Lecture 6
Numerical Integration

Trapezoid rule for integration

$$\int_{x_0}^{x_1} f(x)\,dx$$

Many methods can be used to numerically evaluate the integral

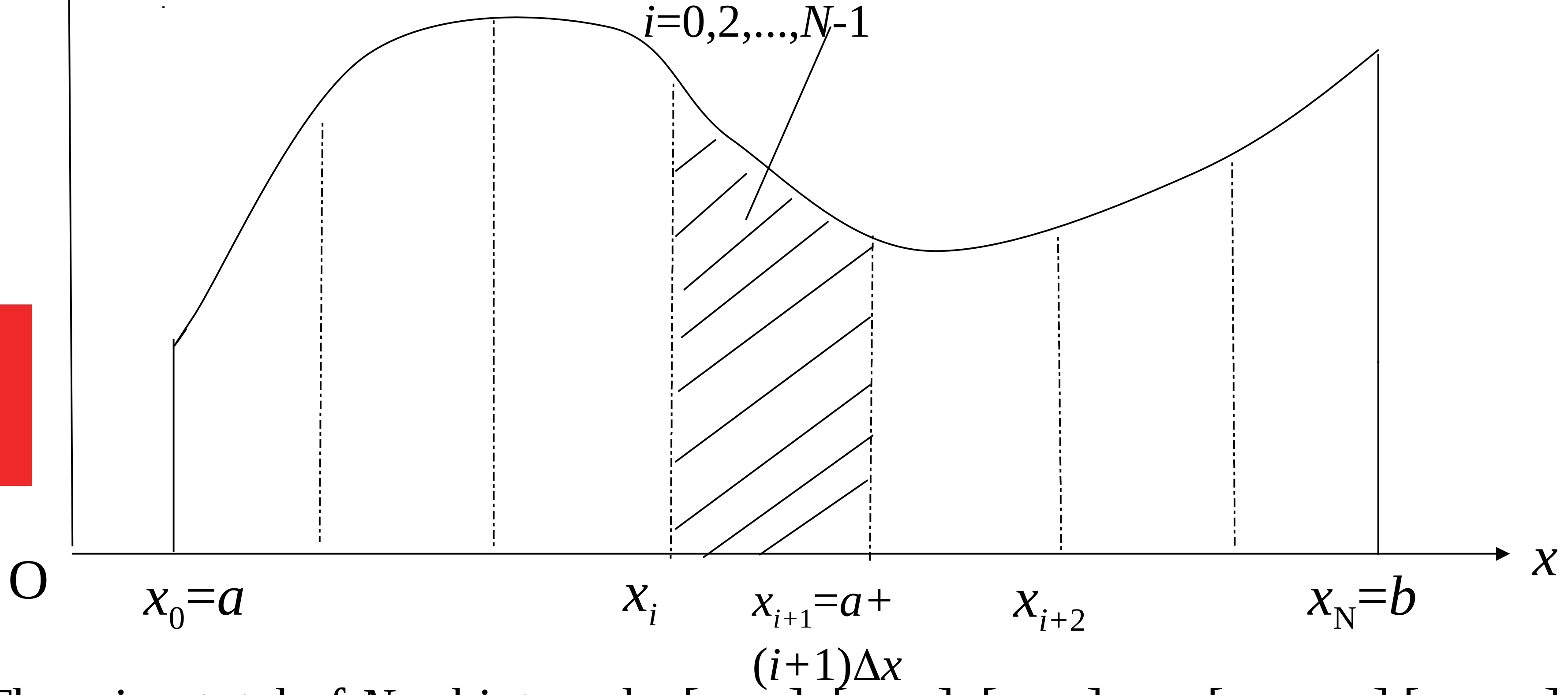
Basically the integral is the area represented between the curve and the vertical axis.

Trapezoid rule for integration

Basically the integral is the area represented between the curve and the x-axis.

$A_i \approx (1/2)[f(x_i)+f(x_{i+1})]\Delta x;$

$i=0,2,\ldots,N-1$



There is a total of N subintervals, $[x_0,x_1]$, $[x_1,x_2]$, $[x_2,x_3]$, … ,$[x_{N-2},x_{N-1}]$,$[x_{N-1},x_N]$.

A_i represents the area under the curve in subinterval i, $\Delta_i=[x_i, x_{i+1}]$

Trapezoidal rule

$$\int_a^b f(x)dx \approx \sum_{i=0}^{i=N-1} A_i = \sum_{i=0}^{i=N-1} \frac{1}{2}\Delta x[f(x_{i+1})+f(x_i)]$$

$$= \Delta x\left\{\frac{1}{2}[f(x_0)+f(x_1)]+\frac{1}{2}[f(x_1)+f(x_2)]+\cdots+\frac{1}{2}[f(x_{N-1})+f(x_N)]\right\}$$

$$= \frac{\Delta x}{2}[f(x_0)+f(x_N)]+\Delta x[f(x_1)+f(x_2)+\cdots+f(x_{N-2})+f(x_{N-1})]$$

$$= \frac{\Delta x}{2}[f(x_0)+f(x_N)]+\Delta x\sum_{i=1}^{i=N-1} f(x_i)$$

The error, is of the order $O(\Delta x)^2$

Simpson’s rule for integration

- The numerical integration can be improved by treating the curve connecting the points $\{x_{\mathrm{i+1}}, f(x_{\mathrm{i+1}})\}$, $\{x_{\mathrm{i}}, f(x_{\mathrm{i}})\}$as a section of a parabola instead of a straight line (as was assumed in trapezoid rule).
- This results in $A_i + A_{i+1} = (\Delta x/3)[f(x_{\mathrm{i}}) + 4f(x_{\mathrm{i+1}}) + f(x_{\mathrm{i+2}})]$.
- For details of the derivation, see the lecture notes by Gilles Cazelais of Camosun College, Cadana,
- http://pages.pacificcoast.net/~cazelais/187/simpson.pdf

Simpson's rule for integration (cont.)

$$\int_a^b f(x)dx = \sum_{i=0,2,4,6,\dots,N-2} A_i + A_{i+1} = \frac{\Delta x}{3} \sum_{i=0,2,4,6,\dots,N-2} f(x_i) + 4f(x_{i+1}) + f(x_{i+2})$$

$$= \frac{\Delta x}{3} \left[\left\{ f(x_0) + 4f(x_{0+1}) + f(x_{0+2}) \right\} + \left\{ f(x_2) + 4f(x_{2+1}) + f(x_{2+2}) \right\} \right.$$

$$\left. + \left\{ f(x_4) + 4f(x_{4+1}) + f(x_{4+2}) \right\} + \dots + \left\{ f(x_{N-2}) + 4f(x_{N-1}) + f(x_N) \right\} \right]$$

$$= \frac{\Delta x}{3} \left[\left\{ f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) \right. \right.$$

$$\left. + 4f(x_5) + 2f(x_6) + \dots + 2f(x_{N-2}) + 4f(x_{N-1}) + f(x_N) \right]$$

Assume *N* a large even number.

Simpson’s rule for integration

$$\int_a^b f(x)\,dx = \frac{\Delta x}{3}\left[\left\{f(x_0)+f(x_N)\right)\right] + \frac{4\Delta x}{3}\left[f(x_1)+f(x_3)+f(x_5)+\ldots+f(x_{N-1})\right.$$

$$+\frac{2\Delta x}{3}\left[f(x_2)+f(x_4)+f(x_6)+\ldots+f(x_{N-2})\right]$$

The number of interval, *N*, matters: if it is too small, large error occurs. The error in Simpson's rule is of the order $O(\Delta x)^4$

Exercise

Write a code to evalate the following integral using both Trapezoid and Simpson's rule. z is a constant set to 1.

Let the integration limits be from x_0=-1.5 to x_1=+5.0.

$$f(x) = \frac{x}{\left(z^2 + x^2\right)^{3/2}}$$

$$\int_{x_0}^{x_1} f(x)\,dx = ?$$

Built-in integration function in Mathematica

- Syntax: **NIntegrate[ ]**
- You can compare the results of Mathematica built-in numerical integration against the one developed by you based on Simpson's and Trapizoid rules.
- Mathematica also provide a powerful symbolic integration functionality:
- Syntax **Integrate[]**.

Antiderivative and Integral

- Give a function $f(x)$, its antiderivative is defined as a function $F(x)$ which fulfills the condition
- $$F'(x) = f(x)$$
- The prime symbol means taking the derivative with respect to the variable, x.
- Fundamental theorem of calculus relates the integral of the function between two limits with the antiderivative to evaluated at these two limits, via
-

Antiderivative in Mathematica

- Given any function $f(x)$, the corresponding antiderivative, $F(x)$, can be obtained via the command
- Integrate[f[x],x]
-
- See C6_Math_built_in_integration_demo1.nb

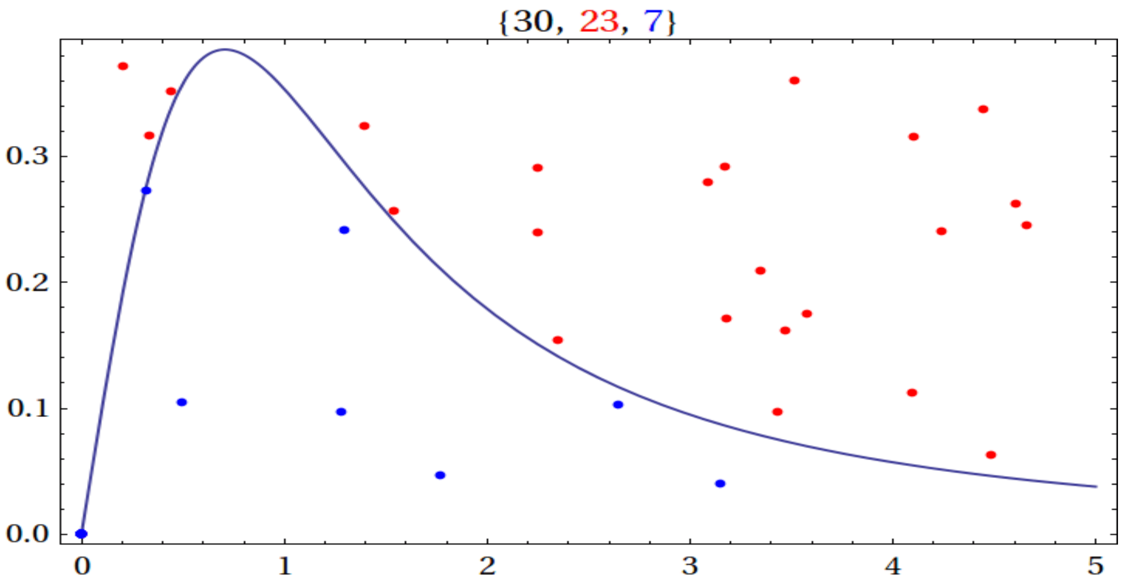
- Logarithmic integral function is formally defined as
-
- http://functions.wolfram.com/GammaBetaErf/LogIntegral/02/
- (*i*) Use Mathematica command **LogIntegral[x]** to plot the function for the interval $0 < x < 1$ (note: the end points are not included).
- (*ii*) Use the command **Nintegrate[]** to generate a set of values {li(0.05),li(0.10),li(0.15), …, li(0.95)}.
- (*iii*) Overlap the ListPlot of (*ii*) on the graph plotted in (*i*). Both code must agree.

- Gamma function is formally defined as
-
- http://functions.wolfram.com/GammaBetaErf/Gamma/02/
- (*i*) Use Mathematica command **Gamma[z]** to plot the gamma function for the interval $1 < z < 5$.
- (*ii*) Use the command **NIntegrate[]** to generate a set of values $\{\Gamma(1.00), \Gamma(1.05), \Gamma(1.10), \ldots, \Gamma(5.00)\}$.
- (*iii*) Overlap the ListPlot of (ii) on the graph plotted in (*i*). Both code must agree.

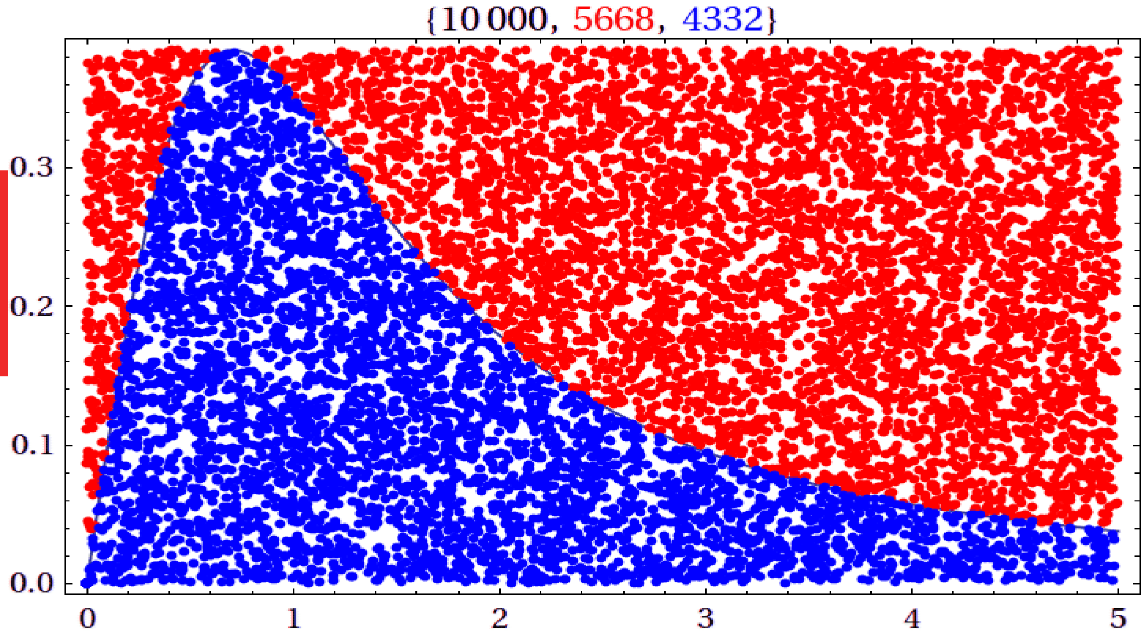
Numerical integration with stochastic method

- Assume $f(x)$ >= 0 for xinit<=x<=xlast.
- Set totalcountmax.
- Set inboxcount = 0, totalcount=0.
- Find Max $f(x)$, and call it fmax.
- Define an area A = fmax*L, where L = xlast-xinit.
- 1. Generate a pair of random numbers (xrand,yrand), with the condition

  xinit<=xrand<=xlast, 0<=yrand<= fmax.
- 2. totalcount=totalcount+1.
- 3. If 0 <=yrand <= f(x=rand), inboxcount = inboxcount + 1
- 4. Stop if totalcount = totalcountmax.
- 5. Repeat step 1.
- The area of the curve f(x) in the interval for [xinit,xlast] is given by
- Area = A*inboxcount/totalcountmax.
- See the implementation of stochastic integration code: C6_stochastic_integration.nb



A=L*fmax=1.9245
L=5-0=5.0
fmax0.3849
at x=0.707107



$$f(x) = \frac{x}{\left(z^2 + x^2\right)^{3/2}}$$

$$\int_{x_0}^{x_1} f(x)\,dx = ?$$

Exercise

Write a code to evalate the following integral using stochasitc method. z is a constant set to 1.

Let the integration limits be from x_0=0 to x_1=+5.0.

$$f(x) = \frac{x}{(z^2 + x^2)^{3/2}}$$

$$\int_{x_0}^{x_1} f(x)dx = ?$$

Exercise

Modify your stochasitc integraton code so that it can integtate a function with both potisive and negative signs in the range of integration. Test it on the following integral. Let the integration limits be from x_0=-2.5 to x_1=+5.0.

$$f(x) = \frac{x}{\left(z^2 + x^2\right)^{3/2}}$$

$$\int_{x_0}^{x_1} f(x)\,dx = ?$$