In the name of $\mathcal{GOD}$

Computational Physics

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Physics Group

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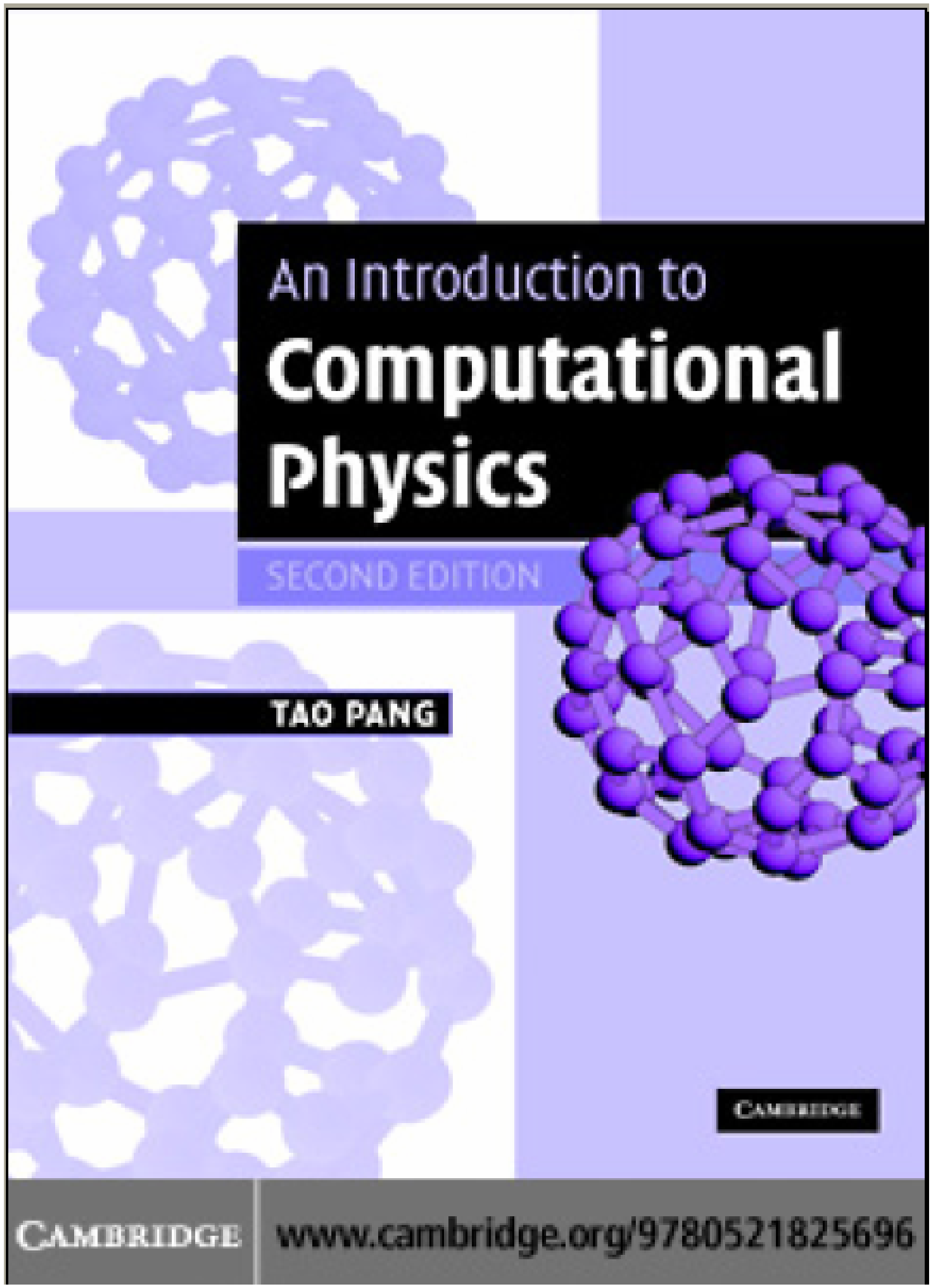
Outline

- Fortran-90 Programming
- Numerical calculus
- Approximation of a function
- Numerical methods for matrices
- Ordinary differential equations
- Partial differential equations
- Monte Carlo simulations
- Molecular dynamics simulations


An Introduction to
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TAO PANG
CAMBRIDGE
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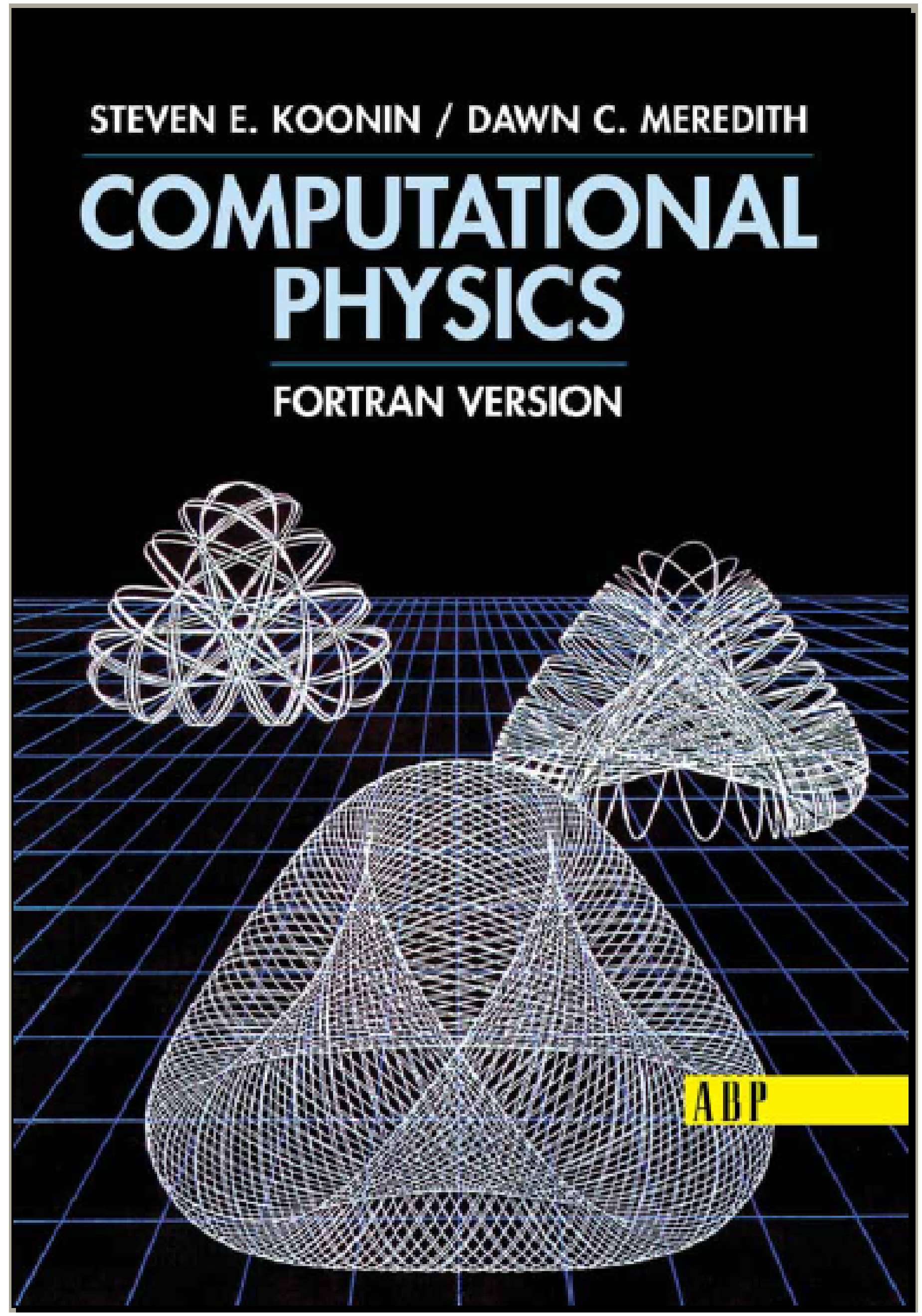
www.cambridge.org/9780521825696


STEVEN E. KOONIN / DAWN C. MEREDITH
COMPUTATIONAL
PHYSICS
FORTRAN VERSION
ABP

Numerical differentiation

Taylor expansion

$$f(x+\Delta x) = f(x) + \frac{\Delta x}{1!} f^{(1)}(x) + \frac{\Delta x^2}{2!} f^{(2)}(x) + \frac{\Delta x^3}{3!} f^{(3)}(x) + \frac{\Delta x^4}{4!} f^{(4)}(x) + \cdots$$

first-order derivative

$$\begin{cases} f(x+\Delta x) = f(x) + \dfrac{\Delta x}{1!} f^{(1)}(x) + \dfrac{\Delta x^2}{2!} f^{(2)}(x) + \cdots \\ f(x-\Delta x) = f(x) - \dfrac{\Delta x}{1!} f^{(1)}(x) + \dfrac{\Delta x^2}{2!} f^{(2)}(x) + \cdots \end{cases}$$

Numerical differentiation

two-point formula

Forward

$$f(x+\Delta x) = f(x) + \frac{\Delta x}{1!} f^{(1)}(x) + \frac{\Delta x^2}{2!} f^{(2)}(x) + \cdots$$

$$f^{(1)}(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x} + O(\Delta x)$$

Backward

$$f(x-\Delta x) = f(x) - \frac{\Delta x}{1!} f^{(1)}(x) + \frac{\Delta x^2}{2!} f^{(2)}(x) + \cdots$$

$$f^{(1)}(x) = \frac{f(x) - f(x-\Delta x)}{\Delta x} + O(\Delta x)$$

three-point formula

Central

$$f(x+\Delta x) - f(x-\Delta x) = \frac{2\Delta x}{1!} f^{(1)}(x) + \frac{2\Delta x^3}{3!} f^{(3)}(x) + \cdots$$

$$f^{(1)}(x) = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} + O(\Delta x^2)$$

Numerical differentiation

five-point formula

$$\begin{cases} f(x+2\Delta x) = f(x) + \frac{2\Delta x}{1!} f^{(1)}(x) + \frac{(2\Delta x)^2}{2!} f^{(2)}(x) + \frac{(2\Delta x)^3}{3!} f^{(3)}(x) + \frac{(2\Delta x)^4}{4!} f^{(4)}(x) + \frac{(2\Delta x)^5}{5!} f^{(5)}(x) + \cdots \\ f(x+\Delta x) = f(x) + \frac{\Delta x}{1!} f^{(1)}(x) + \frac{\Delta x^2}{2!} f^{(2)}(x) + \frac{\Delta x^3}{3!} f^{(3)}(x) + \frac{\Delta x^4}{4!} f^{(4)}(x) + \frac{\Delta x^5}{5!} f^{(5)}(x) + \cdots \\ f(x-\Delta x) = f(x) - \frac{\Delta x}{1!} f^{(1)}(x) + \frac{\Delta x^2}{2!} f^{(2)}(x) - \frac{\Delta x^3}{3!} f^{(3)}(x) + \frac{\Delta x^4}{4!} f^{(4)}(x) - \frac{\Delta x^5}{5!} f^{(5)}(x) + \cdots \\ f(x-2\Delta x) = f(x) - \frac{2\Delta x}{1!} f^{(1)}(x) + \frac{(2\Delta x)^2}{2!} f^{(2)}(x) - \frac{(2\Delta x)^3}{3!} f^{(3)}(x) + \frac{(2\Delta x)^4}{4!} f^{(4)}(x) - \frac{(2\Delta x)^5}{5!} f^{(5)}(x) + \cdots\cdots \end{cases}$$

$$f'(x) = \frac{1}{12h}\left(f(x-2\Delta x) - 8f(x-\Delta x) + 8f(x+\Delta x) - f(x+2\Delta x)\right) + O(\Delta x^4)$$

Numerical differentiation

second-order derivative

three-point formula ?

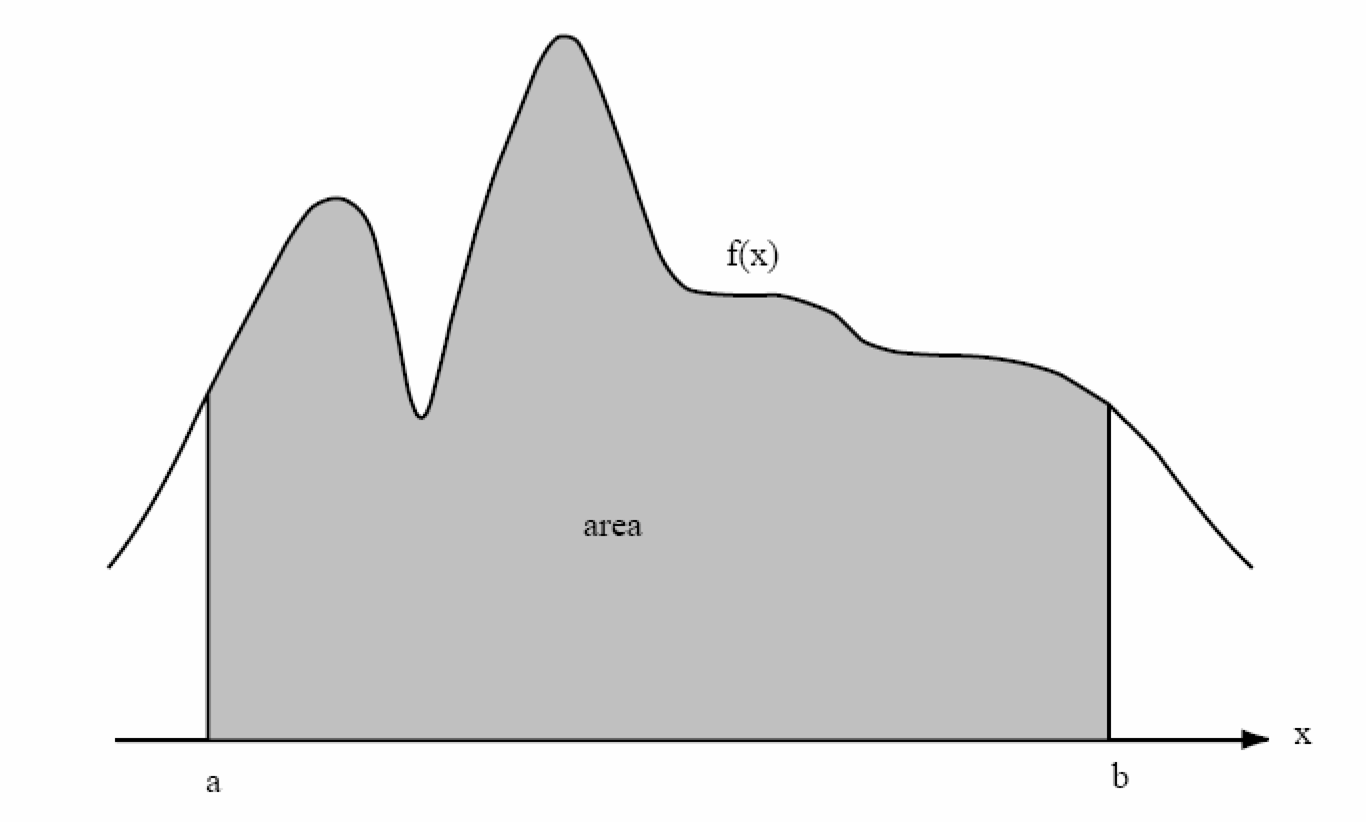
$$f''(x) = \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{2\Delta x} + O(\Delta x^2)$$

five-point formula ?

$$f''(x) = \frac{1}{12\Delta x^2}\{-f(x-2\Delta x) + 16f(x-\Delta x) - 30f(x) + 16f(x+\Delta x) - f(x+2\Delta x)\} + O(\Delta x^4)$$

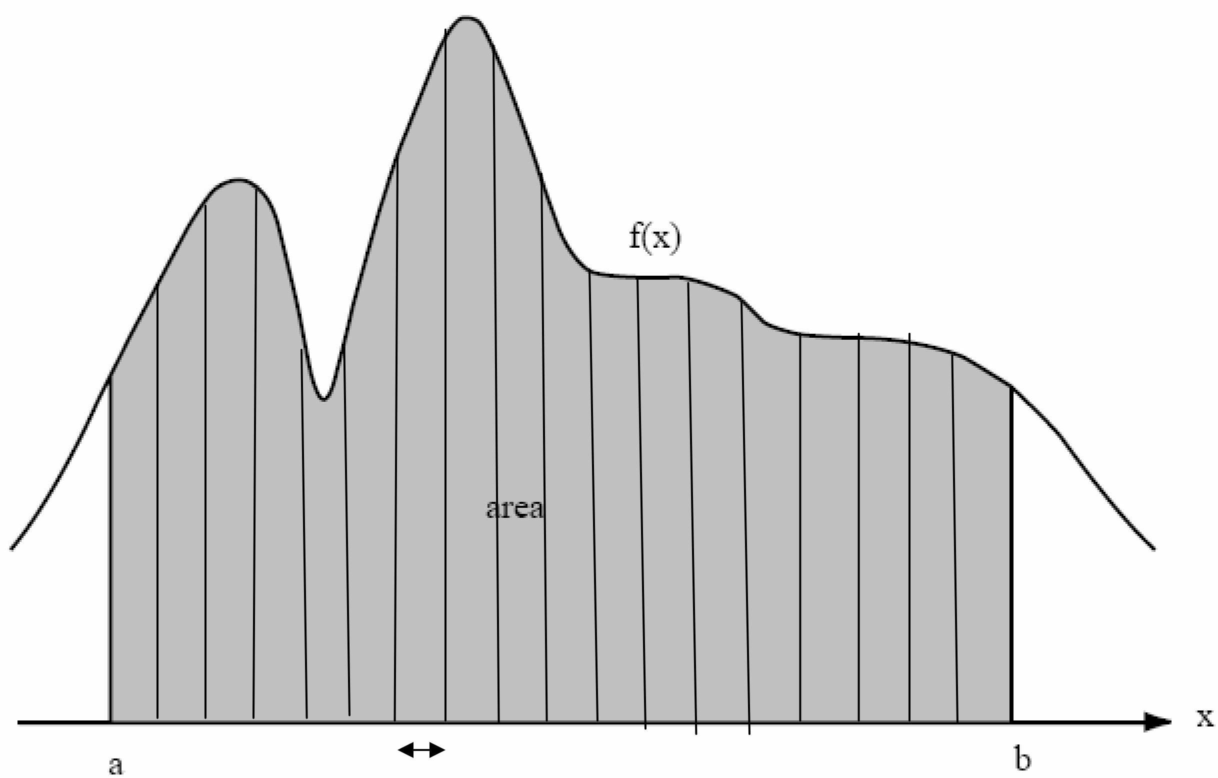
Numerical integration

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



Numerical integration

$$area = \int^{b} f(x)dx$$



$$\Delta x$$

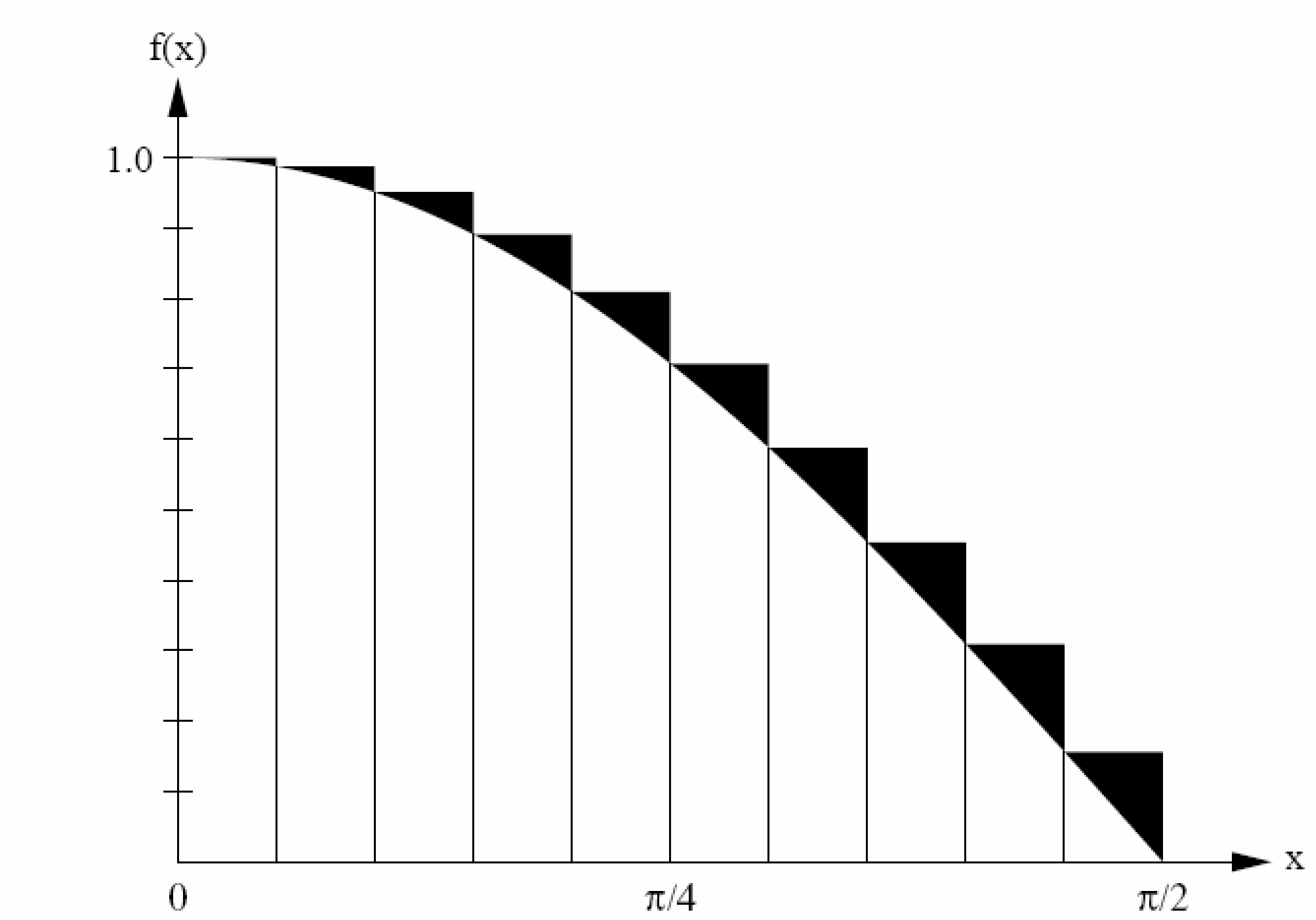
$$\Delta x = \frac{b-a}{n}$$

$$x_i = a + i\Delta x$$

$$x_0 = a \qquad x_n = b$$

Numerical integration

rectangular approximation



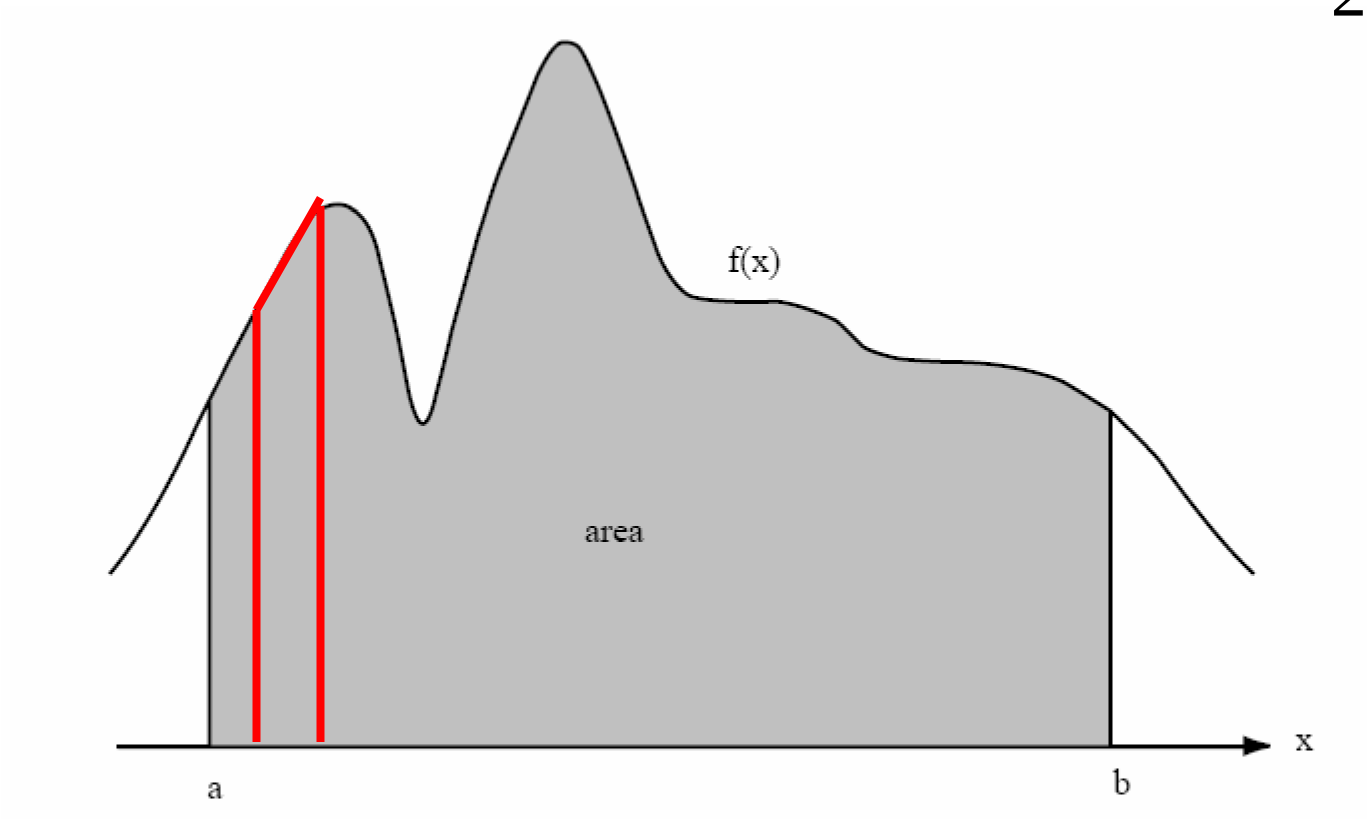
$$F_n = \sum_{i=0}^{n-1} f(x_i)\Delta x$$

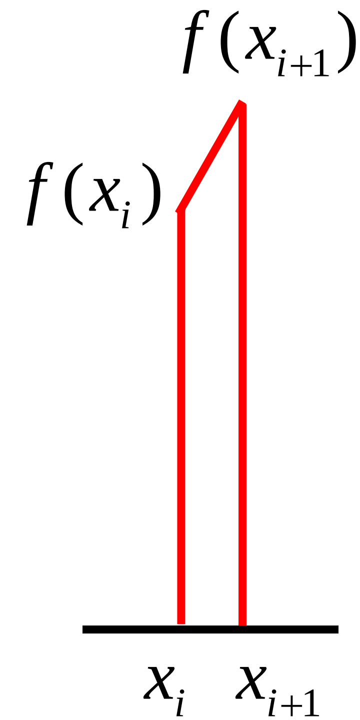
$$f(x) = \cos(x) \qquad , \qquad 0 \le x \le \frac{\pi}{2}$$

Numerical integration

$$S_i = \frac{\Delta x}{2}\left(f(x_i) + f(x_{i+1})\right)$$

trapezoidal rule



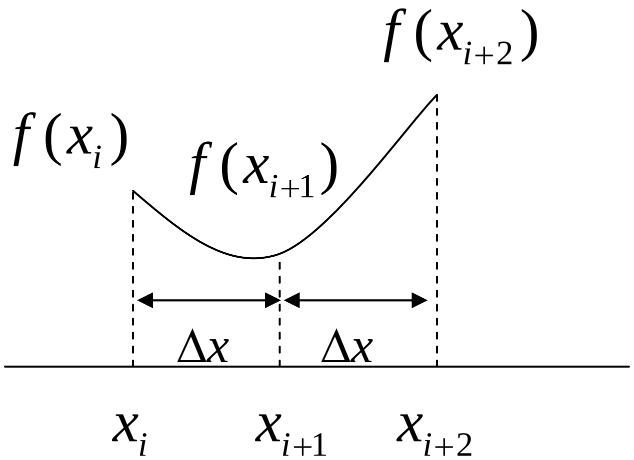


$$F_n = \sum_{i=0}^{n-1} S_i \quad \Rightarrow \quad F_n = \frac{\Delta x}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n) \right]$$

Numerical integration

Simpson's rule

$$area = \int_{x_i}^{x_{i+2}} f(x)dx$$



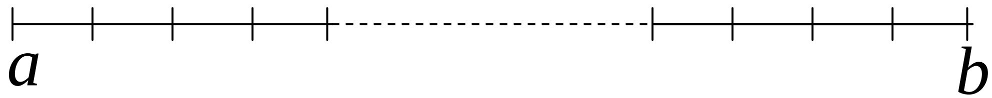
$$\boxed{\begin{aligned} f(x) = {} & f(x_i)\frac{(x-x_{i+1})(x-x_{i+2})}{(x_i-x_{i+1})(x_i-x_{i+2})} \\ & + f(x_{i+1})\frac{(x-x_{i+2})(x-x_i)}{(x_{i+1}-x_{i+2})(x_{i+1}-x_i)} \\ & + f(x_{i+2})\frac{(x-x_i)(x-x_{i+1})}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})} \end{aligned}}$$

$$area = \int_{x_i}^{x_{i+2}} f(x)dx = \frac{\Delta x}{3}[f(x_i) + 4f(x_{i+1}) + f(x_{i+2})]$$

$$\begin{aligned} F_n = \frac{\Delta x}{3}[& f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots \\ & + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)] \end{aligned}$$

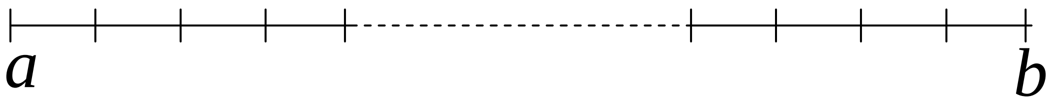
Numerical integration

Weight:



Rectangular approximation:

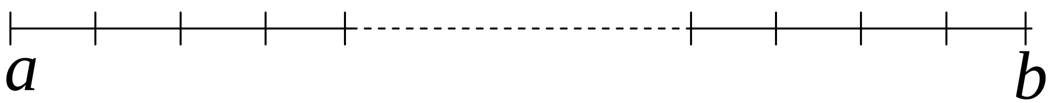
1 1 1 1 1 ……… 1 1 1 1 1



$$F_n = \Delta x \sum_{i=0}^{n} w(x_i)\, f(x_i)$$

Trapezoidal rule:

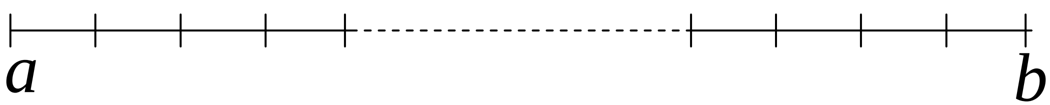
1 2 2 2 2 ……… 2 2 2 2 1



$$F_n = \frac{\Delta x}{2} \sum_{i=0}^{n} w(x_i)\, f(x_i)$$

Simpson’s rule:

1 4 2 4 2 ……… 2 4 2 4 1

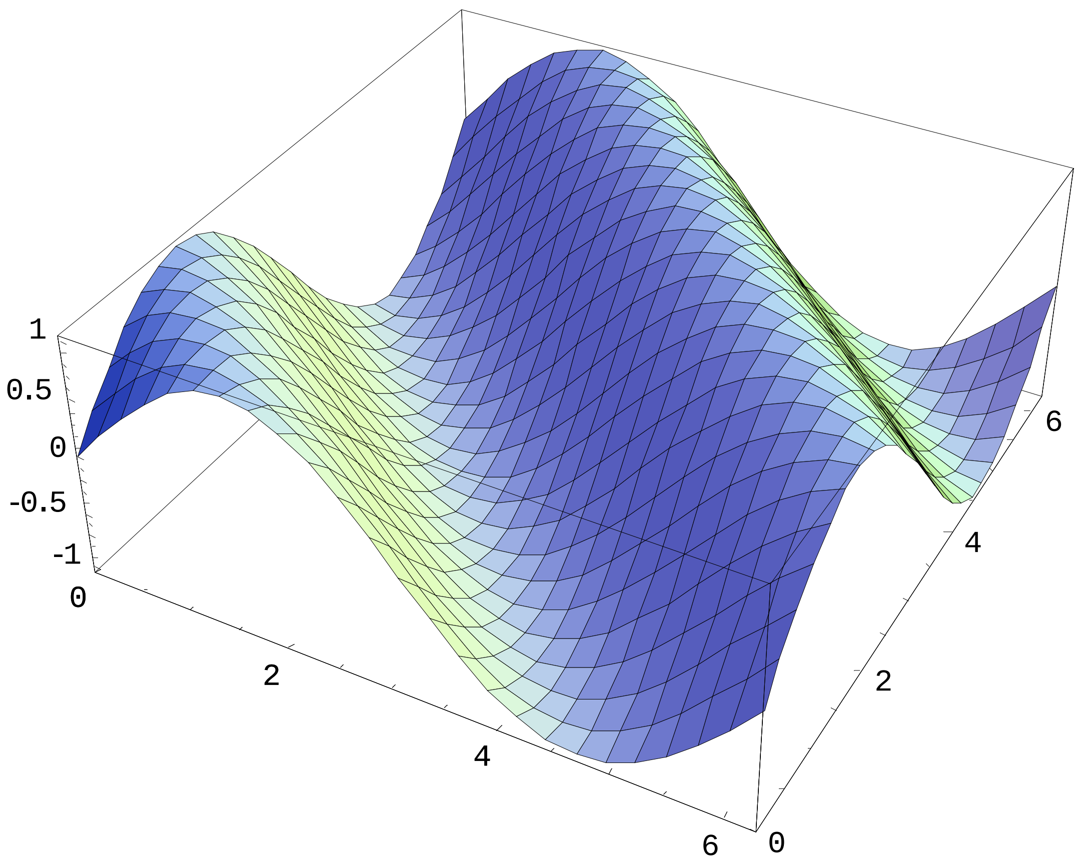


$$F_n = \frac{\Delta x}{3} \sum_{i=0}^{2n+1} w(x_i)\, f(x_i)$$

Numerical integration

2D

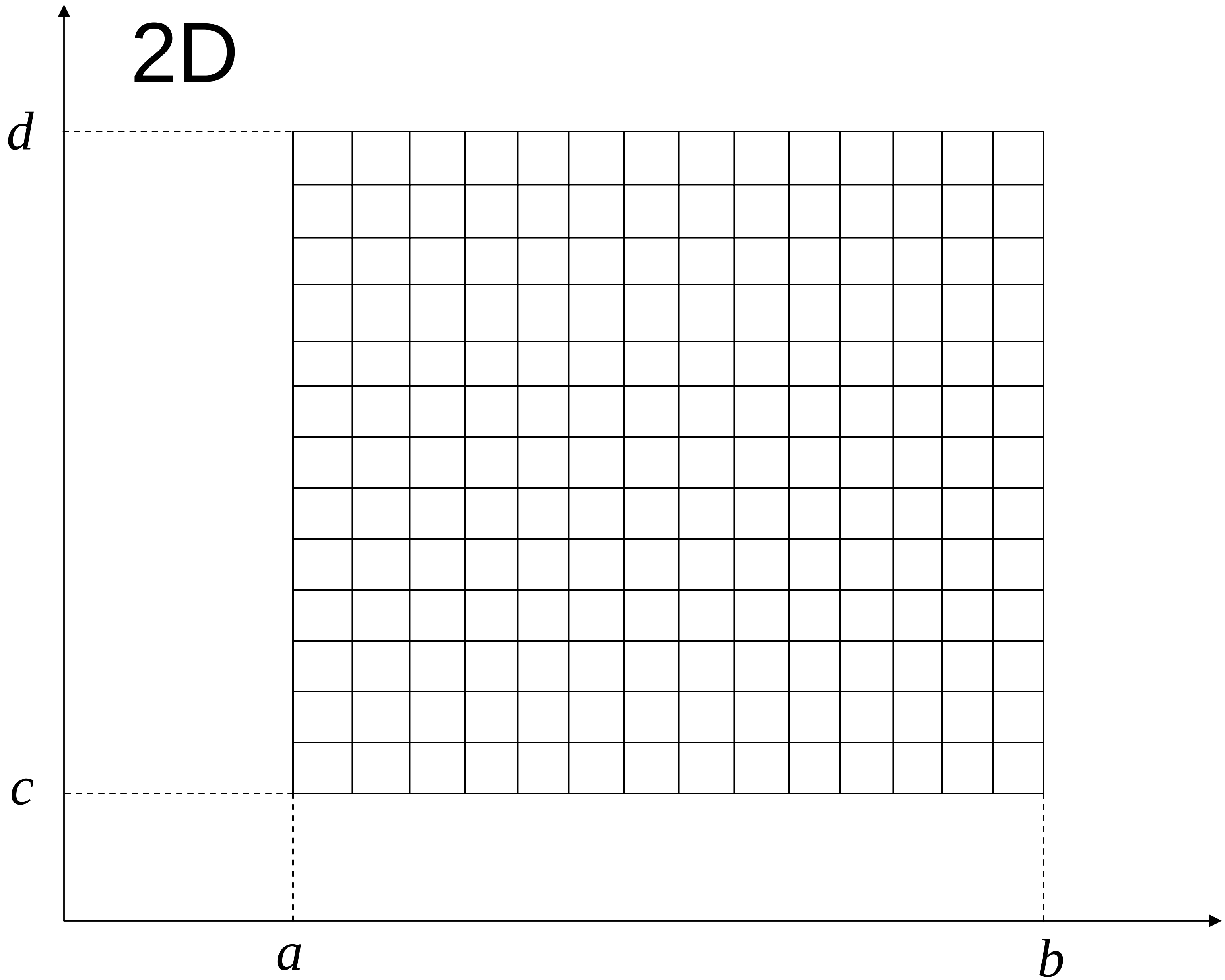
$$I = \int_a^b \int_c^d f(x, y) dxdy$$



$$f(x, y) = \sin(x + y)$$

$$0 \le x \le 2\pi$$
$$0 \le y \le 2\pi$$

Numerical integration



Numerical integration

2D

Rectangular approximation:

?

Trapezoidal rule:

?

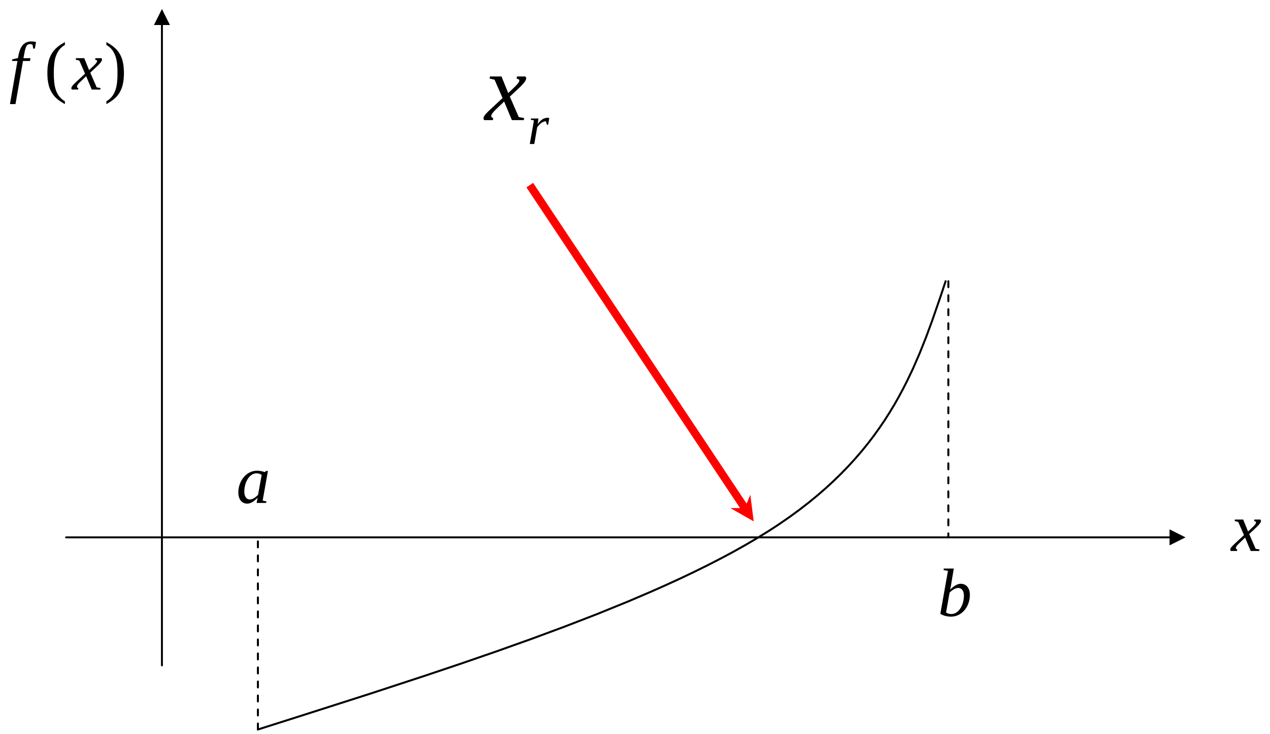
Simpson’s rule:

?

Roots of an equation

Bisection method

$$f(a)f(b) < 0 \Rightarrow x_0 = \frac{a+b}{2}$$

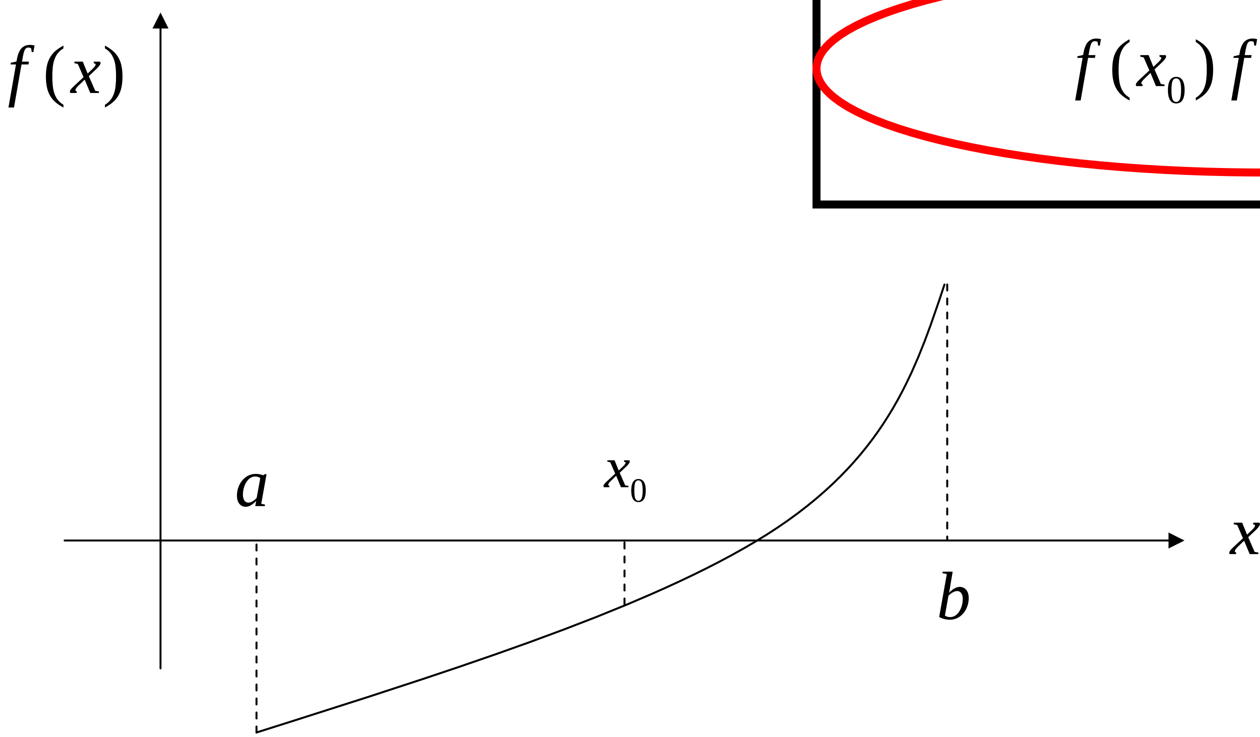


Roots of an equation

Bisection method

$$f(a)\,f(x_0) > 0$$

$$f(x_0)\,f(b) < 0$$

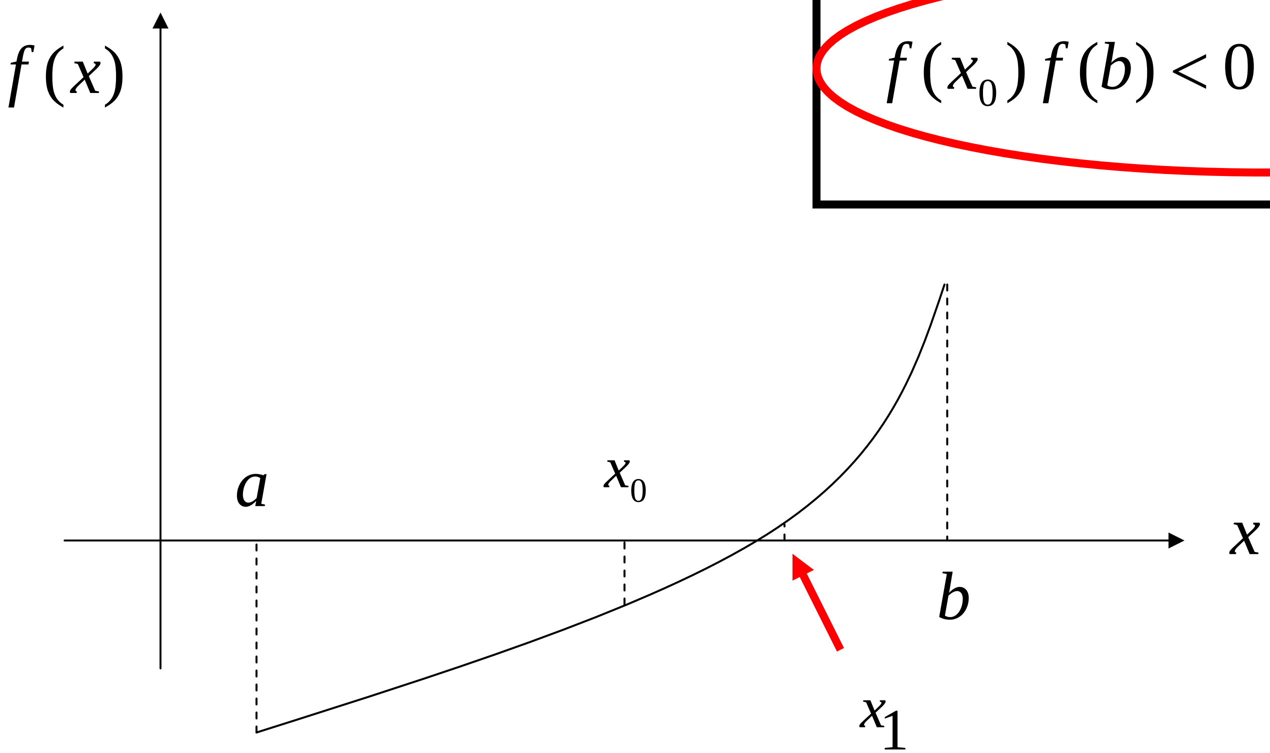


Roots of an equation

Bisection method

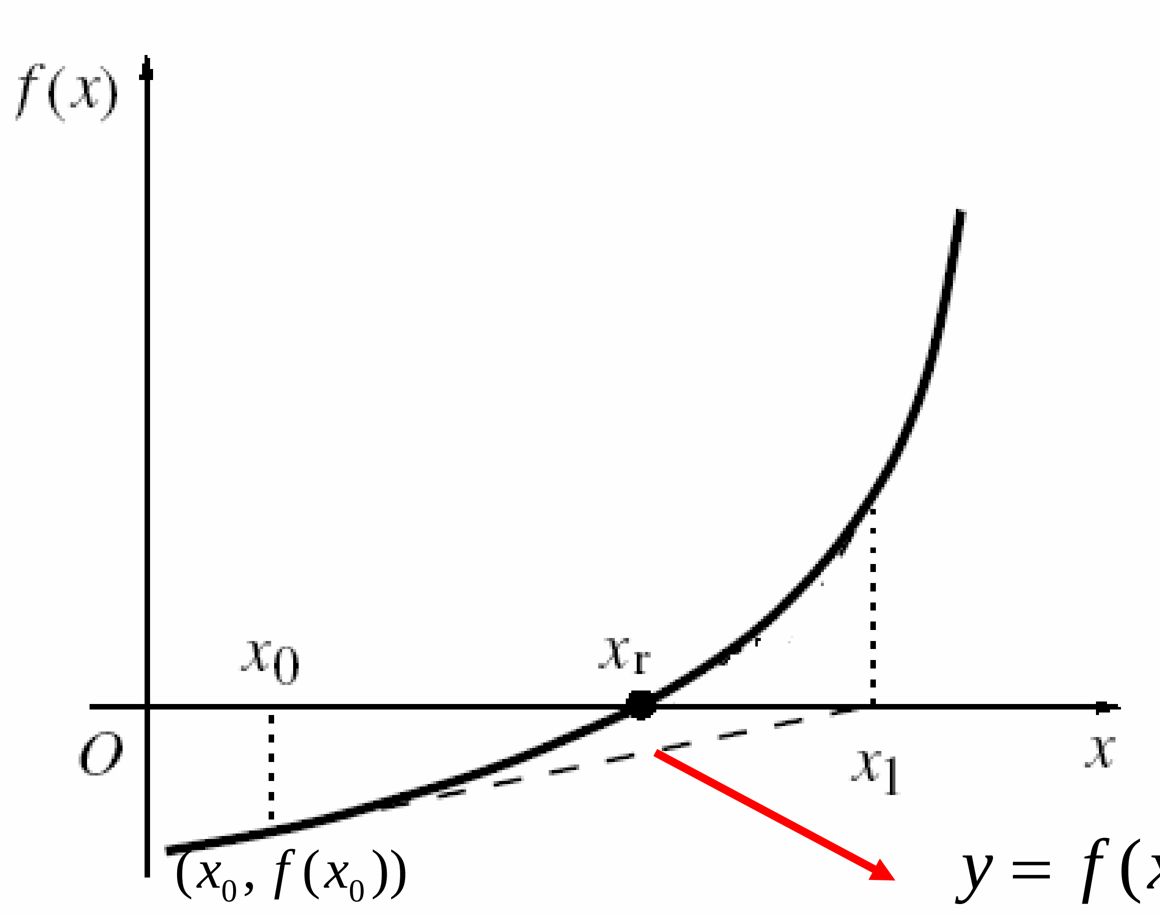
$$f(a)f(x_0) > 0$$

$$f(x_0)f(b) < 0 \Rightarrow x_1 = \frac{x_0 + b}{2}$$



Roots of an equation

The Newton method (*Newton–Raphson method*)

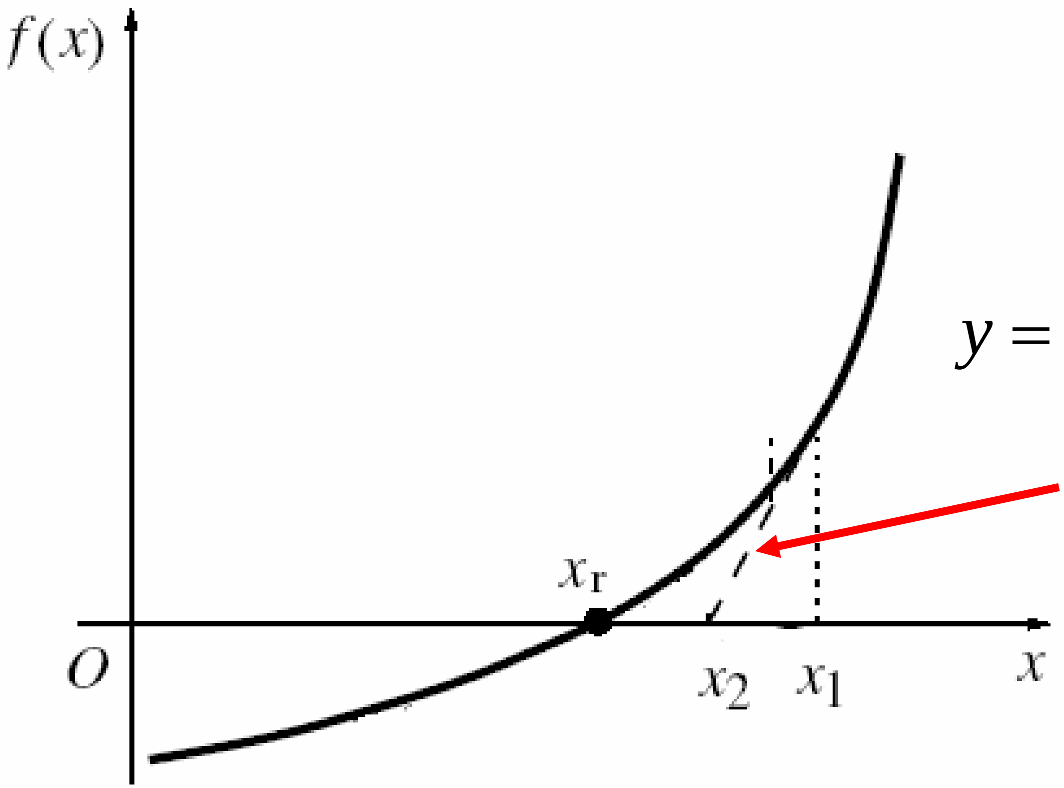


$$y = f(x_0) + (x - x_0) f'(x_0)$$

$$y = 0 \Rightarrow x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

Roots of an equation

The Newton method (*Newton–Raphson method*)



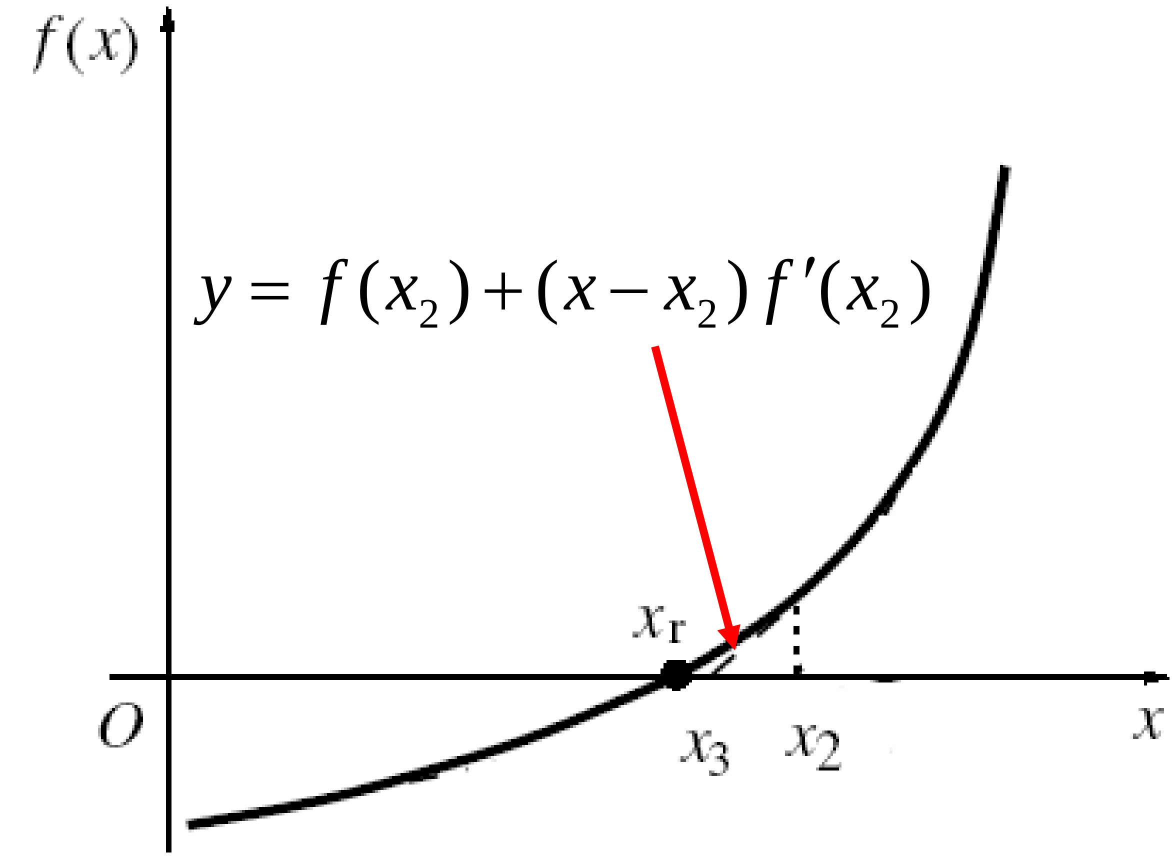
$$y = f(x_1) + (x - x_1) f'(x_1)$$

$$y = 0 \Rightarrow x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

Roots of an equation

The Newton method (*Newton–Raphson method*)

$$y = f(x_2) + (x - x_2) f'(x_2)$$



$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

$$\left| f(x_k) \right| \to 0$$

$$y = 0 \Rightarrow x_3 = x_2 - \frac{f(x_2)}{f'(x_2)}$$

Roots of an equation

Secant method

Newton method

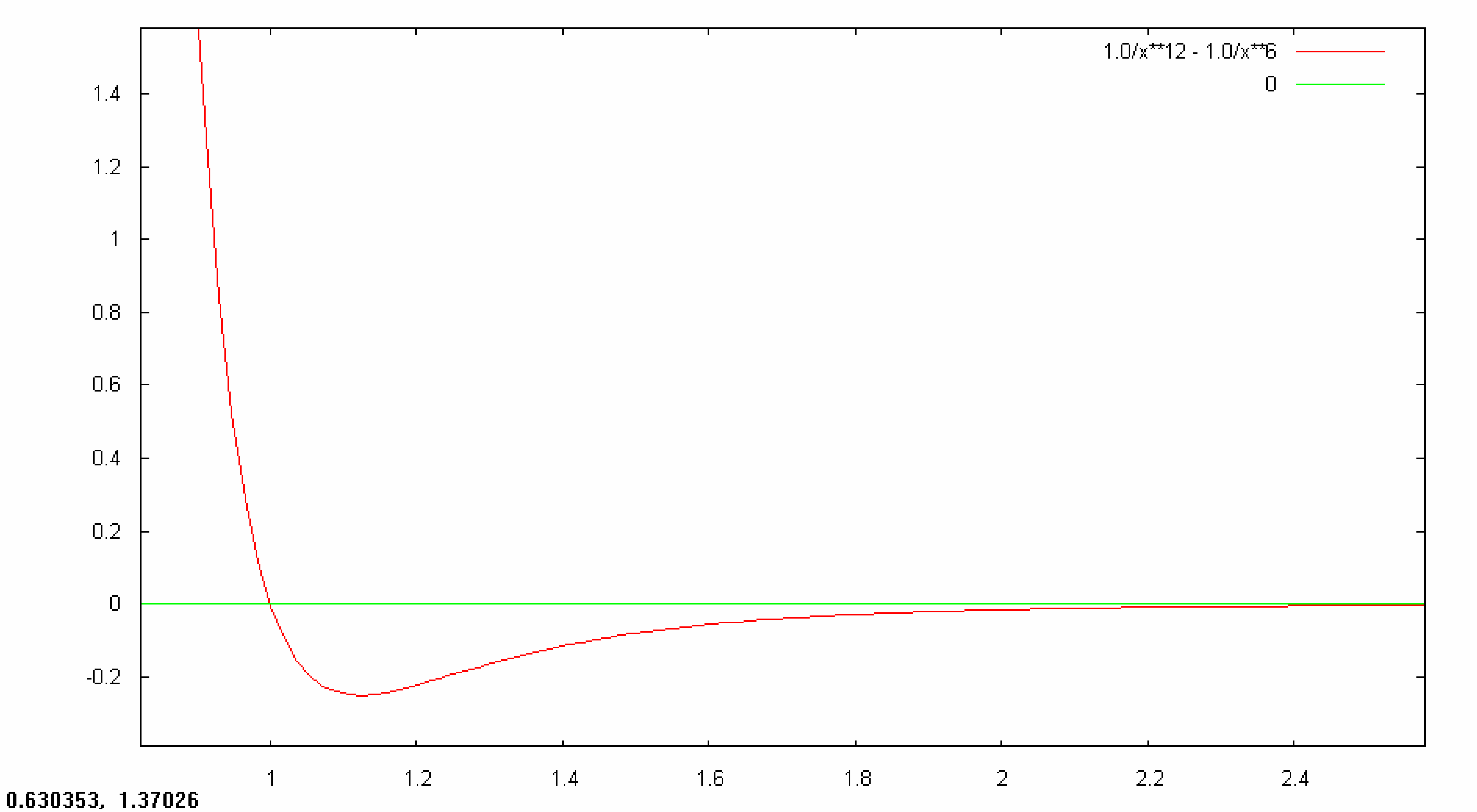
$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

$$f'(x_k) = \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}$$

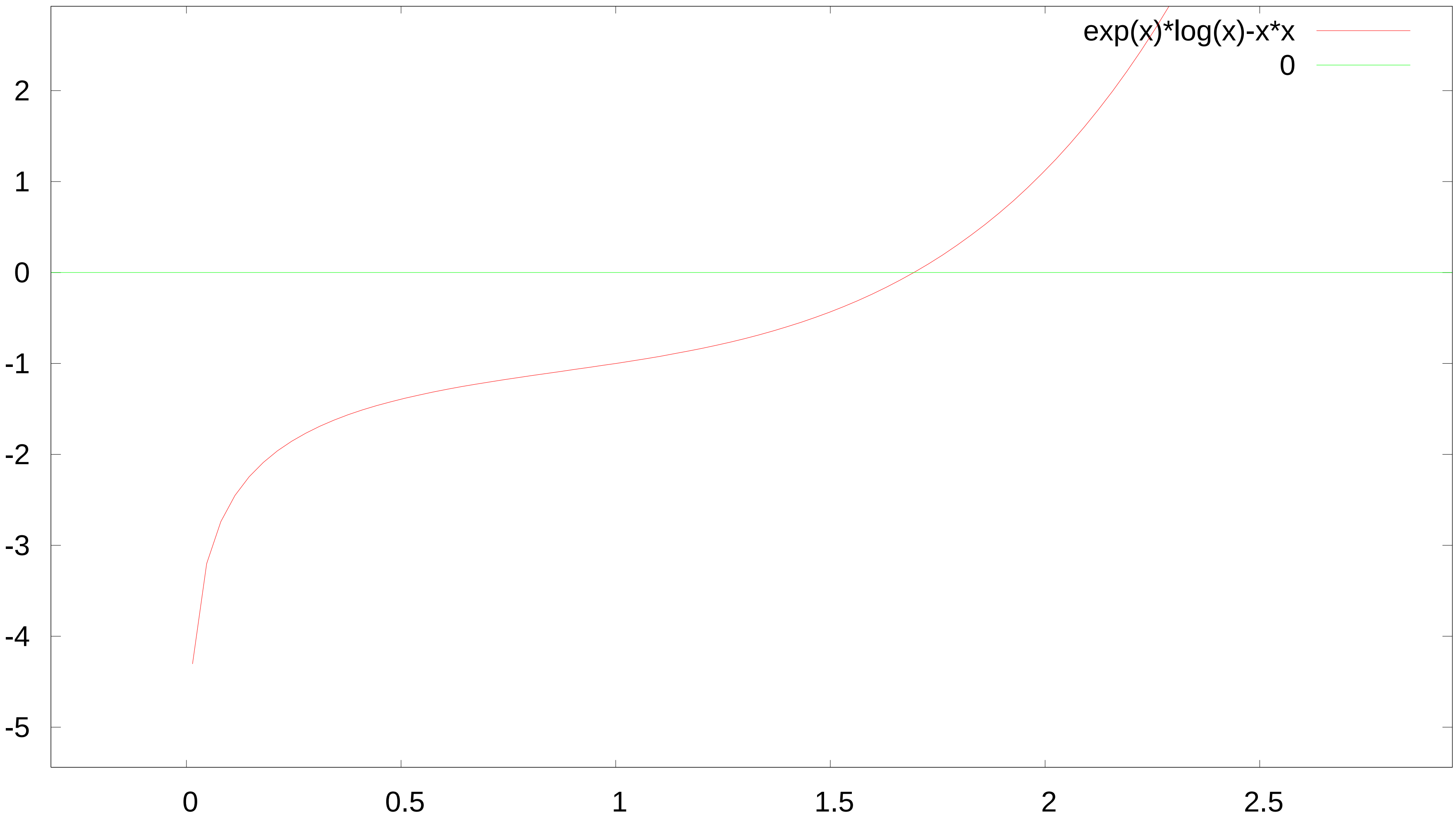
$$\Downarrow$$

Discrete Newton method

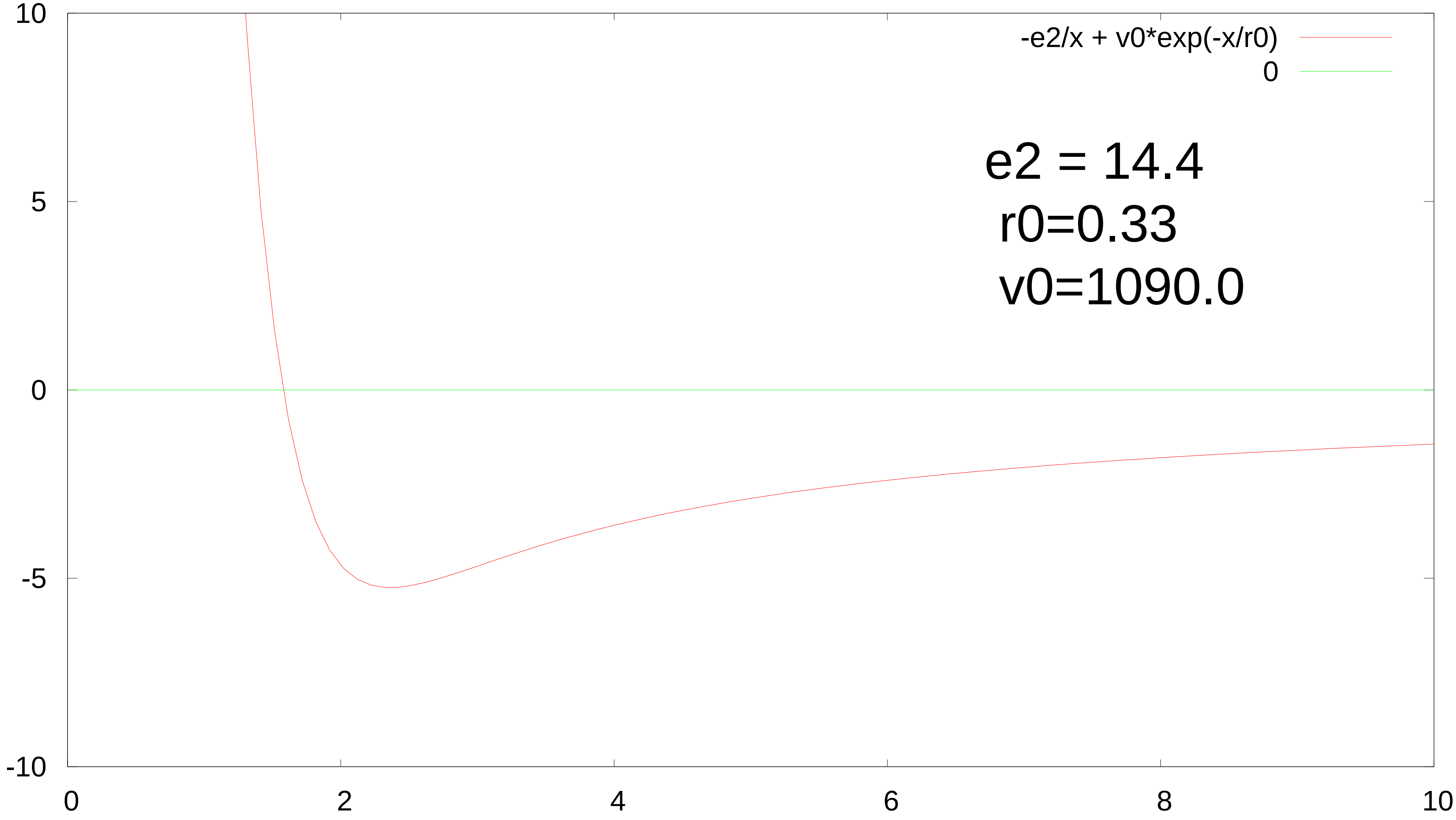
$$x_{k+1} = x_k - (x_k - x_{k-1}) \frac{f(x_k)}{f(x_k) - f(x_{k-1})}$$



1.0/x**12 - 1.0/x**6
0
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
1
1.2
1.4
1.6
1.8
2
2.2
2.4
0.630353, 1.37026



exp(x)*log(x)-x*x
0
2
1
0
-1
-2
-3
-4
-5
0
0.5
1
1.5
2
2.5

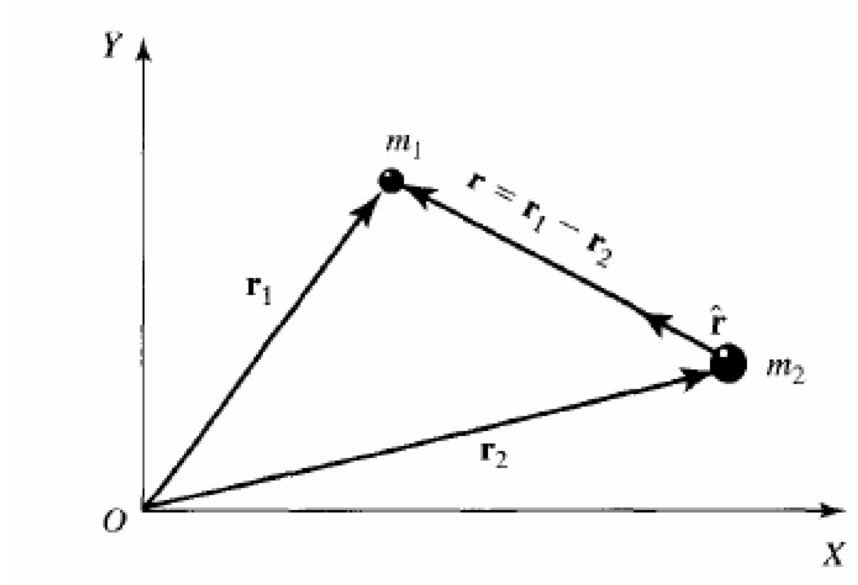

-e2/x + v0*exp(-x/r0)
0
e2 = 14.4
r0=0.33
v0=1090.0
10
5
0
-5
-10
0
2
4
6
8
10

CENTRAL FORCE MOTION

$$m_1\ddot{\vec{r}}_1 = \vec{F}(r)\hat{r}$$

$$m_2\ddot{\vec{r}}_2 = -\vec{F}(r)\hat{r}$$

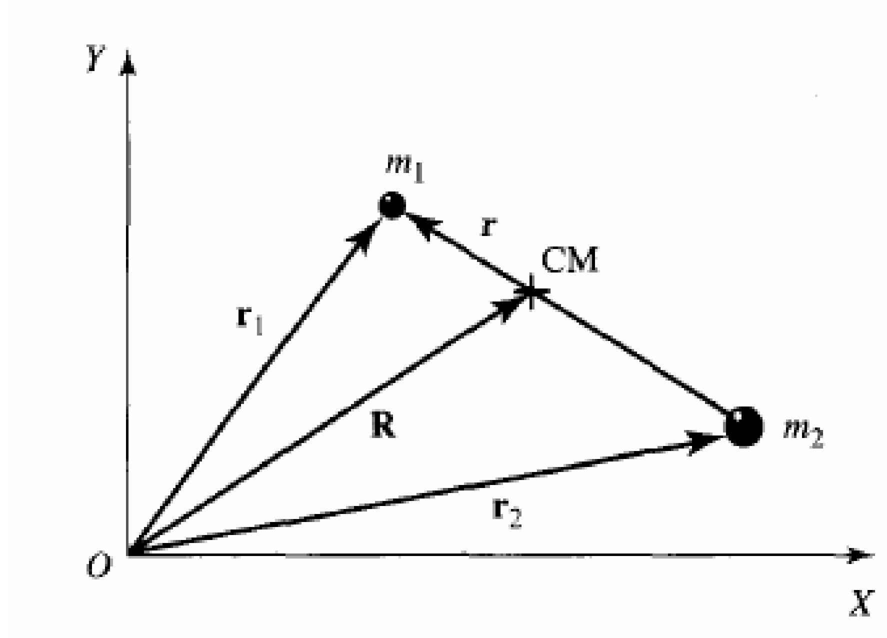
$$\vec{r} = \vec{r}_1 - \vec{r}_2$$



$$\boxed{\begin{gathered} m_1\vec{r}_1 + m_2\vec{r}_2 = (m_1 + m_2)\vec{R} \\ \vec{r} = \vec{r}_1 - \vec{r}_2 \end{gathered}}$$

CENTRAL FORCE MOTION

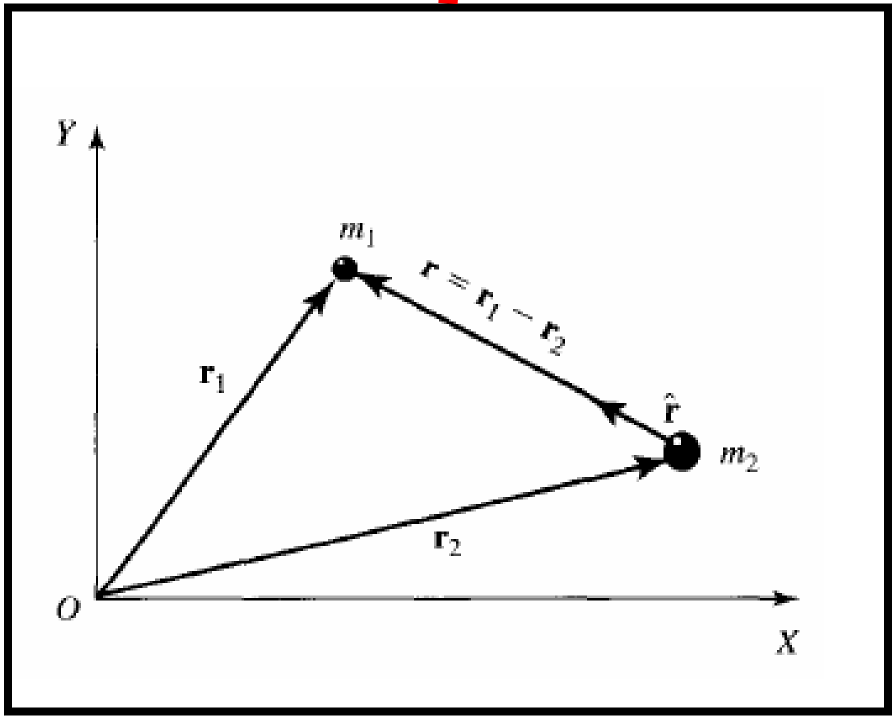
$$m_1\ddot{\vec{r}}_1 = \vec{F}(r)\hat{r}$$
$$m_2\ddot{\vec{r}}_2 = -\vec{F}(r)\hat{r}$$

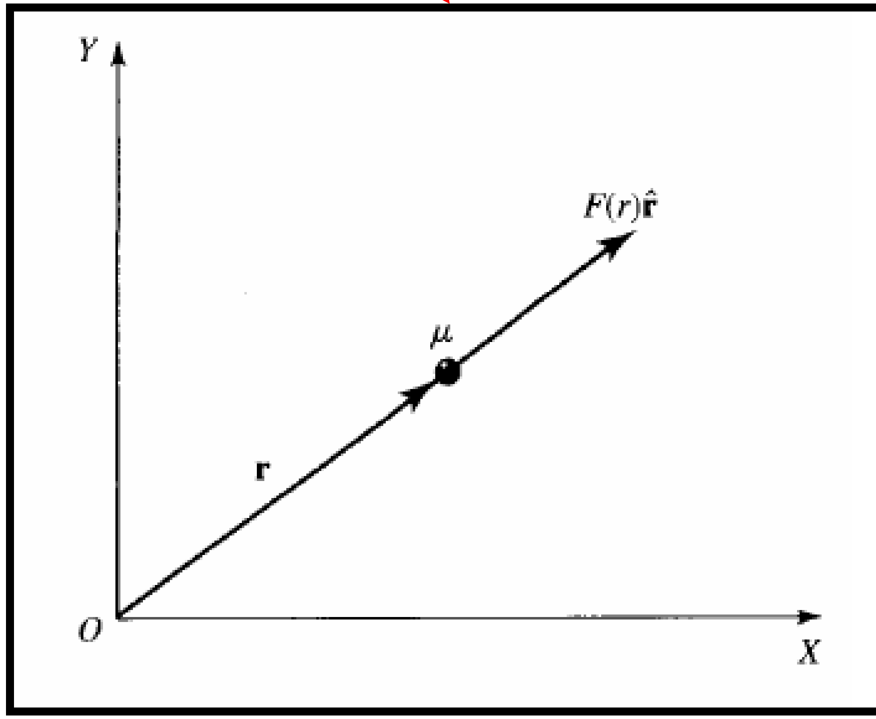


$$\begin{cases} \ddot{\vec{r}}_1 = \dfrac{\vec{F}(r)}{m_1}\hat{r} \\ \ddot{\vec{r}}_2 = -\dfrac{\vec{F}(r)}{m_2}\hat{r} \end{cases} \Rightarrow \ddot{\vec{r}}_1 - \ddot{\vec{r}}_2 = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\vec{F}(r)\hat{r}$$

$$\xrightarrow{\vec{r} = \vec{r}_1 - \vec{r}_2} \ddot{\vec{r}} = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\vec{F}(r)\hat{r} \xrightarrow{\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}} \mu\ddot{\vec{r}} = \vec{F}(r)\hat{r}$$

CENTRAL FORCE MOTION





$$m_1\ddot{\vec{r}}_1 = \vec{F}(r)\hat{r}$$

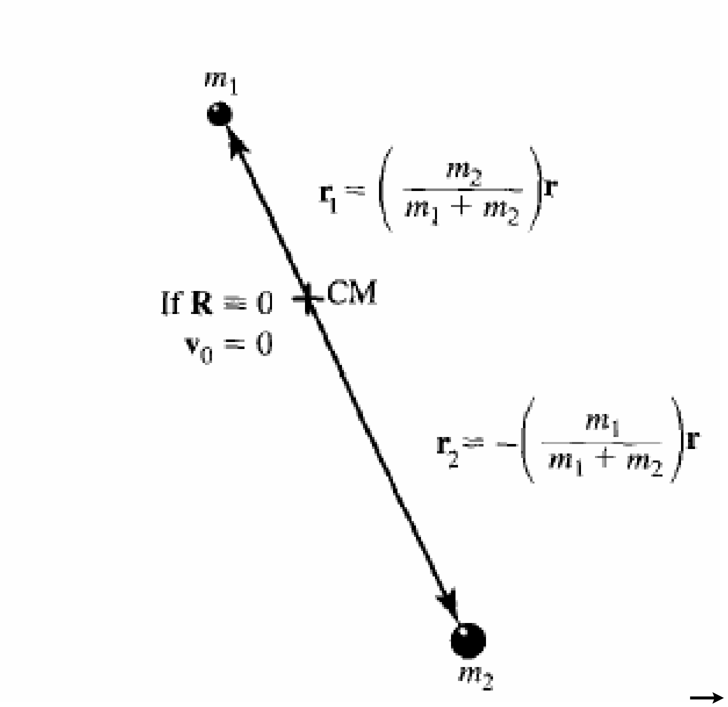
$$m_2\ddot{\vec{r}}_2 = -\vec{F}(r)\hat{r}$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\ddot{\vec{R}} = 0$$

$$\mu\ddot{\vec{r}} = \vec{F}(r)\hat{r}$$

CENTRAL FORCE MOTION



$$\vec{r}_1 = R + \frac{m_2}{m_1+m_2}\vec{r}$$

$$\vec{r}_2 = R - \frac{m_1}{m_1+m_2}\vec{r}$$

$$\mu\ddot{\vec{r}} = \vec{F}(r)\hat{r}$$

$$\vec{r} = r\hat{r}$$
$$\vec{v} = \dot{r}\hat{r} + r\dot{\theta}\hat{\theta}$$
$$\vec{a} = (\ddot{r} - r\dot{\theta}^2)\hat{r} + (2\dot{r}\dot{\theta} + r\ddot{\theta})\hat{\theta}$$

$\Rightarrow$

$$\mu(\ddot{r} - r\dot{\theta}^2) = F(r)$$
$$\mu(2\dot{r}\dot{\theta} + r\ddot{\theta}) = 0$$

CENTRAL FORCE MOTION

$$\mu(2\dot{r}\dot{\theta}+r\ddot{\theta})=0\xrightarrow{\times r}\mu(2r\dot{r}\dot{\theta}+r^2\ddot{\theta})=0\to\frac{d}{dt}(\mu r^2\dot{\theta})=0$$

$$\mu r^2\dot{\theta}=const.=l$$

$$\left\{\begin{array}{l}\mu(\ddot{r}-r\dot{\theta}^2)=F(r)\\ \mu r^2\dot{\theta}=l\Rightarrow\dot{\theta}=\dfrac{l}{\mu r^2}\end{array}\right.\Rightarrow\mu\ddot{r}-\frac{l^2}{\mu r^3}=F(r)$$

CENTRAL FORCE MOTION

$$\mu\ddot{r}-\frac{l^2}{\mu r^3}=F(r)\Rightarrow\mu\frac{dv}{dt}=\frac{l^2}{\mu r^3}+F(r)$$

$$\mu\frac{dr}{dt}\frac{dv}{dr}=\frac{l^2}{\mu r^3}+F(r)\Rightarrow\mu v dv=\left(\frac{l^2}{\mu r^3}+F(r)\right)dr$$

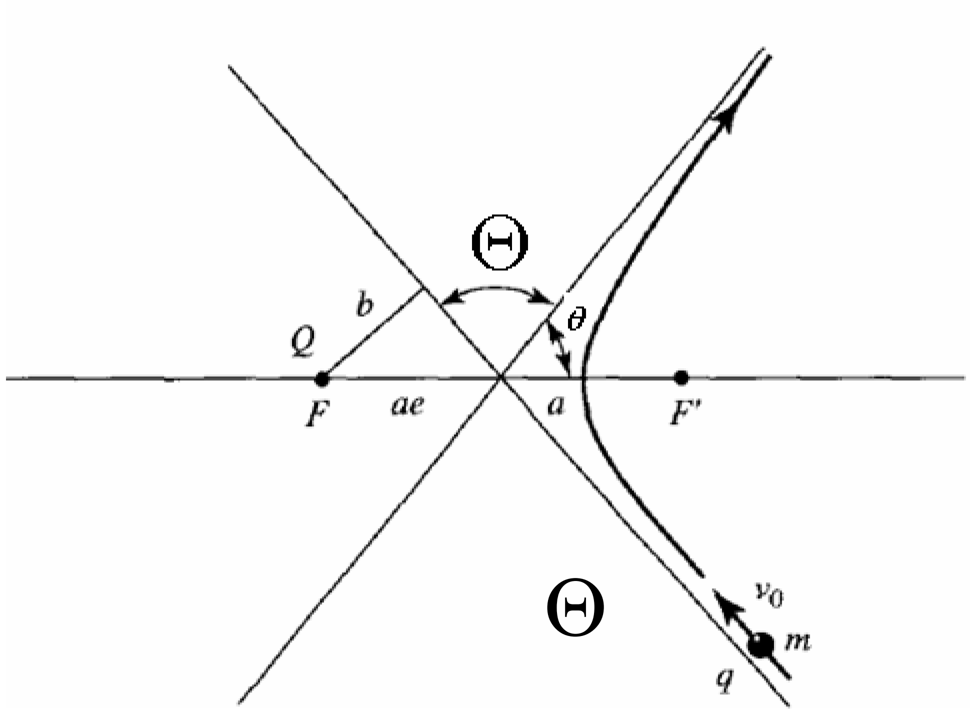
$$\mu v dv=\left(\frac{l^2}{\mu r^3}-\frac{dV}{dr}\right)dr\Rightarrow E=\frac{1}{2}\mu v^2+V(r)+\frac{l^2}{2\mu r^2}=const.$$

CENTRAL FORCE MOTION

$$l = \mu r^2 \dot{\theta} = const.$$

$$E = \frac{1}{2}\mu v^2 + V(r) + \frac{l^2}{2\mu r^2} = const.$$

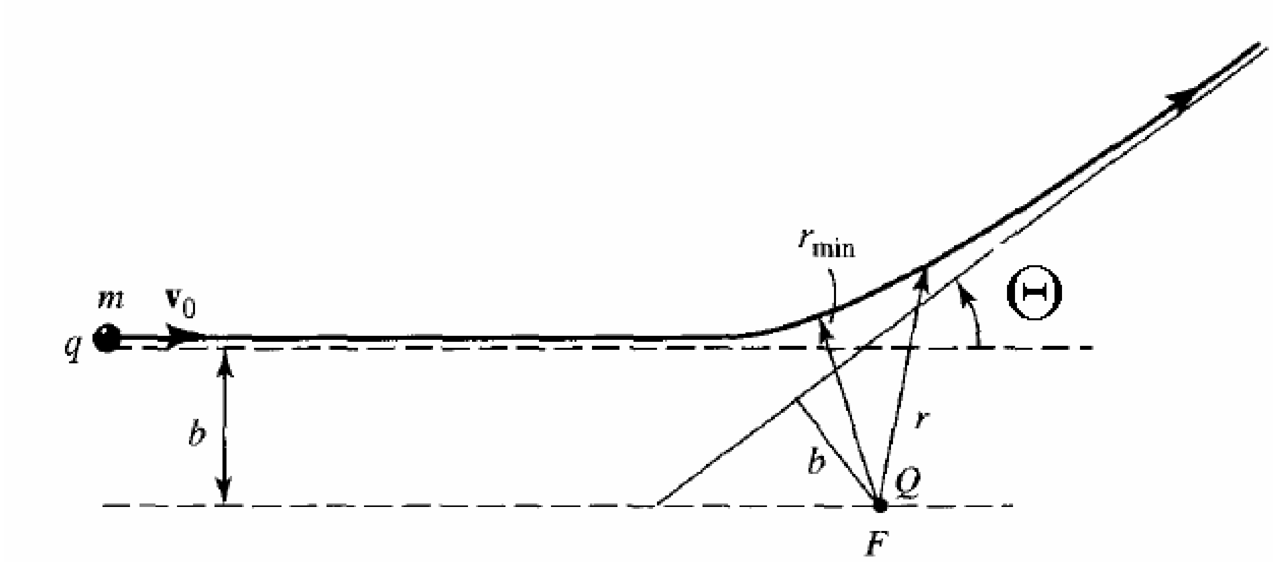
Cross section of scattering



$$E = \frac{1}{2} m v_0^2$$

$$L = m v_0 b$$

$$\Theta = \pi - 2\theta$$



Cross section of scattering

$$l = \mu b v_0 = \mu r^2 \dot{\theta} = const.$$

$$E = \frac{1}{2}\mu v_0^2 = \frac{1}{2}\mu v^2 + V(r) + \frac{l^2}{2\mu r^2} = const.$$

$$\frac{d\theta}{dt} = \dot{\theta} = \frac{b v_0}{r^2}$$

$$\frac{dr}{dt} = v = \pm v_0 \left((1 - \frac{b^2}{r^2}) - \frac{V(r)}{E} \right)^{\frac{1}{2}}$$

Cross section of scattering

$$\frac{\left(\frac{d\theta}{dt}\right)}{\left(\frac{dr}{dt}\right)} = \pm \frac{b}{r^2\left((1-\frac{b^2}{r^2})-\frac{V(r)}{E}\right)^{\frac{1}{2}}} \Rightarrow \frac{d\theta}{dr} = \pm \frac{b}{r^2\left((1-\frac{b^2}{r^2})-\frac{V(r)}{E}\right)^{\frac{1}{2}}}$$

$$\theta = \int_{r_m}^{\infty} \frac{b}{r^2\left((1-\frac{b^2}{r^2})-\frac{V(r)}{E}\right)^{\frac{1}{2}}} dr = -\int_{-\infty}^{r_m} \frac{b}{r^2\left((1-\frac{b^2}{r^2})-\frac{V(r)}{E}\right)^{\frac{1}{2}}} dr$$

$$(1-\frac{b^2}{r_m^2})-\frac{V(r_m)}{E} = 0 \qquad \Theta = \pi - 2\theta$$

Cross section of scattering

$$\sigma = \int \sigma(\Theta) d\Theta$$

$$2\pi I b db = I\sigma(\Theta) d\Omega$$

$$d\Omega = 2\pi Sin\Theta d\Theta$$

$$\sigma(\Theta) = \frac{b}{Sin\Theta}\left|\frac{db}{d\Theta}\right|$$

Write program :

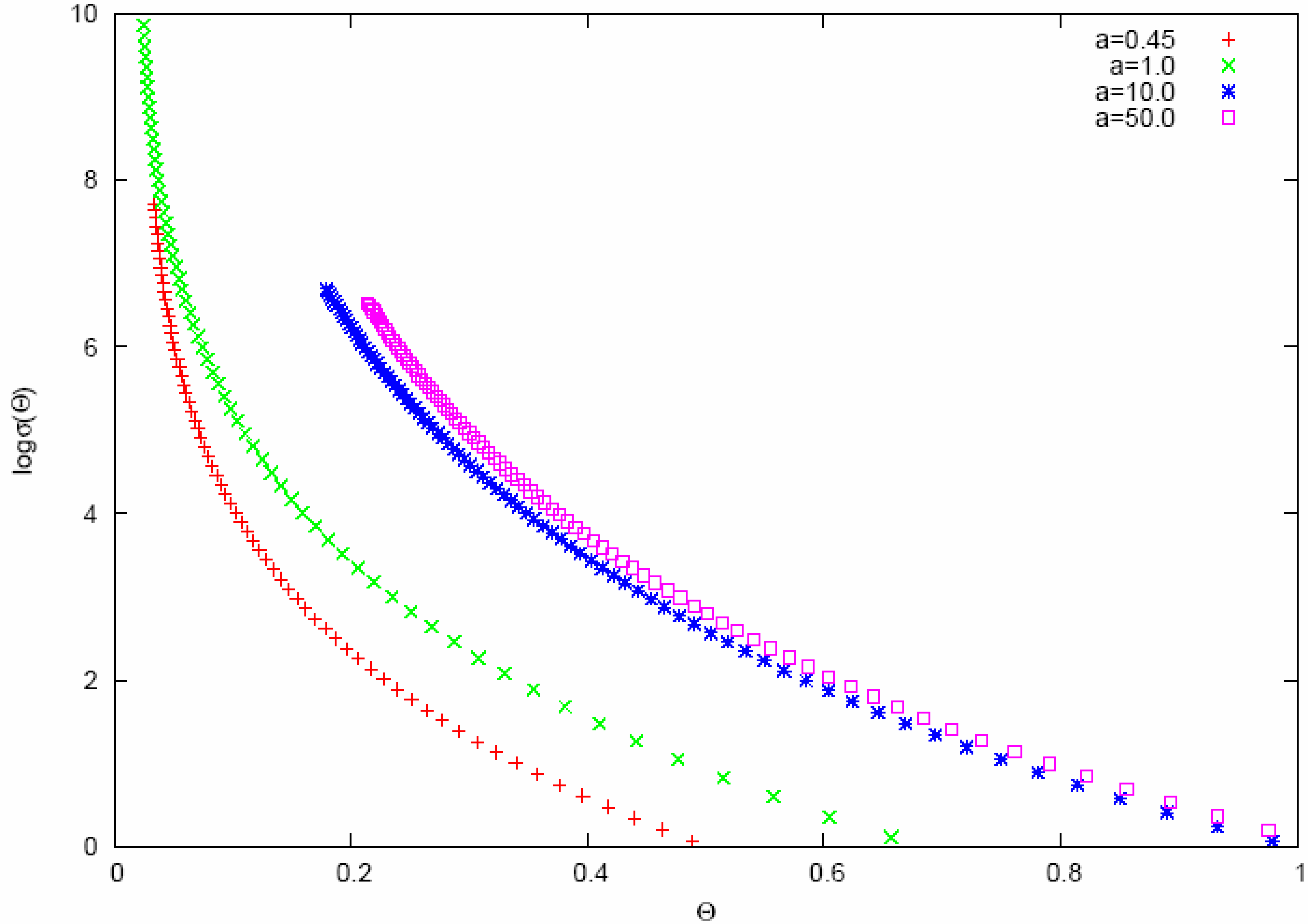
$$V(r) = \frac{\kappa}{r} e^{-r/a}$$

$E = m = \kappa = 1.$ a = 100

$$\Theta(b) = \pi - 2\theta(b) \qquad \sigma(\Theta) = \frac{b}{Sin\Theta}\left|\frac{db}{d\Theta}\right|$$

$$\theta = \int_{r_m}^{\infty} \frac{b}{r^2\left((1-\frac{b^2}{r^2}) - \frac{V(r)}{E}\right)^{\frac{1}{2}}} dr = -\int_{-\infty}^{r_m} \frac{b}{r^2\left((1-\frac{b^2}{r^2}) - \frac{V(r)}{E}\right)^{\frac{1}{2}}} dr$$

$$(1-\frac{b^2}{r_m^2}) - \frac{V(r_m)}{E} = 0$$



a=0.45
a=1.0
a=10.0
a=50.0
log σ(Θ)
Θ
0
0.2
0.4
0.6
0.8
1
2
4
6
8
10