Numerical differentiation and integration

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Introduction

- Many problems are without the analytical solution, it can just be solved by some numerical methods. A few century ago, scientists calculated by hands. Now we use computers to do it, so the numerical method will be more important.

Definition of the differentiation

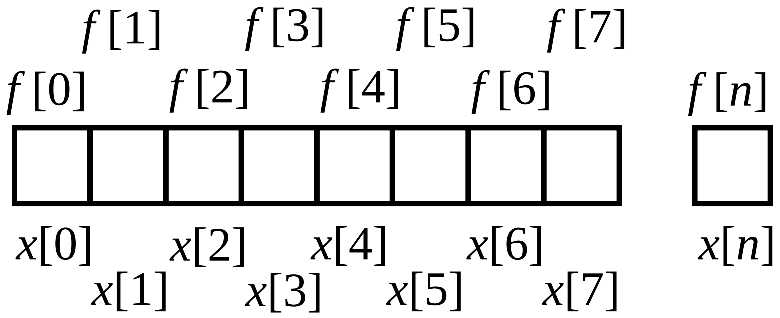
- Give a function $f(x)$, f is continuous in $[a,b]$, and $x \in [a,b]$
- Differential calculate a slope of a curve

$$\frac{d}{dx} f(x) = f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- The grid is discrete in the computer, so the differential equation becomes to difference equation

$$\frac{d}{dx} f(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \to \frac{\Delta f(x)}{\Delta x} = \frac{f(x+h) - f(x)}{h}$$

Difference in computer



$$\frac{\Delta f(x)}{\Delta x} = \frac{f(x+h) - f(x)}{h}$$

- Here h is the distance of the difference grid. For example, h = 2, then

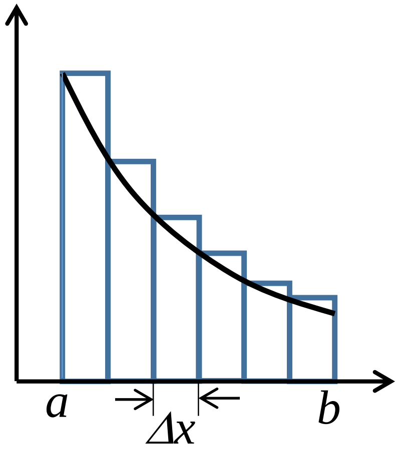
$$\frac{\Delta f(x)}{\Delta x} = \frac{f(x+2) - f(x)}{2} \rightarrow \frac{\Delta f[0]}{\Delta x[0]} = \frac{f[2] - f[0]}{2} \quad \frac{\Delta f[1]}{\Delta x[1]} = \frac{f[3] - f[1]}{2}$$

- It’s the simplest difference, but there are more complex differential equations in our problems, I’ll introduce them in the future.

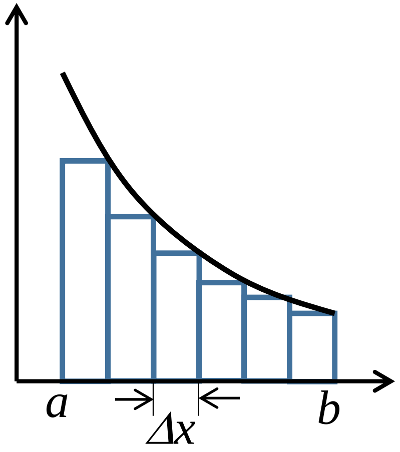
Definition of the integration

- Give a function $f(x)$, f is continuous in $[a,b]$, and $x \in [a,b]$.
- Integration is the area enclosed by the function and the axis

$$\int_a^b f(x)dx = \lim_{\Delta x \to 0} \sum_{i=0}^{n} f(x_i)\Delta x$$



- The figure shows in right, the area of the bigger one is U, the other is L, assume the Riemannian sum of f is I, then its integral exists when
    - $L \leq I \leq U$



Integration in computer

- As the previous slide, we can use rectangular to calculate the integral, its length and width are $f\,[0]$ and Δx. Suppose $\Delta x = 2$, then the integral is
  - $f\,[0]*2 + f\,[2]*2 + \ldots + f\,[n]*2$
- In program, it's convenient to use function, and set start point at a, end point at b, slice into n part, then

$$\Delta x = \frac{b-a}{n}, I = \sum f\,(x + \Delta x)\Delta x$$

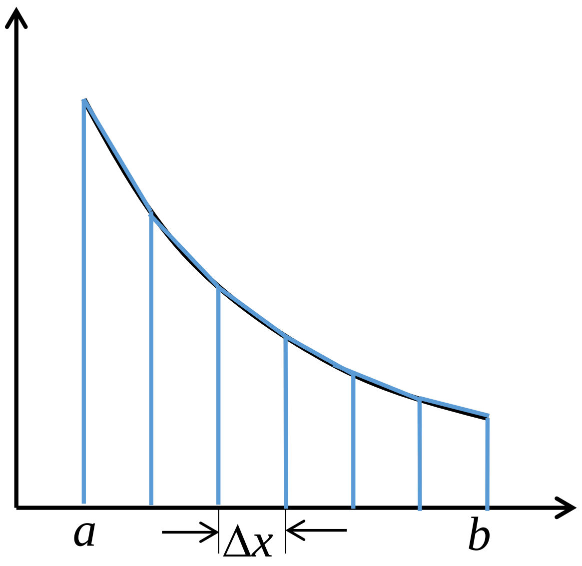
- Obviously, the error is very high unless Δx is very small, it costs computing source, so there are so many numerical methods for Integration.

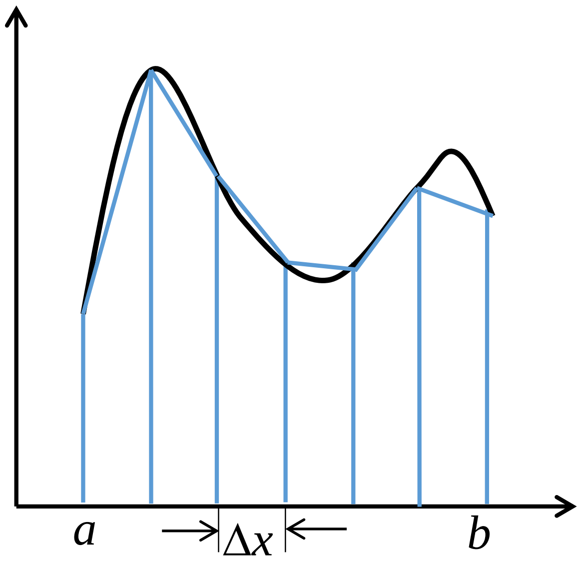
Trapezoidal method

- As the figure shows, when we connect the points of $f(x_i)$ and $f(x_{i+1})$, then the error reduces very fast, it forms a trapezoid, $f(x_i)$ and $f(x_{i+1})$ are its base, Δx is height, so

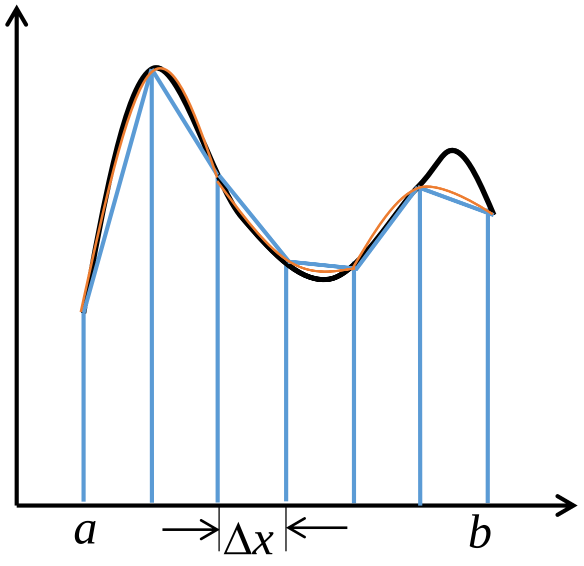
$$\Delta x = \frac{b-a}{n}, I = \sum \frac{[f(x)+f(x+\Delta x)]}{2} \Delta x$$

- Give any curve, the error of trapezoidal method is a little high, so next method we use 3 given points to find a parabola to reduce the error.





Simpson's 1/3 method



- A general form of a parabola is

$$y = ax^2 + bx + c$$

- The integration of y from $-h$ to h is

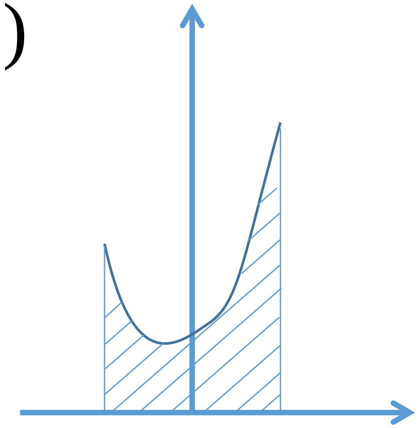
$$A = \int_{-h}^{h} y\,dx = \int_{-h}^{h} (ax^2 + bx + c)\,dx = \left[\frac{a}{3}x^3 + \frac{b}{2}x^2 + cx + d\right]_{-h}^{h}$$

$$= \frac{2a}{3}h^3 + 2ch = \frac{h}{3}(2ah^2 + 6c)$$

- Suppose there are n point in $[a, b]$, then use the first 3 points a, x_0, x_1, so the integration of y is

Simpson's 1/3 method

- Suppose the parabolic pass through $(-h, y_0)$, $(0, y_1)$, (h, y_2)



- $y_0 = ah^2 - bh + c$
- $y_1 = c$
- $y_2 = ah^2 + bh + c$
- Then solve the c and ah^2, we get
- $2ah^2 + 2c = (y_0 + y_2)$, $c = y_1$

$$A = \frac{2a}{3}h^3 + 2ch = \frac{h}{3}(2ah^2 + 6c) = \frac{1}{3}(2ah^2 + 6c) = \frac{h}{3}(y_0 + 4y_1 + y_2)$$

- So $I = \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \ldots + y_n) = \frac{h}{3}(first + 4 \times odd + 2 \times even + last)$

Simpson’s 1/3 method

- In the summation, the factor 4 is from the coefficient, but where is from? As we mentioned before, simpson’s 1/3 method needs 3 point.
- Suppose we have n points, the 0, 1, 2 are in the group a, 2, 3, 4 are in the group b, 4, 5, 6 are in the group c, and so on. There is a point plus 2 times

$$\begin{array}{lcccc} & \boxed{1\ 4\ 1} & \boxed{1\ 4\ 1} & \boxed{1\ 4\ 1} & \boxed{1\ 4\ 1} \\ + & \quad\boxed{1\ 4\ 1} & \boxed{1\ 4\ 1} & \boxed{1\ 4\ 1} & \boxed{1\ 4\ 1} \\ \hline \end{array}$$

1 4 2 4 2 4 2 4 2 4 2 4 2 4 2 4 1

Example

$$I=\int_0^1 e^x dx = e-1 \cong 1.718281828......$$

n	result	error	n	result	error
3	1.718861	5.79E-04	12	1.639652	-7.86E-02
4	1.466244	-2.52E-01	13	1.718282	4.60E-07
5	1.718319	3.70E-05	14	1.651262	-6.70E-02
6	1.55514	-1.63E-01	15	1.718282	2.48E-07
7	1.718289	7.34E-06	16	1.659889	-5.84E-02
8	1.598074	-1.20E-01	17	1.718282	1.46E-07
9	1.718284	2.33E-06	18	1.666549	-5.17E-02
10	1.623194	-9.51E-02	19	1.718282	9.09E-08
11	1.718283	9.53E-07	20	1.671847	-4.64E-02

The result is as the table, as you can see simpson’s 1/3 method is very accuracy, but there is some problem when *n* is even number. Because the method we derive needs 3 points for integration, it’s lack of one point to do that, so the error is so high. Then how do we solve it?

Simpson's 3/8 method

- Its derivation is like 1/3 method, from quadra form

$$f(x) = ax^3 + bx^2 + cx + d$$

- 4 unknown parameters, at least 4 distinct points to find y. Here we use Lagrange interpolation to
- construct y and solve a, b, c, d.
- Suppose there are 4 distinct points
- $(x_0, f(x_0))$, $(x_1, f(x_1))$, $(x_2, f(x_2))$, $(x_3, f(x_3))$, $x_i = x_0 + ih$

Simpson's 3/8 method

$$f(x)=\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}+\frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}$$

$$=\frac{(x-x_1)(x-x_0)(x-x_3)}{(x_2-x_1)(x_2-x_0)(x_2-x_3)}+\frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)(x_3-x_0)}$$

$$=\frac{(x-x_1)(x-x_2)(x-x_3)}{(-h)(-2h)(-3h)}+\frac{(x-x_0)(x-x_2)(x-x_3)}{(h)(-h)(-2h)}$$

$$=\frac{(x-x_1)(x-x_0)(x-x_3)}{(h)(2h)(-h)}+\frac{(x-x_0)(x-x_1)(x-x_2)}{(2h)(h)(3h)}$$

Simpson's 3/8 method

- After integration, the coefficient are
- *a* = 3/8, *b* = 9/8, *c* = 9/8, *d* = 3/8

$$I = \frac{3h}{8}(y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + \ldots + y_n)$$

$$= \frac{3h}{8}(\textit{first} + 3 \times \textit{others} + 2 \times (\textit{multiple of } 3) + \textit{last})$$

- Combine 1/3 and 3/8 method, so that it can be applied in n points, $n \geq 3$
- If there just 2 points, use the trapezoidal method.