Chapter 4: Numerical Differentiation and Integration

Lecture 2:

Numerical Integration

Motivations

- Many integrals cannot be evaluated by integration techniques, for example:

$$\int_0^1 e^{x^2}\,dx,\quad \int_1^2 \frac{\sin x}{x}\,dx,\quad \int_1^2 x^x\,dx,\quad \iint_D e^{(x-y)^2}\,dA,\ldots$$

- Integrand functions are in tabular form, for example:

Time t	1.0	2.0	4.0	5.0
Money flow rate R	6.0	8.0	9.5	12.8

$$\text{Money flow} = \int_1^5 R(t)\,dt$$

Newton-Cotes Methods

- In Newton-Cote Methods, the function is approximated by a polynomial of order *p*
- Computing the integral of a polynomial is easy.

$$f(x) \approx f_p(x) = a_0 + a_1 x + \ldots + a_p x^p$$

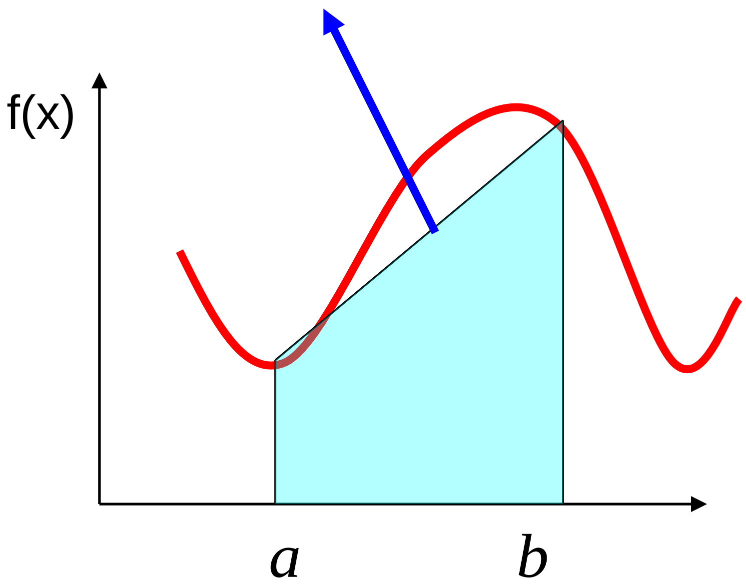
$$\int_a^b f(x)dx \approx \int_a^b f_p(x)\, dx$$

Complicated function

Function given in tabular form

Trapezoidal Rule: single application

$$f(a)+\frac{f(b)-f(a)}{b-a}(x-a)$$



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

$$I\approx\int_a^b\left(f(a)+\frac{f(b)-f(a)}{b-a}(x-a)\right)dx$$

$$=\left(f(a)-a\frac{f(b)-f(a)}{b-a}\right)x\Big|_a^b$$

$$+\frac{f(b)-f(a)}{b-a}\frac{x^2}{2}\Big|_a^b$$

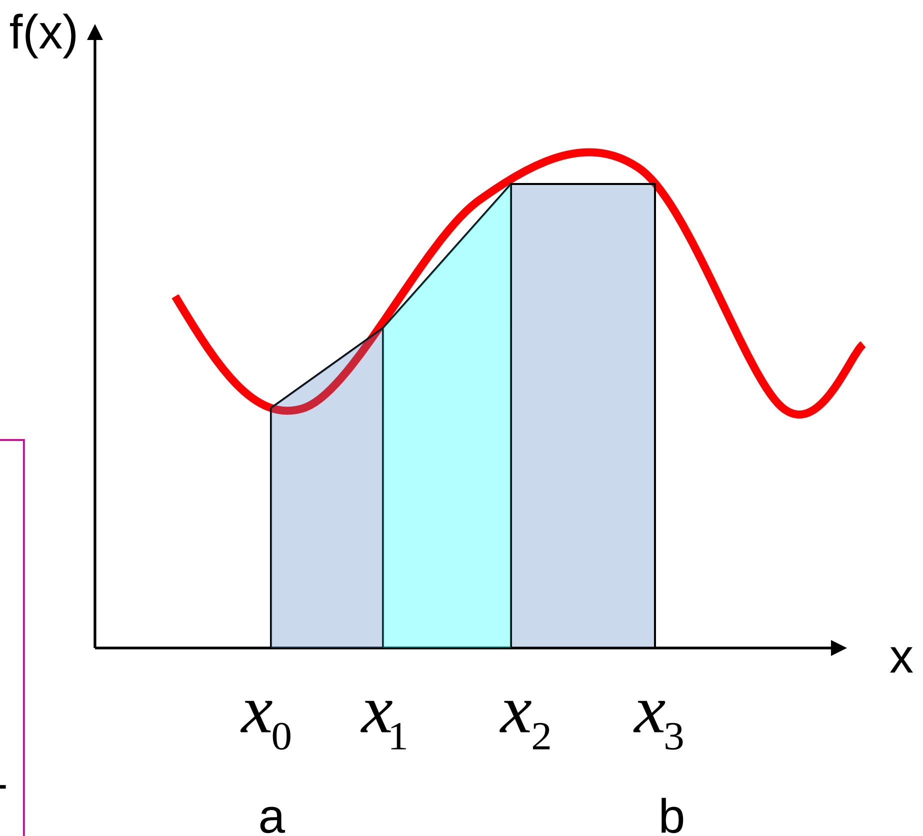
$$=(b-a)\frac{f(b)+f(a)}{2}$$

Trapezoidal Rule: Multiple Application

The interval [a,b] is partitioned into n segments

$$a = x_0 \le x_1 \le x_2 \le \ldots \le x_n = b$$

$$\int_a^b f(x)dx \approx \text{sum of the areas of the trapezoids}$$



$$\int_a^b f(x)dx = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)dx$$

$$\approx \sum_{i=1}^{n} (x_i - x_{i-1}) \frac{f(x_i) + f(x_{i-1})}{2}$$

Trapezoidal Rule:
General Formula and Special case

a) If the interval is divided into n segments (not necessarily equal):

$[a,b]=\bigcup_{i=1}^{n}[x_{i-1},x_i]$, where $a=x_0\le x_1\le x_2\le\ldots\le x_n=b$, then

$$\boxed{\int_a^b f(x)dx \approx \sum_{i=1}^{n}\left(x_i-x_{i-1}\right)\frac{f(x_i)+f(x_{i-1})}{2}}$$

b) **Special Case** (Equally spaced base points): $x_i-x_{i-1}=h, \forall i \quad \Rightarrow \quad h=\dfrac{b-a}{n}$

$$\boxed{\int_a^b f(x)dx \approx \frac{h}{2}\left(f(a)+2\sum_{i=1}^{n-1}f(x_i)+f(b)\right)}$$

Example

Money flows into a bank at different times is given in the Table

Time t (hours)	0.0	1.0	3.0	4.0
Flow rate R (mills $/hour)	0.0	10	12	14

Estimate money flow in these 4 hours

$$F = \int_0^4 R(t)dt \approx \sum_{i=1}^{3} \left(t_i - t_{i-1}\right) \frac{R(t_i) + R(t_{i-1})}{2}$$

$$F = \frac{10+0}{2} + (3-1)\frac{12+10}{2} + \frac{14+12}{2} = 5 + 22 + 13 = 40 \quad \text{(mills \$)}$$

Trapezoidal Rule: Error Estimate

Assumption: $f''(x)$ is continuous on *[a,b]*

Theorem: If Trapezoidal Rule for $h = \dfrac{b-a}{n}$ is used to approximate $\int_a^b f(x)dx$ then

$$Error = -\frac{b-a}{12} h^2 f''(\xi) \quad where\ \xi \in [a,b]$$

$$|Error| \le \frac{b-a}{12} h^2 \max_{x\in[a,b]} |f''(x)|$$

Example: How large do we have to choose n in Trapezoidal rule for approximating $\int_0^{\pi} \sin(x)dx$ to make sure that $|\text{error}| \le \frac{1}{2}\times 10^{-5}$

Solution

$$|Error| \le \frac{b-a}{12} h^2 \max_{x\in[a,b]} |f''(x)|$$

$$b=\pi; \; a=0; \quad f'(x)=\cos(x); \quad f''(x)=-\sin(x)$$

$$|f''(x)| \le 1, x\in[0,\pi] \;\Rightarrow |Error| \le \frac{\pi}{12}h^2$$

We require $\frac{\pi}{12}h^2 \le \frac{1}{2}\times 10^{-5} \Leftrightarrow \frac{\pi^2}{n^2} = h^2 \le \frac{6}{\pi}\times 10^{-5}$

$$\Rightarrow n \ge \frac{\pi^{3/2}}{\sqrt{6}} 10^{5/2} = 718.9. \;\Rightarrow\; n \ge 719$$

Exercise

Given the integral

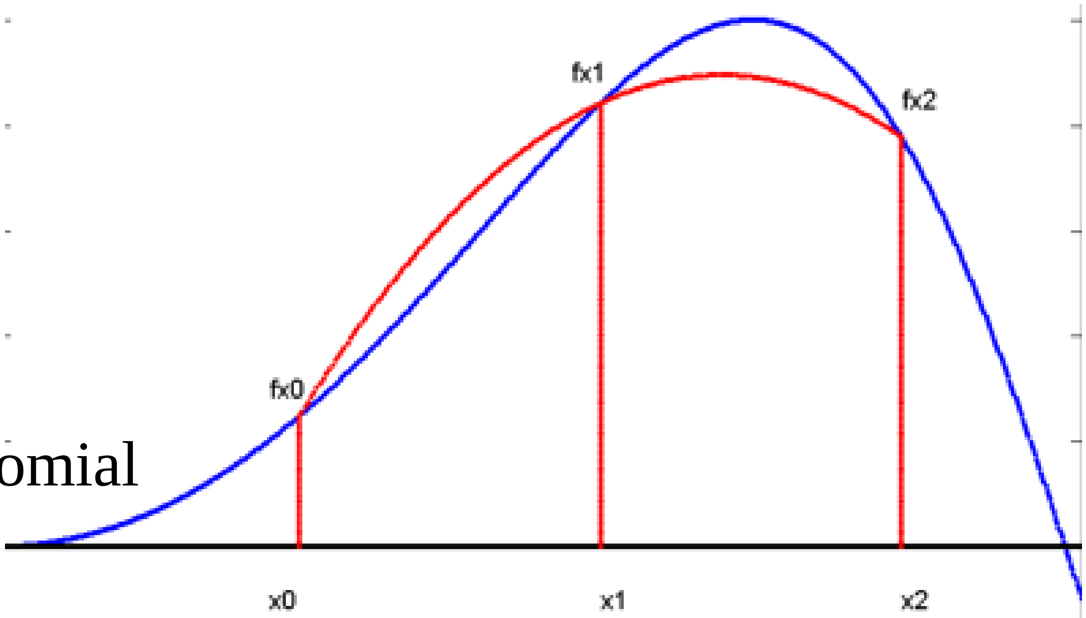
$$I = \int_0^2 \ln(2\,x+1)\,dx$$

a) Evaluate *I* using trapezoidal rule with n=6. Find the relative error.

b) How large do we have to choose the integer *n* in trapezoidal rule to make sure that the error cannot exceed 10^{-8}

Simpson's 1/3 Rule

$$\int_a^b f(x)dx \approx \int_a^b f_p(x)dx$$



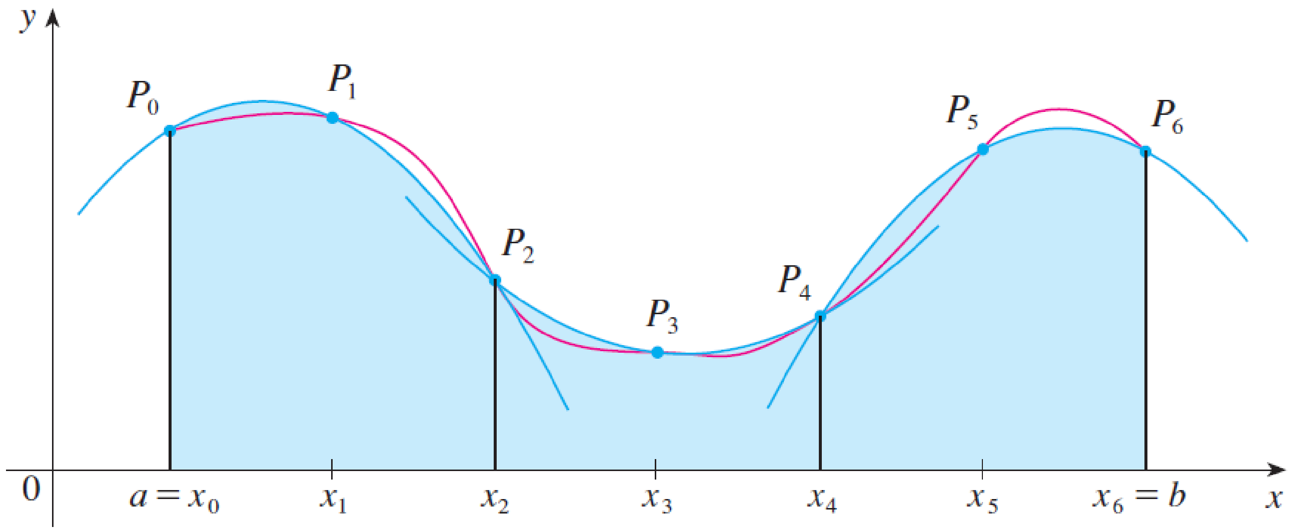
where f_p is a quadratic polynomial interpolation, that is

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

By substitution ***u=x-x0*** we have

$$\int_{x_0}^{x_2} f(x)dx \approx \int_{x_0}^{x_2} f_p(x)dx = (x_2 - x_0)\left(\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}\right)$$

Simpson's 1/3Rule: Multiple Applications



$$x_0 = a < x_1 < x_2 < \ldots < x_n = b, \quad i = 0,1,2,\ldots,n, \qquad n: \text{even}$$

$$\int_a^b f(x)dx = \sum_{i=1}^{n/2} \int_{x_{2(i-1)}}^{x_{2i}} f(x)dx$$

$$\approx \sum_{i=1}^{n/2} \left(x_{2i} - x_{2(i-1)} \right) \frac{f(x_{2(i-1)}) + 4f(x_{2i-1}) + f(x_{2i})}{6}$$

Simpson's 1/3 Rule: Special Case

Data are equally spaced:

$$x_i = a + ih, \quad i = 0, 1, 2, \ldots, n, \; h = \frac{b-a}{n}, \qquad n\text{: even integer}$$

$$\boxed{\int_a^b f(x)dx \approx \frac{h}{3}\left[f(a) + 4\sum_{\substack{i=1 \\ i=odd}}^{n-1} f(x_i) + 2\sum_{\substack{i=2 \\ i=even}}^{n-2} f(x_i) + f(b) \right]}$$

Example

Use 4-segment Simpson's 1/3 Rule to approximate the distance covered by a rocket from t= 8 to t=30 as given by

$$x = \int_{8}^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

a) Use four segment Simpson's Rule to find the approximate value of *x*.
b) Find the true error
c) Find the absolute relative true error

Solution

a) Using 4-segment Simpson's 1/3 Rule,

$$h = \frac{30-8}{4} = 5.5 \qquad t_i = 8 + ih,$$

So

$$f(t_0) = f(8)$$

$$f(t_1) = f(8+5.5) = f(13.5)$$

$$f(t_2) = f(13.5+5.5) = f(19)$$

$$f(t_3) = f(19+5.5) = f(24.5)$$

$$f(t_4) = f(30)$$

Solution (cont.)

$$x = \frac{h}{3}\left[f(t_0) + f(t_n) + 4\sum_{\substack{i=1 \\ i=odd}}^{n-1} f(t_i) + 2\sum_{\substack{i=2 \\ i=even}}^{n-2} f(t_i) \right]$$

$$= \frac{5.5}{3}\left[f(8) + f(30) + 4\sum_{\substack{i=1 \\ i=odd}}^{3} f(t_i) + 2\sum_{\substack{i=2 \\ i=even}}^{2} f(t_i) \right]$$

$$= \frac{22}{12}\left[f(8) + 4f(t_1) + 4f(t_3) + 2f(t_2) + f(30) \right]$$

Solution (cont.)

cont.

$$=\frac{11}{6}\left[f(8)+4f(13.5)+4f(24.5)+2f(19)+\ f(30)\right]$$

$$=\frac{11}{6}\left[177.2667+4(320.2469)+4(676.0501)+2(484.7455)+901.6740\right]$$

$$=11061.64\ m$$

Solution (cont.)

b) In this case, the true error is

$$E_t = 11061.34 - 11061.64 = -0.30 \ m$$

c) The absolute relative true error

$$\left|\in_t\right| = \left|\frac{11061.34 - 11061.64}{11061.34}\right| \times 100\%$$

$$= 0.0027\%$$

Solution (cont.)

Table 1: Values of Simpson's 1/3rd Rule for Example 2 with multiple segments

n	Approximate Value	E_t	$\lvert \epsilon_t \rvert$
2	11065.72	4.38	0.0396%
4	11061.64	0.30	0.0027%
6	11061.40	0.06	0.0005%
8	11061.35	0.01	0.0001%
10	11061.34	0.00	0.0000%

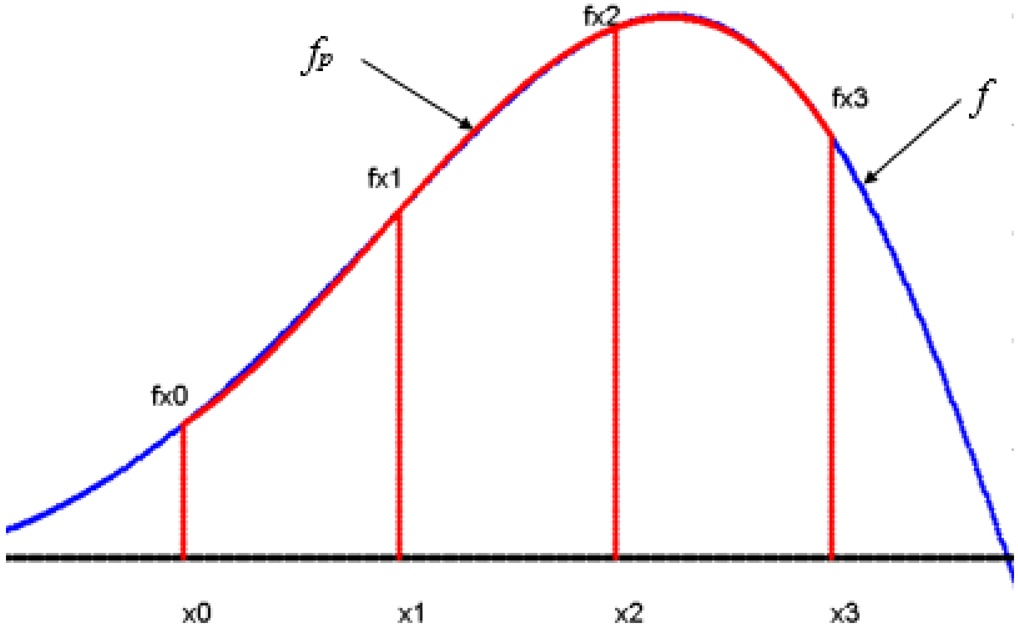
Error in the Multiple Segment Simpson's Rule

Assumption: $f^{(4)}(x)$ is continuous on *[a,b]*

Theorem: If Simpson's Method for $h = \dfrac{b-a}{n}$ is used to approximate $\int_a^b f(x)dx$ then

$$E_r = -\frac{b-a}{180} h^4 f^{(4)}(\xi) \quad where\ \xi \in [a,b]$$

$$|E_r| \le \frac{b-a}{180} h^4 \max_{x\in[a,b]} \left| f^{(4)}(x) \right|$$



SIMPSON'S 3/8 RULE

Similar to 1/3 Simpson's method, *f* approximately by function *fp* where *fp* is a cubic polynomial interpolation, that is

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

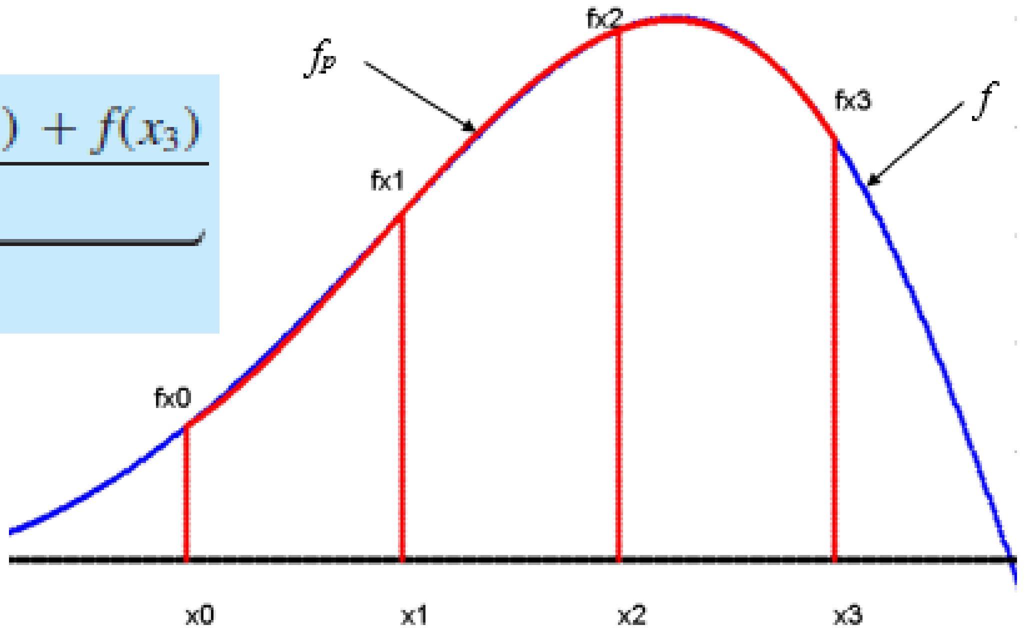
$$+ \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} f(x_3)$$

SIMPSON'S 3/8 RULE

By substitution ***u=x-x0*** we have

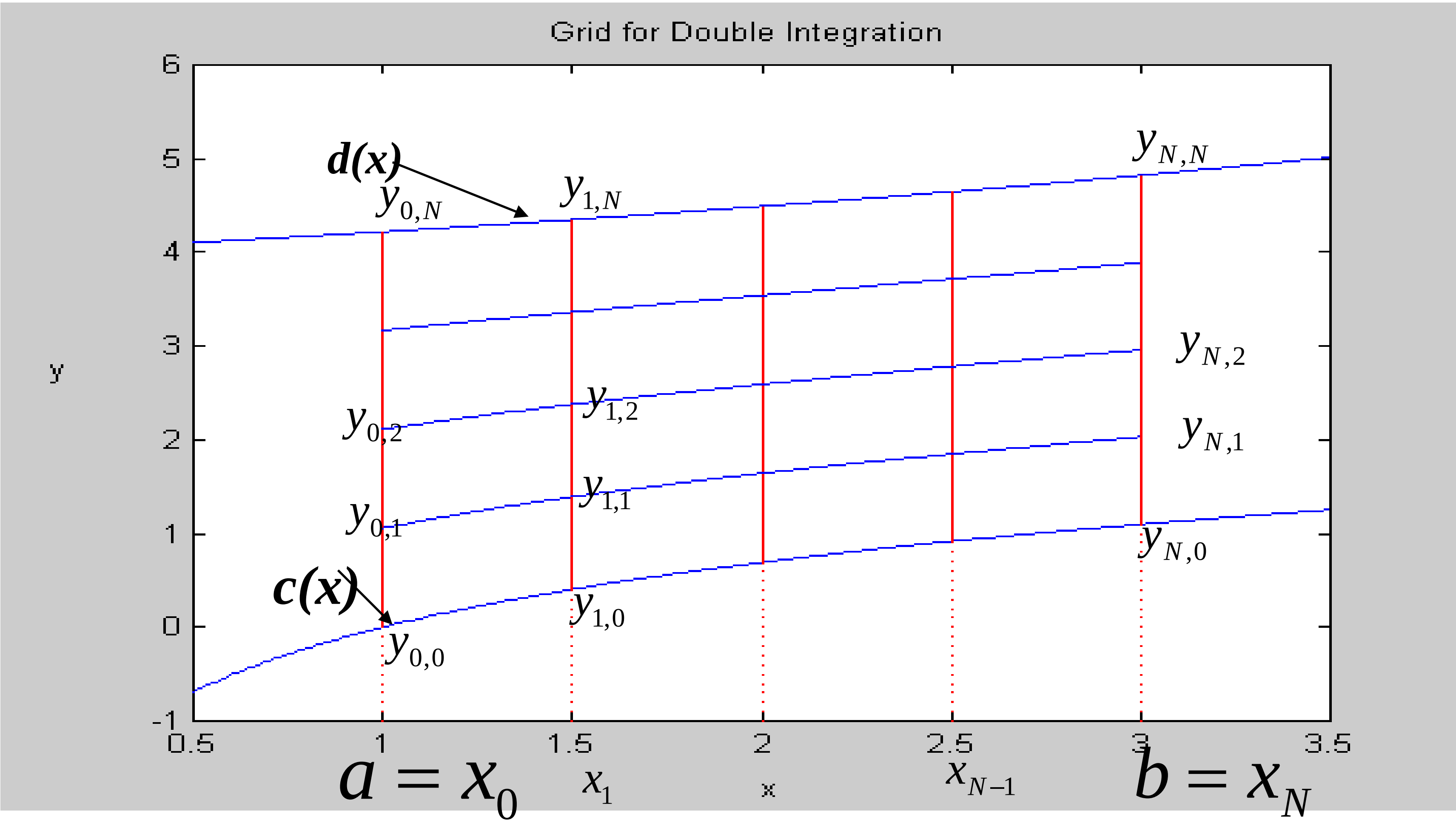
$$\int_a^b f(x)dx \approx \frac{3h}{8}\{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\} \qquad h=\frac{x_3-x_0}{3}$$

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}}_{\text{Average height}}$$



$$E_r \cong -\frac{3}{80}h^5 f^{(4)}(\xi)$$

Numerical Integration in a Two Dimensional Domain



- A double integration in the domain is written as

$$I = \int_a^b \left[\int_{c(x)}^{d(x)} f(x, y) dy \right] dx$$

- The numerical integration of above equation is to reduce to a combination of one-dimensional problems

Procedure:

- **Step 1:** Define $$G(x) = \int_{c(x)}^{d(x)} f(x, y) dy$$

So, the solution is $$I = \int_a^b G(x) dx$$

- **Step 2:** Divided the range of integration [a,b] into N equispaced intervals with the interval size

$$h_x = \frac{b - a}{N}$$

So, the grid points will be denoted by $x_0, x_1, \ldots, x_N$

and then we have

$$G(x_i) = \int_{c(x_i)}^{d(x_i)} f(x_i, y) dy,$$

- **Step 3:** Divided the domain of integration $\left[c(x_i), d(x_i)\right]$ into N equi-spaced intervals with the interval size

$$h_y = \frac{\left[d(x_i) - c(x_i)\right]}{N}$$

So, the grid points denoted by $y_{i,0}, y_{i,1}, \ldots, y_{i,N}$

- **Step 4:** By Applying numerical integration for one-dimensional (for example the trapezoidal rule) we have

$$G(x_i) = \frac{h_y}{2}\left\{ f(x_i, y_{i,0}) + 2\sum_{j=1}^{N-1} f(x_i, y_{i,j}) + f(x_i, y_{i,N}) \right\}$$

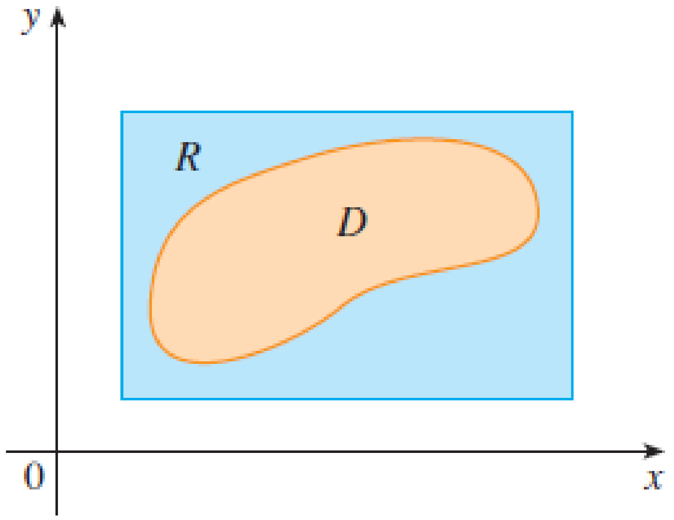
for $i = 0,1,2,\ldots,N$

- **Step 5:** By applying numerical integration (for example trapezoidal rule) in one-dimensional domain we have the solution of double integration is

$$I = \frac{h_x}{2}\left\{ G(x_0) + 2\sum_{i=1}^{N-1} G(x_i) + G(x_N) \right\}$$

A simple method

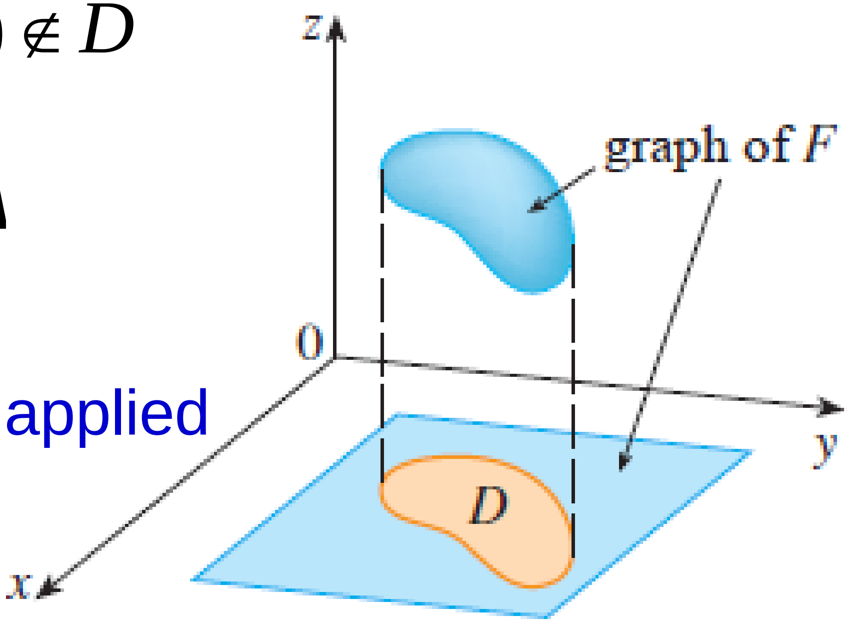
Let D be a bounded region,
enclosed in a rectangle R



Define

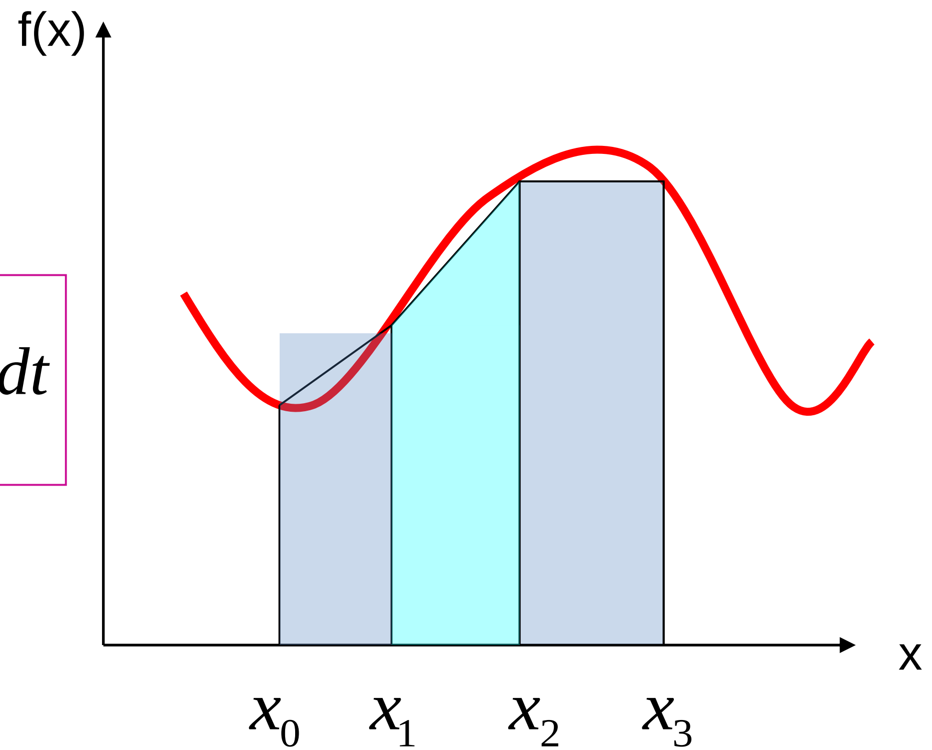
$$F(x,y)=\begin{cases} f(x,y), & \text{if } (x,y)\in D \\ 0, & \text{if } (x,y)\notin D \end{cases}$$

$$\iint_D f(x,y)dA=\iint_R F(x,y)dA$$



Equally spaced data rules can be applied

Improper Integrals



$$t = 1/x, \quad \int_a^{\infty} f(x)dx = \int_0^{1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right) dt$$

$f(a) = \infty$, use a rule for $a' = x_1 \leq x_2 \leq \ldots \leq x_n = b$

use right-end point rule in $[x_0, x_1]$

For example, trapezoidal rule:

$$\int_a^b f(x)dx \approx f(x_1)(x_1 - x_0) + \sum_{i=2}^{n} (x_i - x_{i-1}) \frac{f(x_i) + f(x_{i-1})}{2}$$

Exercise 1

Trapezoidal Rule: Given the integral

$$I = \int_0^{\pi/2} \sin(x^2)\,dx$$

a) Evaluate I with n=6. Estimate the error.

b) How large do we need to choose n so that the $|E_r| \leq 10^{-8}$

Exercise 2

Simpson's 1/3 rule: Given the integral

$$I = \int_{0}^{\pi/2} \sin(x^2)\,dx$$

a) Evaluate I with n=6. Estimate the error.

b) How large do we need to choose n so that the $|E_r| \le 10^{-8}$

Exercise 3

Simpson's 3/8 rule: Given the integral

$$I = \int_0^{\pi/2} \sin(x^2)dx$$

a) Approximate I. Estimate the error.

b) Use it in conjunction with Simpson's 1/3 rule to approximate I for 5 segments

Quiz

Given the integral $$I = \int_0^1 e^{-x^2}\,dx$$

a) Evaluate I using Simpson's 1/3 rule with n=6.
b) How large do we need to choose n so that Simpson's 1/3 rule gives $|E_r| \leq 10^{-8}$
c) Approximate I using Simpson's 3/8 rule. Use it in conjunction with Simpson's 1/3 rule to approximate I for 5 segments