Lecture 16: Numerical Integration

Rajen Kumar Sinha

Department of Mathematics
IIT Guwahati

Numerical Integration

Recall the technique of anti-differentiation. To find the value of

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

we need to find a function $F(x)$ with the property that $F'(x) = f(x)$. Then

$$\int_a^b f(x)\,dx = F(b) - F(a).$$

Example: If $f(x) = x^2$ then $F(x) = \frac{x^3}{3}$.
There are many elementary functions that do not have simple anti-derivatives.
Example:

$$\int_0^2 e^{-x^2}\,dx; \qquad \int_0^1 \sin(xe^x)\,dx; \qquad \int_0^\pi \cos(3\cos\theta)\,d\theta$$

These integrals are not amenable to the techniques learned in elementary calculus.

Question. Suppose we are given the values of a function $f(x)$ at a few points, say x_0, x_1,..., x_n, can that information be used to estimate

$$\int_a^b f(x)\,dx \text{ (an integral)?}$$

$x_0 \quad f(x_0)$
$x_1 \quad f(x_1)$
$\vdots$
$x_n \quad f(x_n)$

Answer: Yes

The problem of numerical integration is to estimate the number

$$I(f) = \int_a^b f(x)dx. \tag{1}$$

Basic Idea: To approximate

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

where $p_k(x)$ is the polynomial of degree $\leq k$ with

$$p_k(x_i) = f(x_i), \quad i = 0, \ldots, k.$$

The error in the approximation is given by

$$E(f) = I(f) - I(p_k).$$

This approximation is usually written as a weighted sum

$$I(p_k) = A_0 f(x_0) + A_1 f(x_1) + \cdots + A_k f(x_k),$$

where A_i's are weights and $f(x_0), \ldots, f(x_k)$ are function values.

By Newton's divided difference interpolating polynomial, we have

$$f(x) = p_k(x) + \underbrace{f[x_0, \ldots, x_k, x]\psi_k(x)}_{\text{Error term}},$$

where

$$\begin{aligned} p_k(x) &= f(x_0) + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) \\ &\quad + \cdots + f[x_0, x_1, \cdots, x_k](x - x_0)(x - x_1)\cdots(x - x_{k-1}), \\ \psi_k(x) &= \prod_{j=0}^{k}(x - x_j). \end{aligned}$$

Rectangle Rule: Let $k = 0$. Then

$$f(x) \approx p_0(x) = f(x_0).$$

Hence

$$I(p_k) = \int_a^b f(x_0)\,dx = (b-a)f(x_0)$$

If $x_0 = a$, then this approximation becomes

$$I(f) \approx R = (b-a)f(a)$$

which is called rectangle rule.

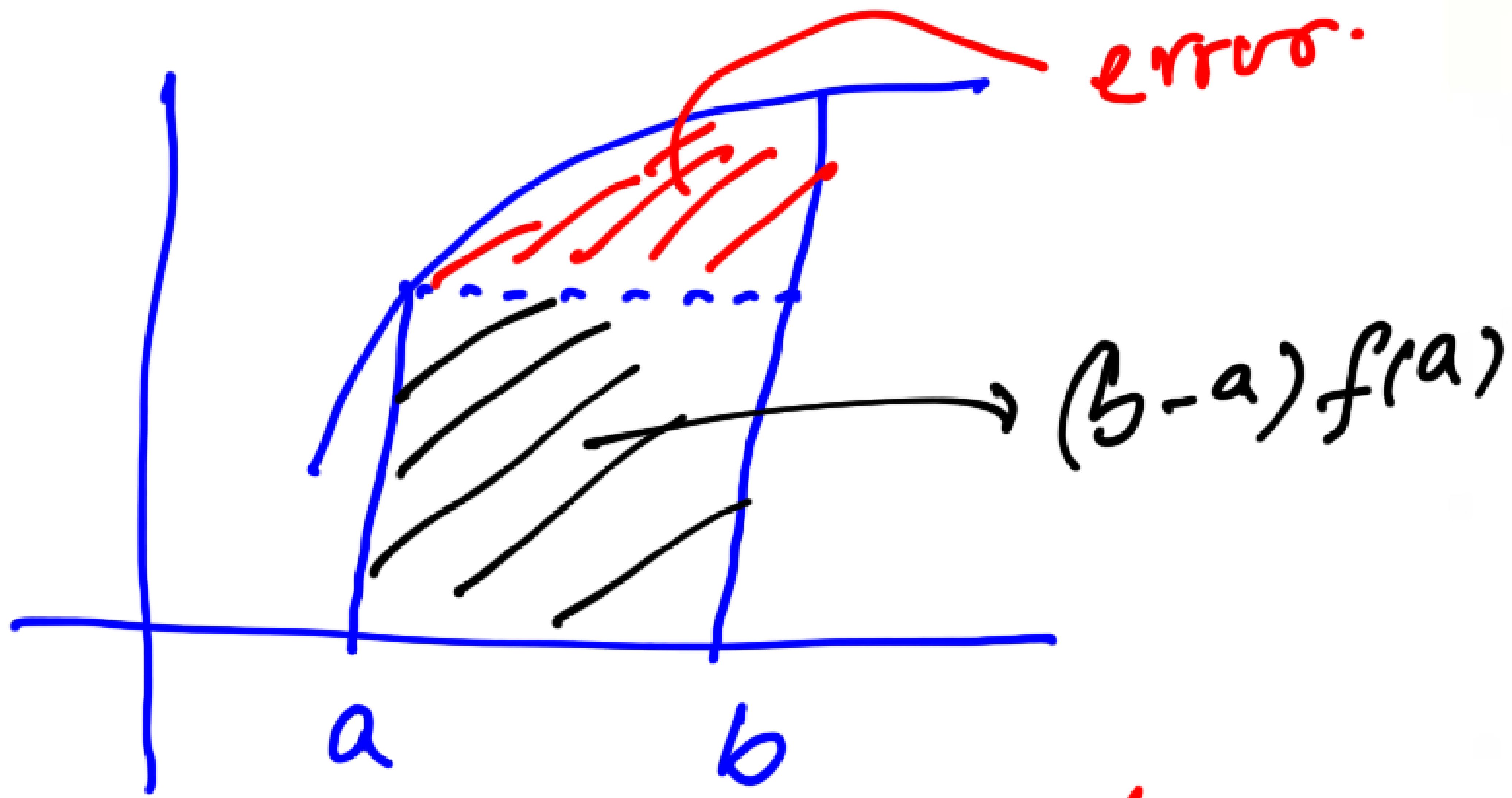
$k = 0$

$I(p_0) = f(x_0)$

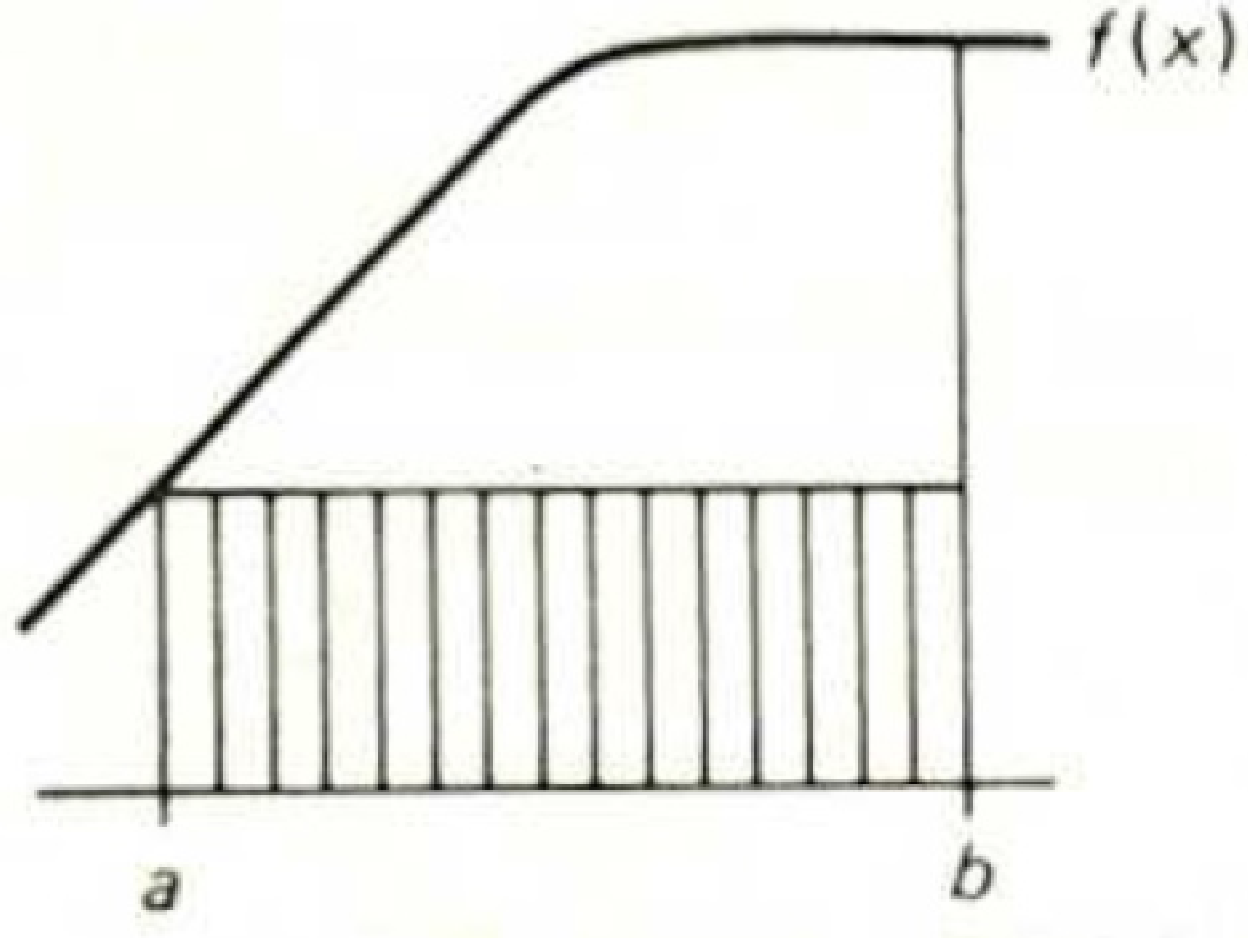
$I(f) \approx I(p_0)$

$I(p_0) = \int_a^b f(x_0)\,dx$

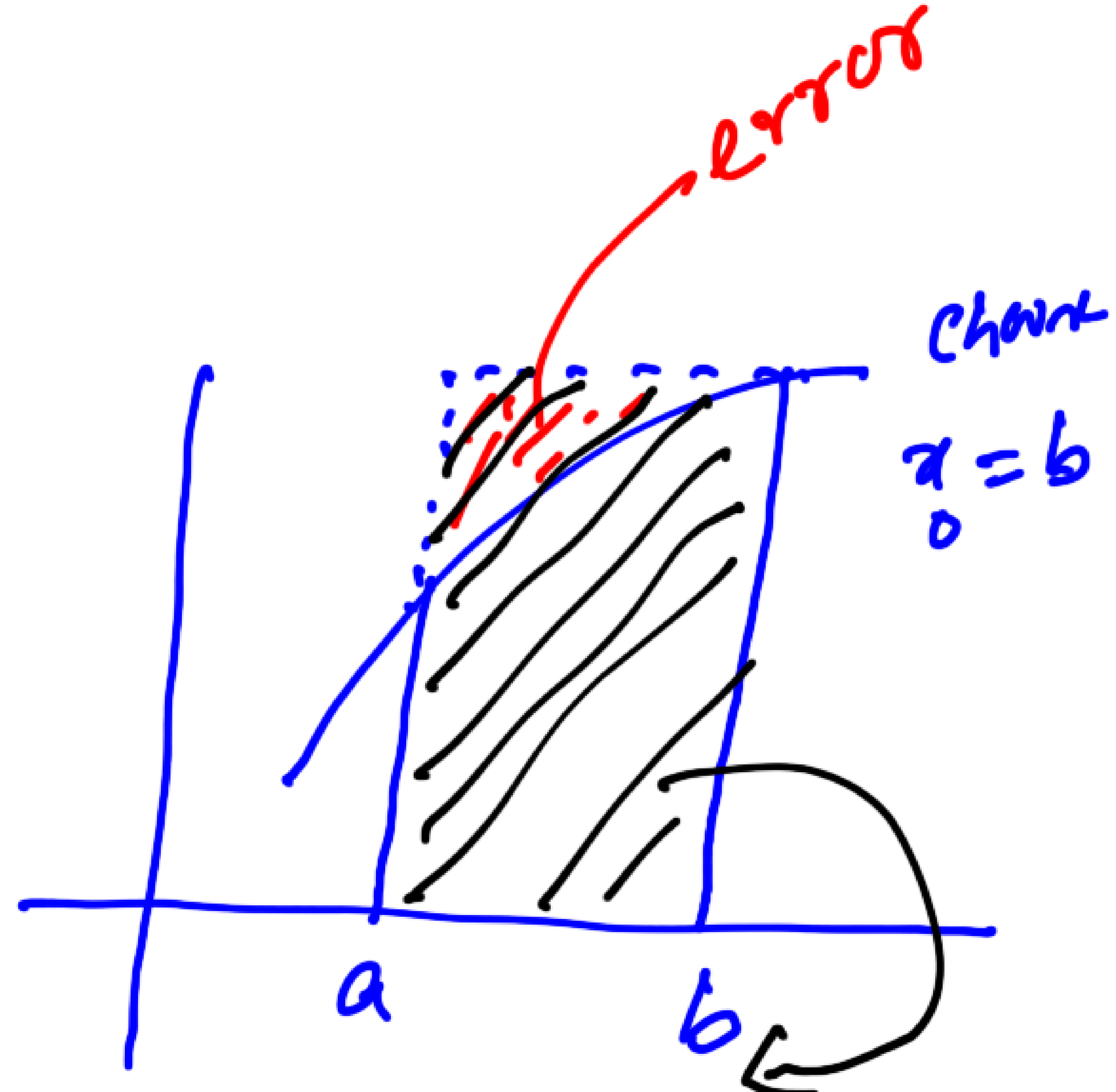
$= (b-a)f(x_0)$



Left rectangle rule.



Rectangle rule



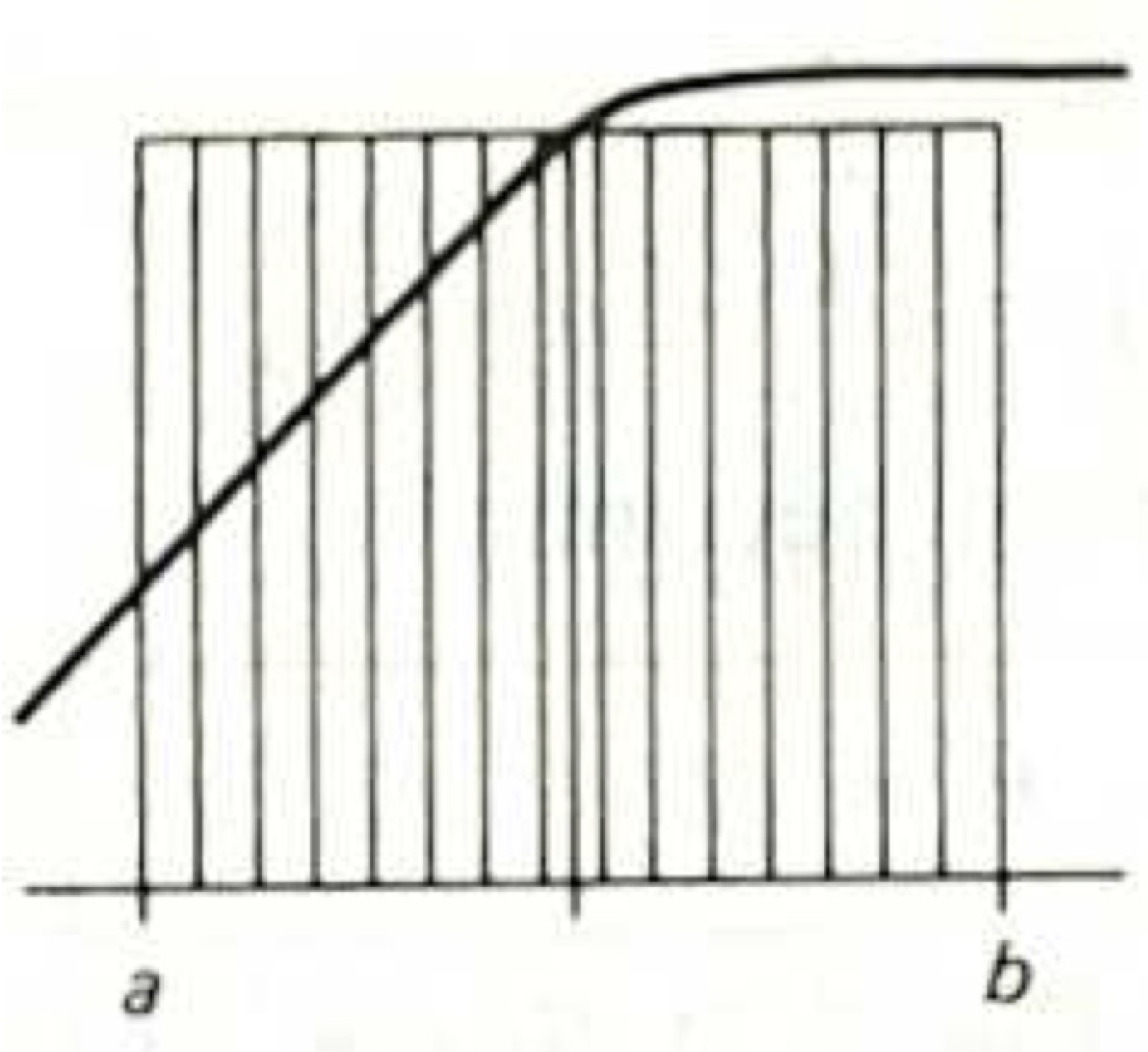
$(b-a) f(b)$

Right rectangle rule

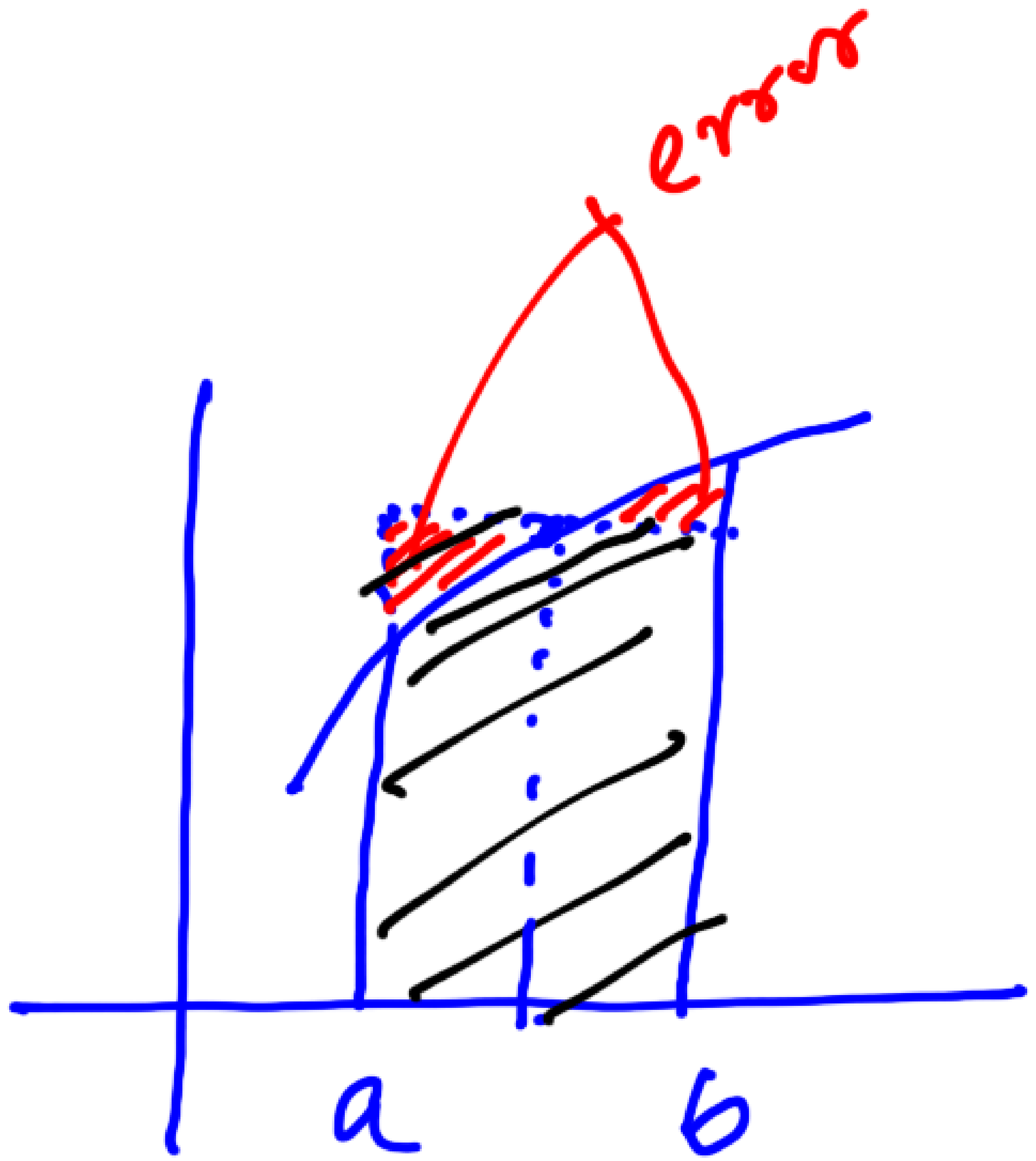
Mid-point Rule: If $x_0 = (a+b)/2$, then the formula

$$I(f) \approx M = (b-a) f\left(\frac{a+b}{2}\right)$$

is known as the mid-point rule.



Midpoint rule



$(b-a) f\left(\frac{a+b}{2}\right)$

Mid-point rule.

$p_1(x) = f(x_0) + f[x_0,x_1](x-x_0)$

$f(x) \approx p_1(x)$

$\int_a^b f(x)dx \approx \int_a^b p_1(x)dx.$

Trapezoidal Rule: Let $k = 1$. Then

$$f(x) \approx f(x_0) + f[x_0, x_1](x - x_0)$$

Choose $x_0 = a$ and $x_1 = b$ to have

$$I(p_1) = \int_a^b \{f(a) + f[a, b](x - a)\}\, dx$$

$\int_a^b \{f(a) + f[a,b](x-a)\} dx$

$= f(a)(b-a) + f[a,b] \left.\frac{(x-a)^2}{2}\right|_a^b$

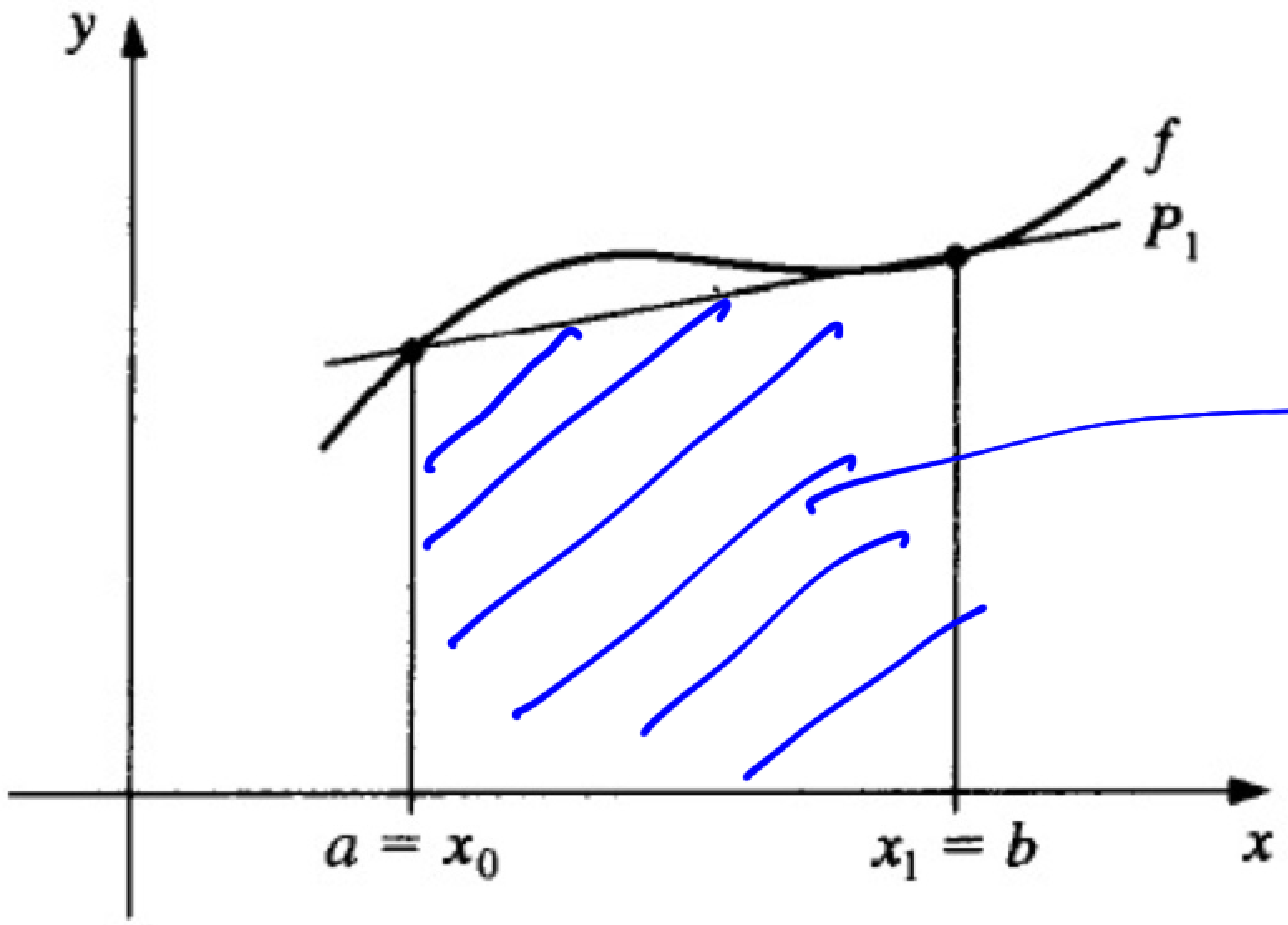
$= f(a)(b-a) + f[a,b]\frac{(b-a)^2}{2}$

$= f(a)(b-a) + \frac{f(b)-f(a)}{(b-a)} \times \frac{(b-a)^2}{2}$

or

$$I(f) \approx T = \frac{1}{2}(b - a)[f(a) + f(b)],$$

which yields the trapezoidal rule.



$\frac{(b-a)}{2}\left[f(a)+f(b)\right]$

(Trapezoidal rule)

$p_2(x) = f(x_0) + f[x_0, x_1](x - x_0)$
$+ f[x_0, x_1, x_2](x - x_0)(x - x_1)$

Simpson's Rule: Let $k = 2$. Then

$$f(x) \approx p_2(x)$$

If we choose $x_0 = a$, $x_1 = (a+b)/2$, $x_2 = b$, then the interpolating polynomial $p_2(x)$ is in the form

$$p_2(x) = f(a) + f[a,b](x-a) + f[a,b,\frac{a+b}{2}](x-a)(x-b).$$

Then

$$\begin{aligned} I(p_2) = \int_a^b p_2(x)dx &= f(a)(b-a) + f[a,b](b-a)^2/2 \\ &\quad + f[a,b,\frac{a+b}{2}] \int_a^b (x-a)(x-b)dx \\ &= f(a)(b-a) + f[a,b](b-a)^2/2 \\ &\quad + f[a,\frac{a+b}{2},b](b-a)^3/6. \end{aligned}$$

Using the fact that

$$f[a, b, \frac{a+b}{2}] = f[a, \frac{a+b}{2}, b],$$

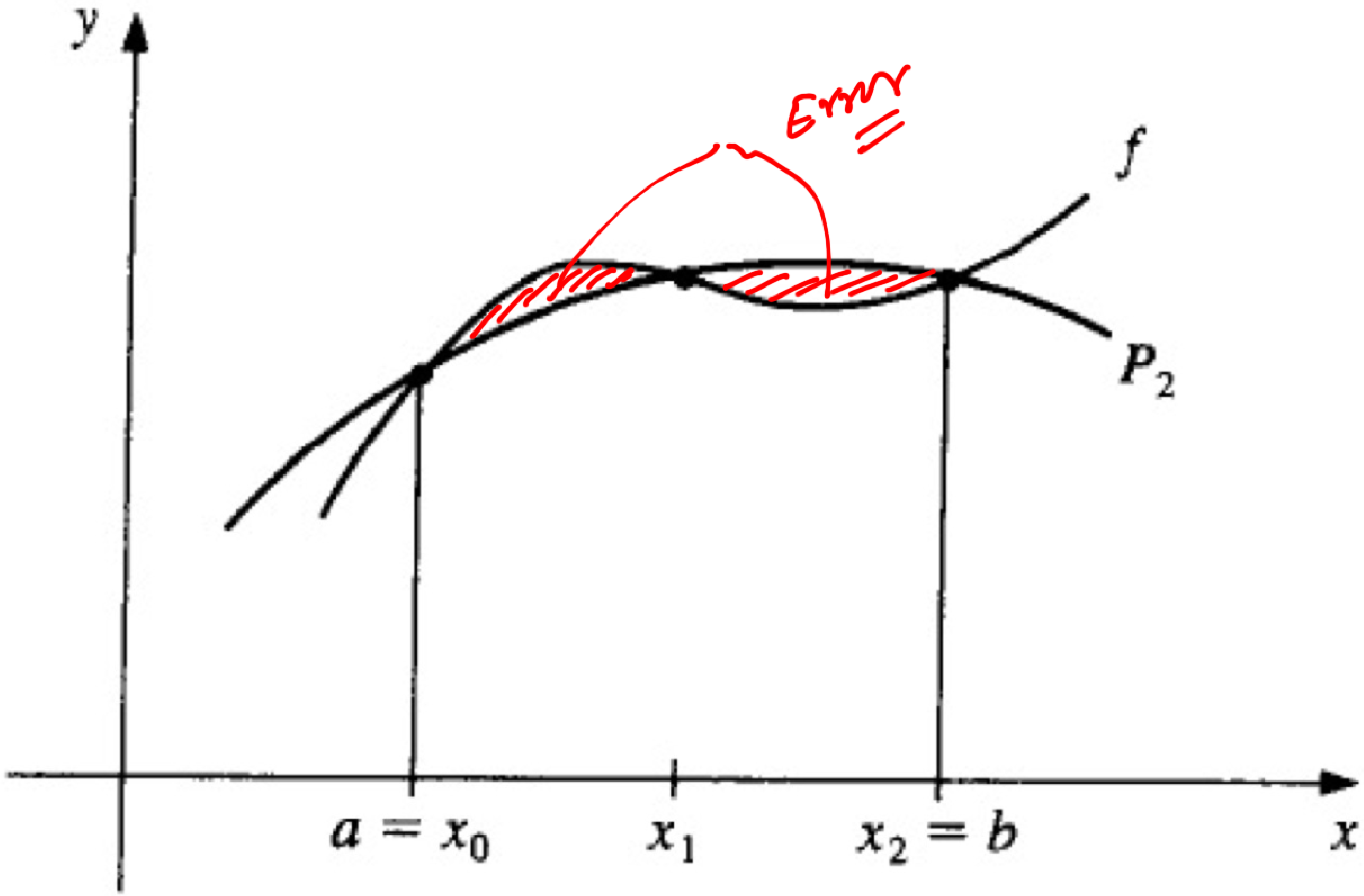
we get

$$\begin{aligned}
\int_a^b p_2(x)dx &= (b-a)\Big\{ f(a) + (f(b) - f(a))/2 \\
&\quad -2\left(f(b) - 2f\left(\frac{a+b}{2}\right) + f(a)\right)/6 \Big\} \\
&= \frac{(b-a)}{6}\left\{ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right\}.
\end{aligned}$$

Thus, the quadrature formula reads

$$I(f) \approx S = \frac{b-a}{6}\left\{ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right\},$$

which is Simpson's rule.



(Simpson's rule)

$$p_3(x) = f(x_0) + f[x_0,x_1](x-x_0) + f[x_0,x_1,x_2](x-x_0)(x-x_1) + f[x_0,x_1,x_2,x_3](x-x_0)(x-x_1)(x-x_2)$$

Corrected Trapezoidal Rule: Let $k = 3$. Then

$$f(x) \approx p_3(x)$$

we know $f[a,a] = f'(a)$

$f[b,b] = f'(b)$

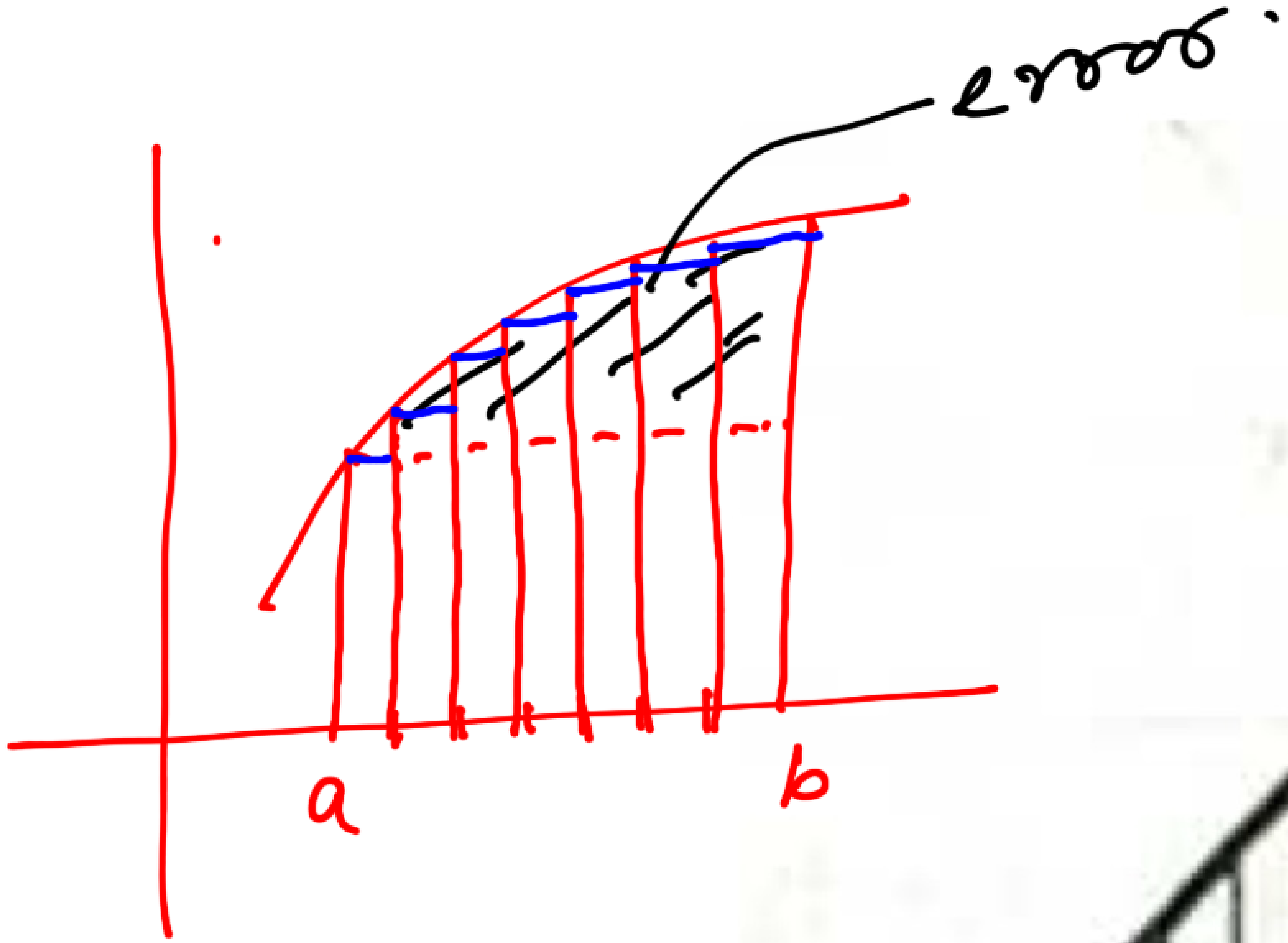
Choosing $x_0 = x_1 = a$, $x_2 = x_3 = b$, we notice that

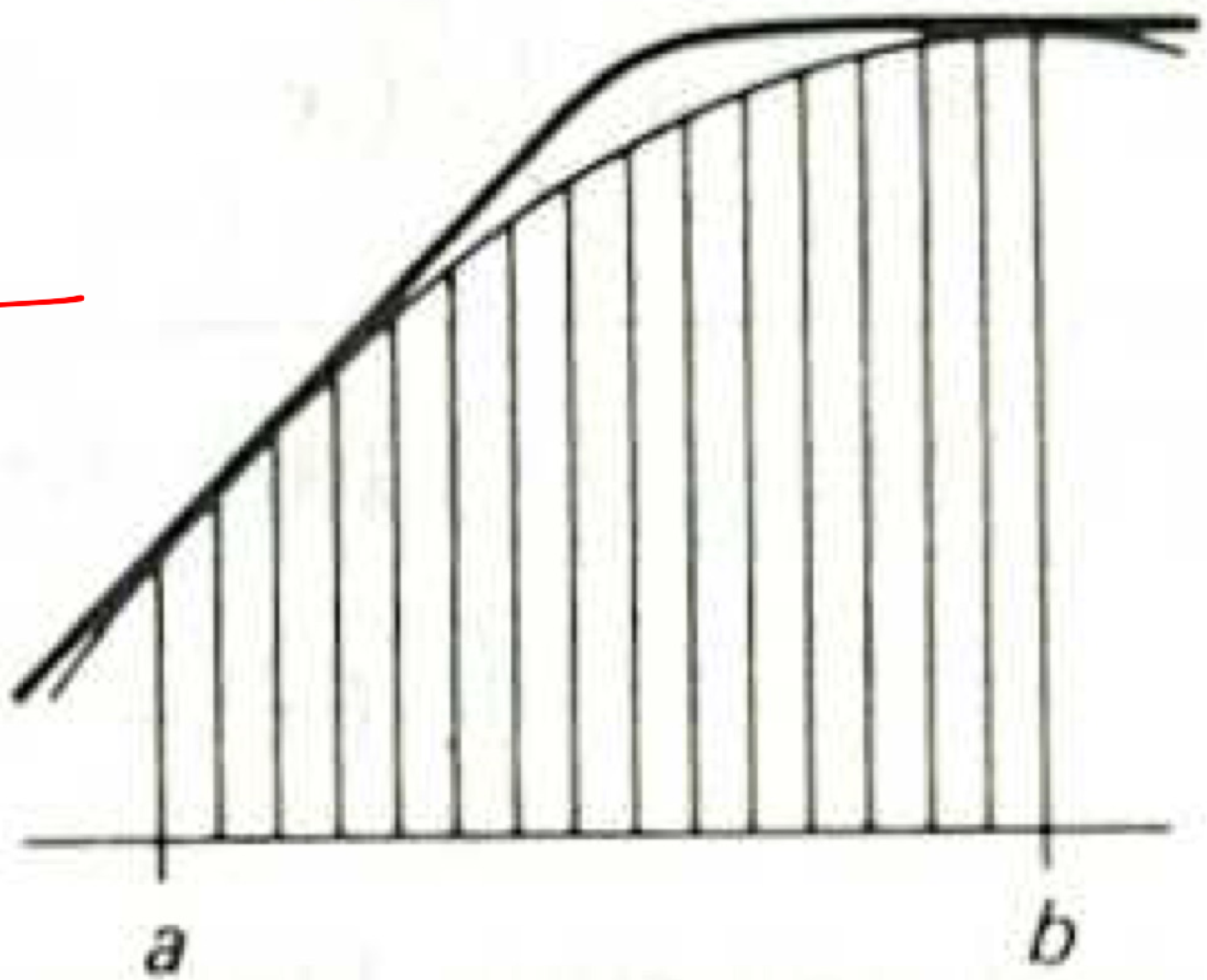
$$\begin{aligned} p_3(x) \quad = \quad & f[a] + f[a,a](x-a) + f[a,a,b](x-a)^2 \\ & + f[a,a,b,b](x-a)^2(x-b). \end{aligned}$$

An obvious calculation leads to

$$I(p_3) = \int_a^b p_3(x)dx = \underbrace{\frac{(b-a)}{2}[f(a)+f(b)]}_{\text{Trapezoidal rule}} + \underbrace{\frac{(b-a)^2}{12}[f'(a)-f'(b)]}_{\text{correction term.}}$$

is known as corrected trapezoid rule.





Corrected trapezoid rule

*** Ends ***