s)\,ds - \frac{1}{2}\left[F(0)+F(n)\right] + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!}\left[F^{(2k-1)}(n) - F^{(2k-1)}(0)\right]$$

where

$F^{(k)}$ is the k-th derivative of F and the B_{2k} are the Bernoulli numbers

n	Bn
0	1
1	−1/2 = −0.5
2	1/6 ≈ 0.1667
4	−1/30 ≈ −0.0333
6	1/42 ≈ 0.02381
8	−1/30 ≈ −0.0333
10	5/66 ≈ 0.07576
12	−691/2730 ≈ −0.2531
14	7/6 ≈ 1.1667

B_n=0 for n≥3, odd

Error Order

Make the transformation: $x = sh + a$

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

or

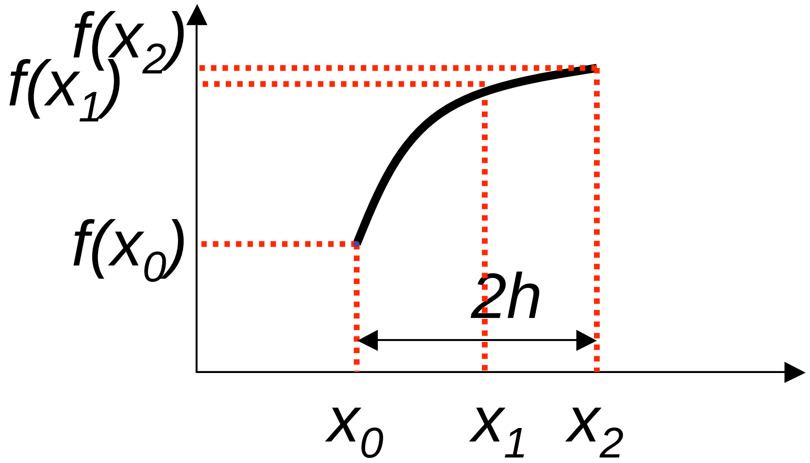
$$\int_a^b f(x)\,dx = \underbrace{h\sum_{i=1}^{n-1} f(x_i) + \frac{h}{2}[f(a)+f(b)]}_{\text{Trapezoidal Rule}} - \frac{h^2}{12}[f'(b) - f'(a)] + O(h^4)$$

We see that the error from the trapezoidal rule is of order h^2.

The precision can be improved by setting h smaller and smaller but we will eventually hit rounding errors and computing time limitations. Look for methods with higher order of the error.

Simpson's Rule

$$n = 2 \qquad \int_a^b p(x)\,dx = h\sum_{i=0}^{n} f(x_i)\alpha_i = 2h\,\frac{f(x_0)+4f(x_1)+f(x_2)}{6}$$



Error order h^4 (interpolating polynomial of 2nd order)

Composite Simpson's rule:

$$\int_a^b f(x)\,dx \approx \frac{2h}{6}\begin{bmatrix} f(a)+4f(a+h)+f(a+2h)+ \\ f(a+2h)+4f(a+3h)+f(a+4h)+ \\ \cdots+ \\ f(b-2h)+4f(b-h)+f(b) \end{bmatrix}$$

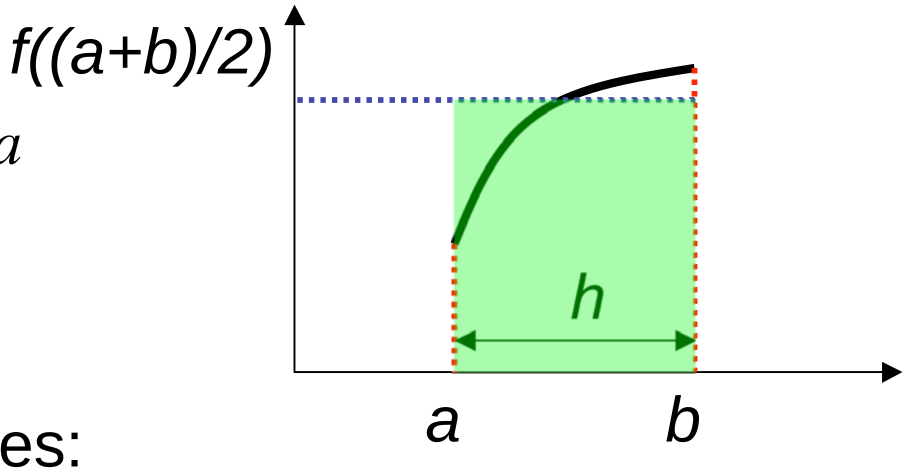
Note: range divided into an even multiple of h

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

Midpoint Rule

It is sometimes preferable to sample the function at the midpoint of the interval rather than at the ends (e.g., if the function has a singularity at the endpoint). Simplest example:

$$\int_a^b f(x)\,dx \approx hf\left(\frac{a+b}{2}\right) \qquad h = b-a$$



The composite midpoint rule gives:

$$\int_a^b f(x)\,dx \approx 2h\big(f(a+h) + f(a+3h) + \cdots + f(b-h)\big)$$

The error order is h^2

Extrapolation Method

Let R_{ij} be our estimate of the integral when 2^{i-1} intervals are used and j is the order of the interpolating polynomial (previously n). E.g., j=1 is Trapezoidal Rule, j=2 is Simpson's Rule. Look at the error formula:

$$\int_a^b f(x)\,dx = T_S(h) + \alpha_2 h^2 + \alpha_4 h^4 + \cdots$$

where $T_S(h)$ is e.g. the Trapezoidal rule. Now take $h \to \frac{h}{2}$

$$\int_a^b f(x)\,dx = T_S(h/2) + \alpha_2 h^2/4 + \alpha_4 h^4/16 + \cdots$$

so

$$\int_a^b f(x)\,dx - \frac{4T_S(h/2) - T_S(h)}{3} = -\alpha_4 h^4/4 + \cdots$$

i.e., can get a higher order error by combining results from different step sizes (recall extrapolation method for derivatives).

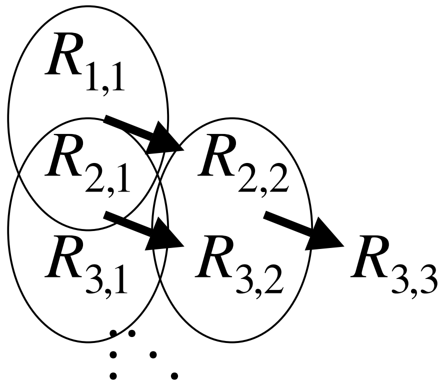
Extrapolation Method

There is a general formula for calculating the higher order terms - Richardson Formula:

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

See Scherer lecture notes for derivation

So we can gain higher order of error at the same time as making the step size smaller (technique called Romberg integration).



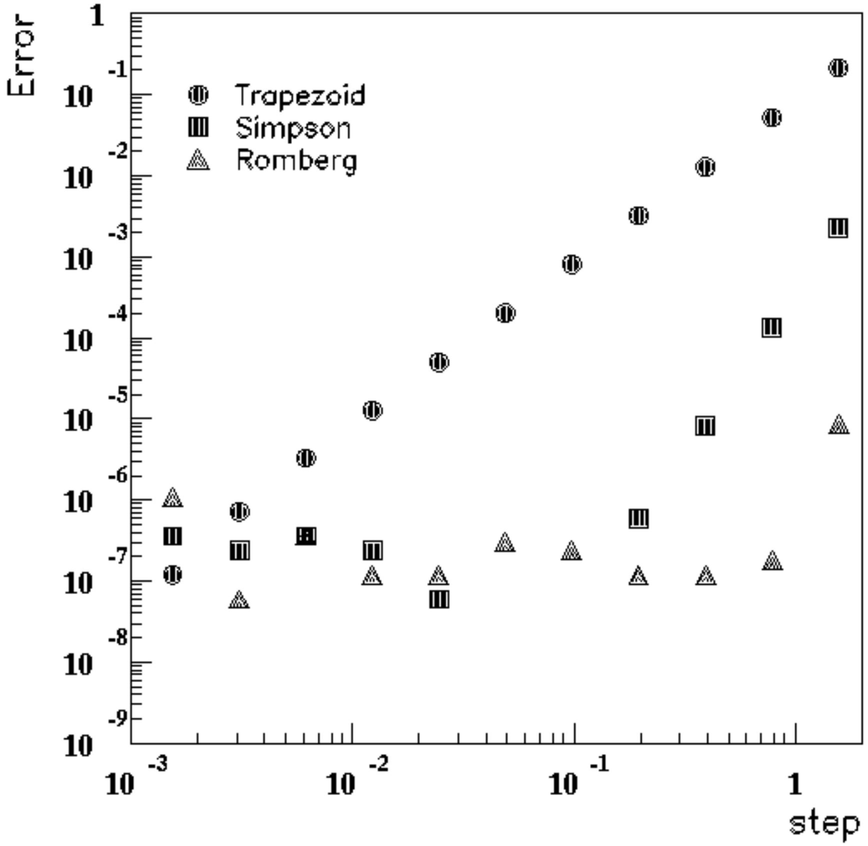
So, e.g., can get up h^6 precision by extrapolating the trapezoidal rule calculations with spacing h,h/2,h/4

Example

Let's investigate a concrete example:

$$K = \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2 \theta}\, d\theta$$

We know the exact value for some k, e.g., k=1 →K=1.0



Romberg Integration (3 step)

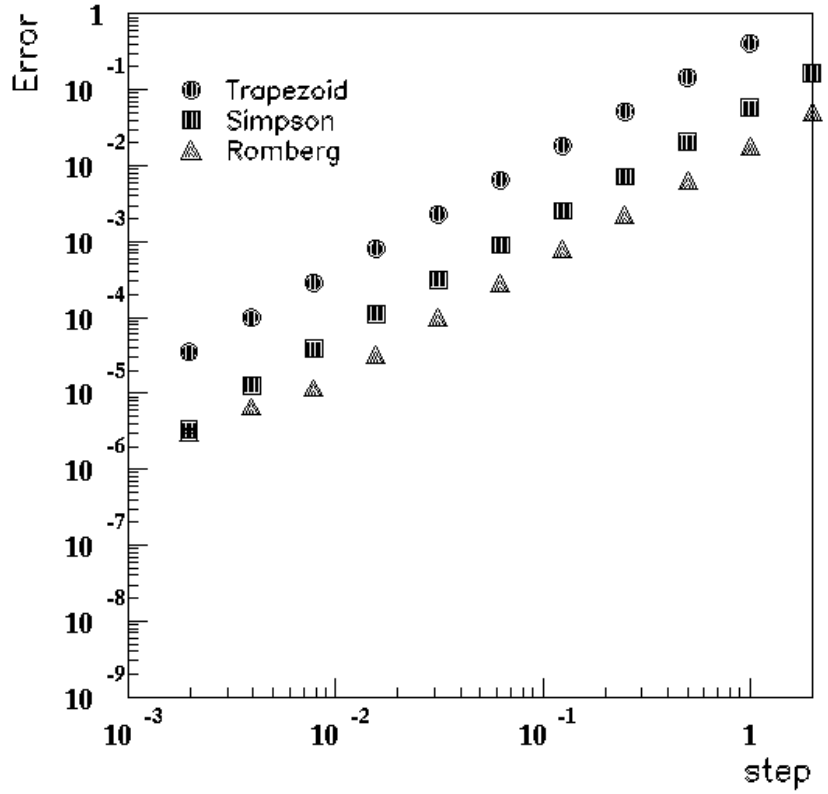
i	*j* = *1*	*2*	*3*
1	0.785398126		
2	0.94805944	1.00227988	
3	0.987115741	1.00013447	0.999991417

Trapezoidal rule used 3 times

Example

Next example:

$$K = \int_0^2 \sqrt{4 - x^2}\, dx = \pi$$



Convergence much slower because of infinite slope at x=2

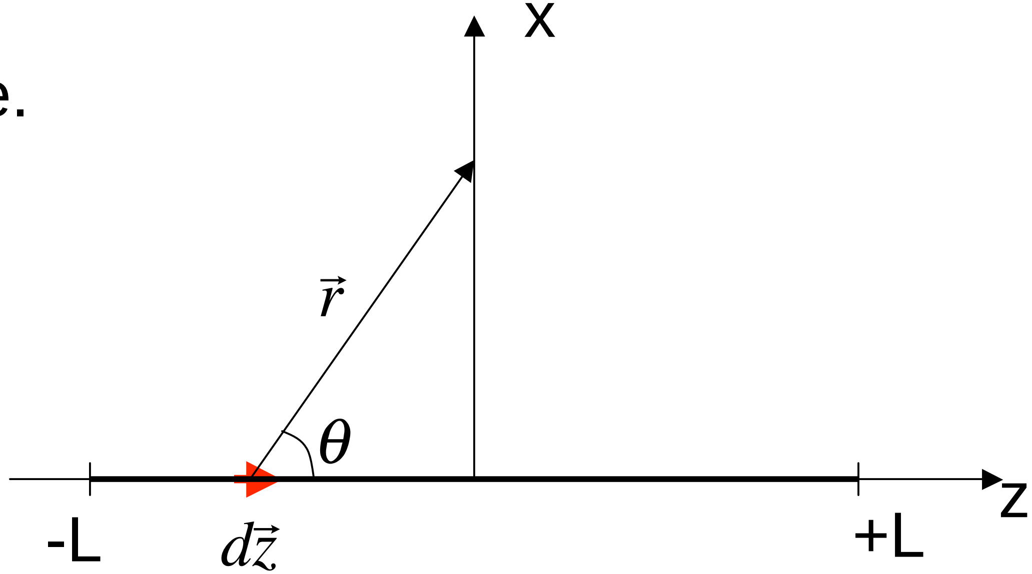
$$\frac{d\sqrt{4 - x^2}}{dx} = \frac{1}{2}\frac{-2x}{\sqrt{4 - x^2}} = \frac{-x}{\sqrt{4 - x^2}} \xrightarrow[x \to 2]{} -\infty$$

Magnetic Field

Current I flowing in wire.
Biot-Savart Law:

$$d\vec{B} = \frac{\mu_0 I}{4\pi}\frac{d\vec{z}\times\vec{r}}{r^3}$$

$$d\vec{z}\times\vec{r} = r\,dz\sin\theta\hat{y}$$



$$\vec{B} = B\hat{y},\quad B = \int_{-L}^{L}\frac{\mu_0 I}{4\pi}\frac{r\sin\theta}{r^3}\,dz = \int_{-L}^{L}\frac{\mu_0 I}{4\pi}\frac{x}{(x^2+z^2)^{3/2}}\,dz$$

Consider L→∞, x small: Ampere's Law gives $B = \frac{\mu_0 I}{2\pi r}$ where r is

the distance from the wire. Try our numerical calculations.

Magnetic Field

Note that Ampere's law applied to an infinite length wire. To reproduce the result numerically, need to have L>>r.

$$r = x = 1, \left(\frac{x}{\sqrt[3]{x^2+z^2}}\right)_{\min} = \left(\frac{1}{\sqrt[3]{1^2+L^2}}\right), \left(\frac{x}{\sqrt[3]{x^2+z^2}}\right)_{\max} = \left(\frac{1}{\sqrt[3]{1^2+0}}\right)$$

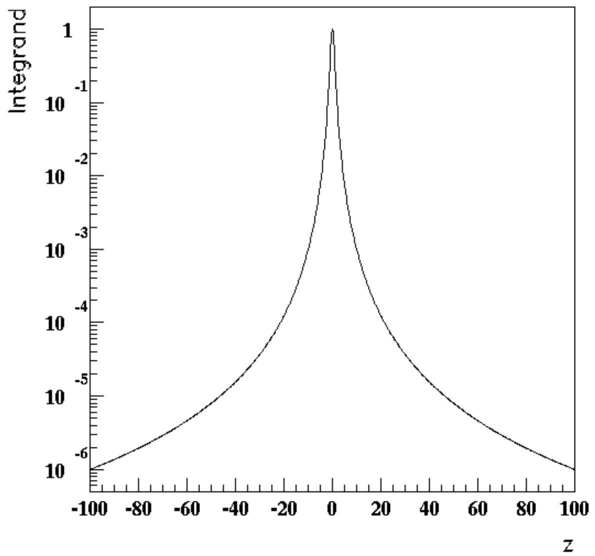
$$\left(\frac{x}{\sqrt[3]{x^2+z^2}}\right)_{\min} \Big/ \left(\frac{x}{\sqrt[3]{x^2+z^2}}\right)_{\max} = \left(\frac{1}{\sqrt[3]{1^2+L^2}}\right)$$

$$\text{for this ratio } \le \varepsilon, \quad L > \sqrt{\varepsilon^{-2/3} - 1} \approx \varepsilon^{-1/3}$$

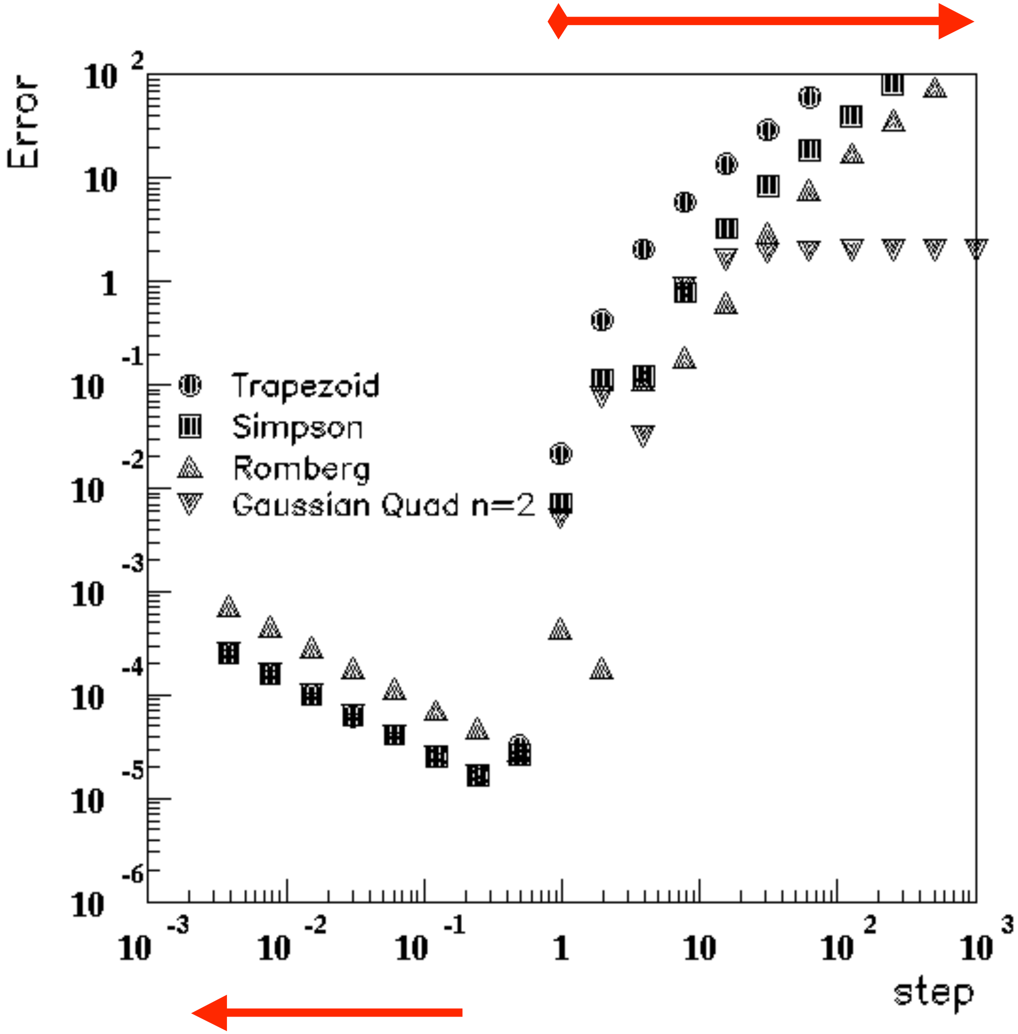
For $L = 1000, \varepsilon = 10^{-9}$

Magnetic Field

Take x=1, L=1000



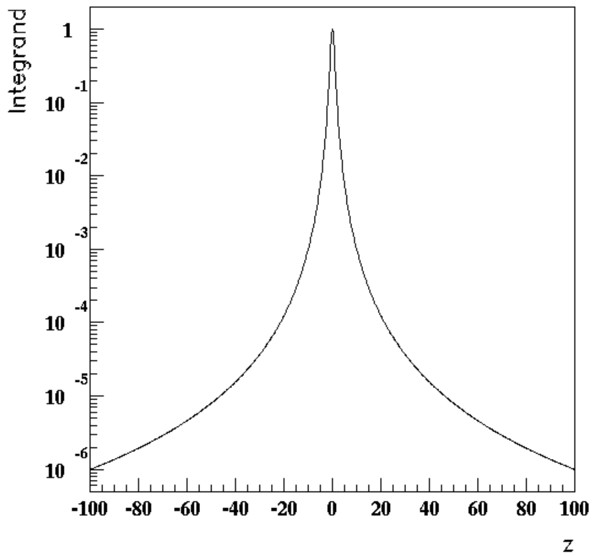
Step too big

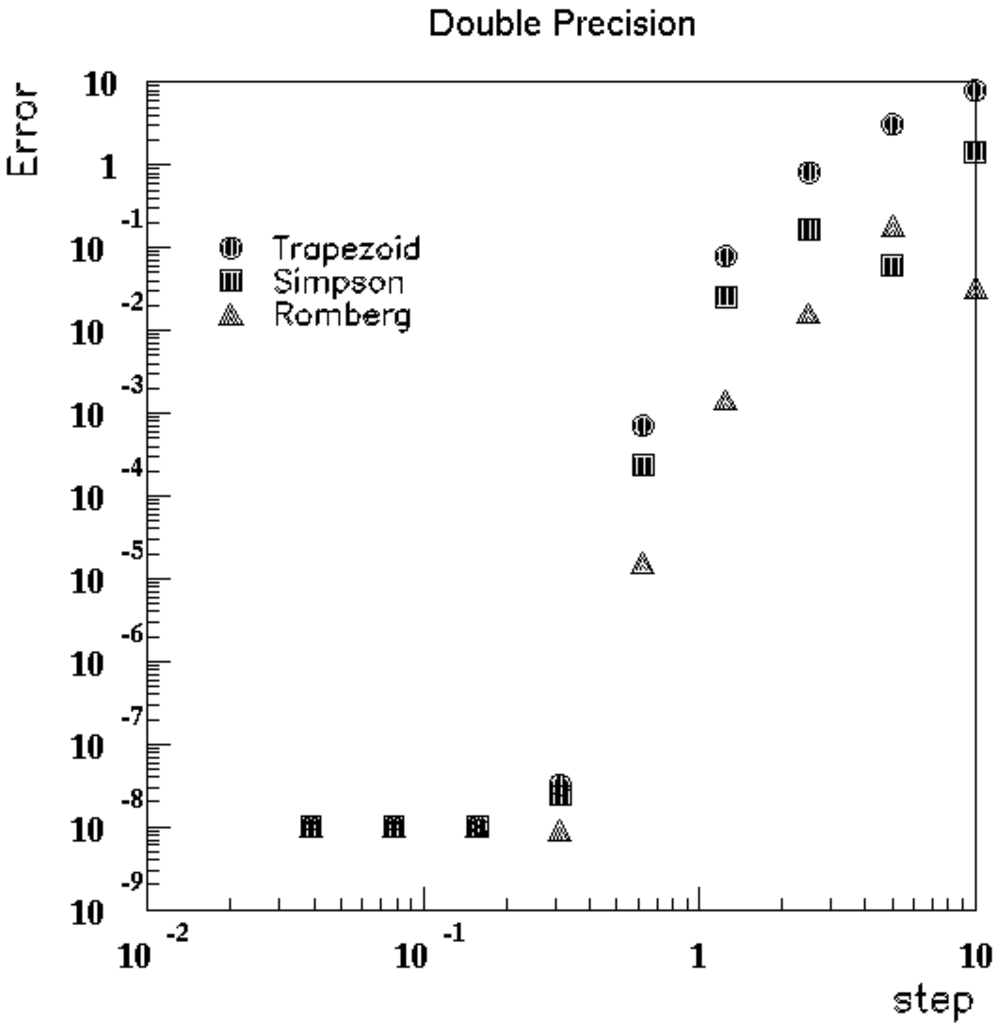


Rounding errors

Magnetic Field

Try double precision: L=10000





Gaussian Quadrature

We now move away from the requirement of equidistant points for the integration. General technique called Gaussian quadrature which yields polynomial accuracy of order (2n-1) using n^{th} order polynomials.

Consider the scalar product of two functions in the interval [-1,1]

$$\langle fg \rangle = \int_{-1}^{1} f(x) g(x)\, dx$$

Now consider an orthogonal set of polynomials on this interval, such that

$$\langle P_i P_j \rangle = \delta_{ij}$$

E.g., Legendre polynomials (1,x,x^2-1/3,…)

Gaussian Quadrature

Assume we have a polynomial *p(x)* of order 2n-1. We can interpolate this polynomial at n points x_i using our usual Lagrange method of order n-1:

$$\tilde{p}(x) = \sum_{j=1}^{n} L_j(x) p(x_j)$$

We can rewrite *p(x)* as

$$p(x) = \tilde{p}(x) + (x - x_1)(x - x_2)\cdots(x - x_n) q(x)$$

where $q(x)$ is a polynomial of degree n - 1

If we pick the x_i as the roots of an n^{th} order polynomial from an orthogonal set (e.g., Legendre Polynomials), then

$$P_n(x) = (x - x_1)(x - x_2)\cdots(x - x_n)$$

$$\int_{-1}^{1} P_n(x) q(x) = 0 \quad \text{since } q(x) = \sum_{j=0}^{n-1} a_j P_j(x)$$

Gaussian Quadrature

So, $$\int_{-1}^{1} p(x)\,dx = \int_{-1}^{1} \tilde{p}(x)\,dx = \int_{-1}^{1} \sum_{j=1}^{n} L_j(x)\,p(x_j)\,dx = \sum_{j=1}^{n} w_j\,p(x_j)$$

where the w_j are determined by the choice of x_j which in turn come from the choice of orthogonal set of polynomials.

$$w_j = \int_{-1}^{1} L_j\,dx$$

Note what we have achieved: 2n-1 accuracy using a polynomial of degree n by picking sampling points in special way.

Procedure (Legendre polynomials):

1. Choose which order you want to use (n)
2. Find the n roots of P_n *(look them up in a table)*
3. Find the corresponding Lagrange Polynomials
4. Calculate the weight factors
6. Evaluate the integral

Gaussian Quadrature

E.g., use Legendre polynomials, n=2

$$P_2(x) = x^2 - \frac{1}{3} \quad \text{with roots } \; x_1 = \sqrt{1/3} \quad x_2 = -\sqrt{1/3}$$

The Lagrange polynomials are

$$L_i(x) = \frac{(x-x_0)\cdots(x-x_{i-1})(x-x_{i+1})\cdots(x-x_n)}{(x_i-x_0)\cdots(x_i-x_{i-1})(x_i-x_{i+1})\cdots(x_i-x_n)}$$

$$L_1 = \frac{(x-x_2)}{(x_1-x_2)} = \frac{x+\sqrt{1/3}}{\sqrt{1/3}-\left(-\sqrt{1/3}\right)} = \frac{x+\sqrt{1/3}}{2\sqrt{1/3}} \quad w_1 = \int_{-1}^{1} L_1 \, dx = 1$$

$$L_2 = \frac{x-\sqrt{1/3}}{-2\sqrt{1/3}} \quad w_2 = \int_{-1}^{1} L_2 \, dx = 1$$

Note that these can be used for any integrand you want to evaluate

Gaussian Quadrature

So, this gives the 2-point rule: $\int_{-1}^{1} f(x)\,dx \approx f\left(-\sqrt{1/3}\right) + f\left(\sqrt{1/3}\right)$

For different integration limits, make a change of variables:

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

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\frac{a+b}{2} + \frac{b-a}{2}u\right)\frac{b-a}{2}\,du$$

for our example

$$\int_a^b f(x)\,dx \approx \frac{b-a}{2}\left[f\left(\frac{a+b}{2} - \frac{b-a}{2}\sqrt{1/3}\right) + f\left(\frac{a+b}{2} + \frac{b-a}{2}\sqrt{1/3}\right)\right]$$

e.g., $K = \int_0^{\pi/2} \sqrt{1-\sin^2\theta}\,d\theta \approx \frac{\pi/2}{2}\left[\cos\left(\frac{\pi/2}{2} - \frac{\pi/2}{2}\sqrt{1/3}\right) + \cos\left(\frac{\pi/2}{2} + \frac{\pi/2}{2}\sqrt{1/3}\right)\right]$

$$= \frac{\pi}{4}[0.9454092 + 0.3258856] = 0.9984726$$

Gaussian Quadrature

Of course, can apply composite Gaussian Quadrature, or use a higher order Legendre polynomial.

n	x_i	w_i
1	0	2
2	$\pm\sqrt{1/3}$	1
3	0 $\pm\sqrt{3/5}$	8/9 5/9
4	±0.339981 ±0.861136	0.652145 0.347855
5	0 ±0.538569 ±0.906180	0.568889 0.478629 0.236927

Gaussian Quadrature

One can also choose different sets of orthogonal polynomials by breaking up the integral as follows $\int_a^b w(x) f(x)\, dx$

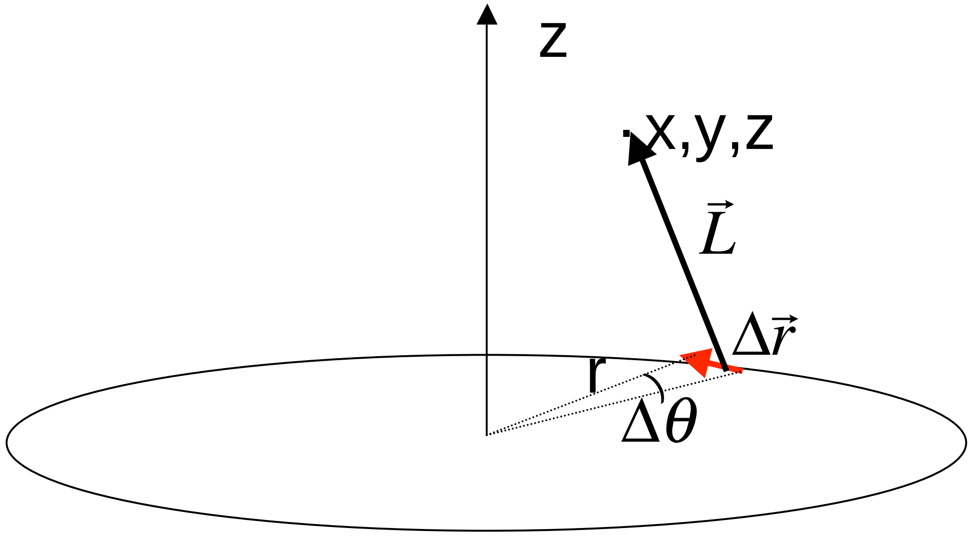
Interval	*w(x)*	*Orthogonal Polynomials*
[-1,1]	1	Legendre
(-1,1)	$(1-x)^{\alpha}(1-x)^{\beta}$ $\alpha,\beta>-1$	Jacobi
(-1,1)	$1/\sqrt{(1-x^2)}$	Chebyshev (first kind)
[-1,1]	$\sqrt{(1-x^2)}$	Chebyshev (second kind)
[0,∞)	e^{-x}	Laguerre

Orthogonality: $\int_a^b w(x) P_N(x) P_M(x)\, dx = 0 \quad M \neq N$

The weights are given by $w_i = \int_a^b w(x) L_i(x)\, dx$

Field due to Current Loop

Example: the magnetic field due to a current loop:



Magnetic field can be calculated analytically for points along the axis, but not for other points. Magnetic field will have components in all directions. Need to calculate them one at a time.

Field due to a Current Loop

Calculation of the magnetic field due to a current loop at a point P off the axis of the loop. Following integrals appear:

$$I = \int_{-1}^{1} \frac{x}{(a-x)^{3/2}\sqrt{1-x^2}}\,dx \qquad \text{take } a = \frac{5}{4}$$

Note singularity at endpoints !

Note that $\frac{1}{\sqrt{1-x^2}}$ already appears in integral, so we use this as the weight function and use the roots of the Chebyshev polynomials of the first kind. For n=4, these are

$$x_1 = \cos{\pi/8},\, x_2 = \cos{3\pi/8},\, x_3 = -\cos{3\pi/8},\, x_4 = -\cos{\pi/8}$$

giving

$$w_1 = w_2 = w_3 = w_4 = \pi/4$$

so that $$I \approx w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3) + w_4 f(x_4) = 5.02$$

where $$f(x) = \frac{x}{(a-x)^{3/2}}$$

Correct answer ≈5.33

Exercizes

1. Compare the Trapezoidal rule, Simpson's rule, the Romberg extrapolation method, and Gaussian quadrature with Legendre Polynomials for the following integral (try different values of θ_m) for different step sizes:

$$\sqrt{8}\int_0^{\theta_m} \frac{d\theta}{\sqrt{\cos\theta - \cos\theta_m}}$$