Numerical Analysis MTH614

Spring 2012, Korea University

Numerical Integration

Trapezoidal rule

To derive the Trapezoidal rule for approximating $\int_a^b f(x)dx$, let the linear polynomial $p_1(x)$ such that

$$p_1(x) = \frac{(b-x)f(a) + (x-a)f(b)}{b-a} \qquad (1)$$

Then, we integrate $p_1(x)$ from a to b,

$$\int_a^b p_1(x) = (b-a)\left(\frac{f(a)+f(b)}{2}\right) \qquad (2)$$

Consequently,

$$\int_a^b p_1(x) \approx T_1(f) = (b-a)\left(\frac{f(a)+f(b)}{2}\right). \qquad (3)$$

where $h = (b-a)/n \text{ and } x_i = a + i \cdot h \text{ for } 0, 1, \ldots, n.$

For each sub-interval $[x_i, x_{i+1}]$ of the $[a, b]$

$$\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx$$
$$= \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx. \quad (1)$$

If we apply the trapezoidal rule for (1)

$$\int_a^b f(x)dx \approx \frac{h}{2}\sum_{i=1}^{n}[f(x_{i-1}) + f(x_i)]. \quad (2)$$

Therefore we have

$$T_n(f) \equiv \frac{h}{2}[f(x_0) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(x_n)]. \quad (3)$$

For example, integrate the exponential function

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

```
%%%%%%%%%%%%%%%%%%%%%%%%%% trape.m %%%%%%%%%%%%%%%%%%%%%%%%%%%%%
clear; clc; a=0; b=1; % end points of interval
f=inline('exp(x)','x');
n=[1 2 4 8 16 32 64 128 256 512 1024 2048];
% number of subintervals
error0=0;
fprintf('   n        numerical sum        error        ratio \n')
for iter=1:length(n)
 h=(b-a)/n(iter);
 T=0;
 for i=1:n(iter)
     T=T+f(a+(i-1)*h)+f(a+(i)*h);
 end
 T=(h/2)*T;
 error=abs(exp(1)-1-T);
 ratio=error0/error;
 if iter==1
 fprintf('%4.0f      %16.14f     %5.4e      \n',n(iter),T,error)
 else
 fprintf('%4.0f      %16.14f     %5.4e   %5.2f \n',n(iter), ...
     T,error,log(ratio)/log(2))
 end
 error0=error;
end
```

n	numerical sum	error	ratio
1	1.85914091422952	1.4086e-001	
2	1.75393109246483	3.5649e-002	1.98
4	1.72722190455752	8.9401e-003	2.00
8	1.72051859216430	2.2368e-003	2.00
16	1.71884112857999	5.5930e-004	2.00
32	1.71842166031633	1.3983e-004	2.00
64	1.71831678685009	3.4958e-005	2.00
128	1.71829056808348	8.7396e-006	2.00
256	1.71828401336682	2.1849e-006	2.00
512	1.71828237468610	5.4623e-007	2.00
1024	1.71828196501581	1.3656e-007	2.00
2048	1.71828186259824	3.4139e-008	2.00

Simpson's rule

Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher order polynomials.

Instead of using a linear connection, given three points a , $c = (a+b)/2$, and b are connected with a parabola such that

$$p_2(x) = f(a)\frac{(x-b)(x-c)}{(a-b)(a-c)} + f(b)\frac{(x-a)(x-c)}{(b-a)(b-c)} + f(c)\frac{(x-a)(x-b)}{(c-a)(c-b)}. \quad (1)$$

The result of the integration is

$$\int_a^b p_2(x)dx = \frac{h}{3}[f(a) + 4f(c) + f(b)],\ h = \frac{b-a}{2}. \quad (2)$$

This gives Simpson's rule

$$\int_a^b p_2(x)dx \approx S_2(f) \equiv \frac{h}{3}[f(a) + 4f(c) + f(b)]. \quad (3)$$

Let us derive the general form of Simpson's rule.

For any even number n, the endpoints a and b of each interval [a,b] divide the real line into partitions n equal segments with a stepsize h such that $a = x_0, x_1, \ldots, x_{n-1}, x_n = b.$

The total integral can be represented as

$$\begin{aligned}\int_a^b f(x)dx &= \int_{x_0}^{x_n} f(x)dx \\ &= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_n-2}^{x_n} f(x)dx.\end{aligned} \tag{1}$$

For each subinterval $[x_i, x_{i+2}]$, we apply Simpson's rule to (1)

$$\frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2) + \frac{h}{3}[f(x_2) + 4f(x_3) + f(x_4)] + \cdots + \frac{h}{3}[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)] \tag{2}$$

Therefore, we obtain

$$S_n(f) \equiv \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \cdots + 2y_{n-2} + 4y_{n-1} + y_n) \tag{3}$$

$$= \sum_{i=1}^{n/2} \frac{h}{3}(y_{2i-2} + 4y_{2i-1} + y_{2i}). \tag{4}$$

For example, use Simpson's rule to integral $I = \int_0^1 e^x dx = e - 1.$

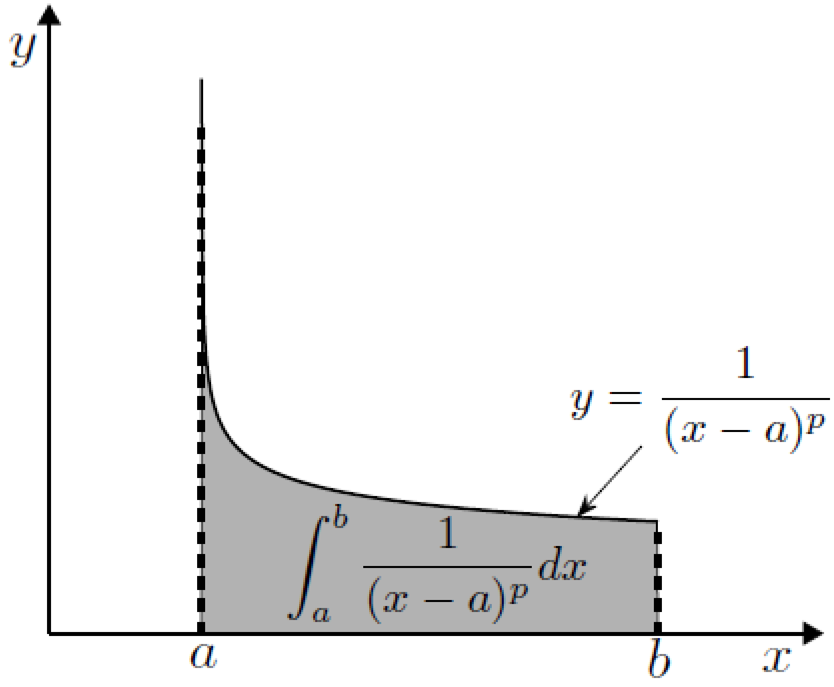
```
%%%%%%%%%%%%%%%%%%%%%%%%%%% simpson.m %%%%%%%%%%%%%%%%%%%%%%%%%%%
clear; clc; a=0; b=1; % end points of interval
f=inline('exp(x)','x');
n=[2 4 8 16 32 64 128 256 512];
% number of subintervals
error0=0;
fprintf('   n        numerical sum        error       ratio \n')

for iter=1:length(n)
 h=(b-a)/n(iter);
 S=0;
 for i=1:n(iter)/2
     S=S+f(a+2*(i-1)*h)+4.0*f(a+(2*i-1)*h)+f(a+2*i*h);
 end
 S=(h/3)*S;
 error=abs(exp(1)-1-S);
 ratio=error0/error;
 if iter==1
 fprintf('%4.0f      %16.14f     %5.4e      \n',n(iter),S,error)
 else
 fprintf('%4.0f      %16.14f     %5.4e   %5.2f \n',n(iter), ...
     S,error,log(ratio)/log(2))
 end
 error0=error;
end
```

n	numerical sum	error	ratio
2	1.71886115187659	5.7932e-004	
4	1.71831884192175	3.7013e-005	3.97
8	1.71828415469990	2.3262e-006	3.99
16	1.71828197405189	1.4559e-007	4.00
32	1.71828183756177	9.1027e-009	4.00
64	1.71828182902802	5.6897e-010	4.00
128	1.71828182849461	3.5560e-011	4.00
256	1.71828182846127	2.2233e-012	4.00
512	1.71828182845918	1.3789e-013	4.01

Improper integration

As the notion of integration is extended either to an interval of integration on which the function is unbounded, or to an interval wit h one or more infinite endpoints. In either case, the function has a singularity at one of the endpoints.



(1)

In this lecture, we show that the improper integrals can be reduced to problems of this form

$$\int_a^b \frac{dx}{(x-a)^p}, \tag{1}$$

P-test in calculus states the improper integral with a singularity at the left end point converges if and only if $0 < p < 1,$ and define

$$\int_a^b \frac{1}{(x-a)^p}dx = \left.\frac{(x-a)^{1-p}}{1-p}\right|_a^b = \frac{(b-a)^{1-p}}{1-p}$$

If f is a function that can be written in the form

$$f(x) = \frac{g(x)}{(x-a)^p},$$

where $0 < p < 1$ and $g \in C^5[a,b],$ then the improper integral also exists.

In that case, we can construct the fourth Taylor polynomial

$$\begin{aligned} P_4(x) &= g(a) + g'(a)(x-a) + \frac{g''(a)}{2!}(x-a)^2 + \frac{g^{(3)}(a)}{3!}(x-a)^3 + \frac{g^{(4)}(a)}{4!}(x-a)^4 \\ &= \sum_{k=0}^{4} \frac{g^{(k)}(a)}{k!}(x-a)^k. \end{aligned} \tag{2}$$

Then, we can separate

$$\int_a^b \frac{g(x)}{(x-a)^p}dx = \underbrace{\int_a^b \frac{g(x)-P_4(x)}{(x-a)^p}dx}_{(a)} + \underbrace{\int_a^b \frac{P_4(x)}{(x-a)^p}dx}_{(b)}. \quad (1)$$

Rewrite part (b) as

$$\begin{aligned} \int_a^b \frac{P_4(x)}{(x-a)^p}dx &= \sum_{k=0}^{4} \int_a^b \frac{g^{(k)}(a)}{k!}(x-a)^{k-p}dx \\ &= \sum_{k=0}^{4} \frac{g^{(k)}(a)}{k!(k-p+1)}(b-a)^{k-p+1}. \quad (2) \end{aligned}$$

and part (a) follows that $\int_a^b \frac{g(x)-P_4(x)}{(x-a)^p}dx \approx \int_a^b G(x)dx$ (3)

where $G(x)$ is given

$$G(x) = \begin{cases} \dfrac{g(x)-P_4(x)}{(x-a)^p} & a < x \le b \\ 0 & x = a. \end{cases} \quad (4)$$

Therefore, we obtain numerical solution from (2) and (3).

For example, integrate the exponential function $\int_0^1 \frac{e^x}{\sqrt{x}} dx$.

First of all, let us separate the exponential function using $P_4(x)$,

$$\int_0^1 \frac{e^x}{\sqrt{x}} dx = \int_0^1 \frac{e^x - P_4(x)}{\sqrt{x}} + \int_0^1 \frac{P_4(x)}{\sqrt{x}} \quad (1)$$

where $P_4(x)$ is given as

$$P_4(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \frac{x^4}{4!} \quad (2)$$

and then define $G(x)$ such that

$$G(x) = \begin{cases} \frac{e^x - P_4(x)}{\sqrt{x}} & 0 < x \leq 1 \\ 0 & x = 0. \end{cases} \quad (3)$$

Next, the part (a) of the equation is calculated at discrete points

$$\{x_i | x_i = h \cdot i, \; h = (1/4), \; \text{for } i = 0, \ldots, 4.\}.$$

We find that

x	0.0000	0.25	0.50	0.75	1.00
G(x)	0.0000	0.0000170	0.0001013	0.0026026	0.0099485

$$\int_0^1 G(x)\,dx \approx \frac{0.25}{3}\left[0 + 4(0.0000170) + 2(0.0004013) + 4(0.0026026) + (0.0099485)\right] \quad (1)$$
$$= 0.0017691$$

The part (b) can be calculated

$$(b):\ \int_0^1 \frac{P_4(x)}{\sqrt{x}}\,dx = \int_0^1 \left(x^{-\frac{1}{2}} + x^{\frac{1}{2}} + \frac{1}{2}x^{\frac{3}{2}} + \frac{1}{6}x^{\frac{5}{2}} + \frac{1}{24}x^{\frac{7}{2}}\right)dx$$
$$= \left[2x^{\frac{1}{2}} + \frac{2}{3}x^{\frac{3}{2}} + \frac{1}{5}x^{\frac{5}{2}} + \frac{1}{21}x^{\frac{7}{2}} + \frac{1}{108}x^{\frac{9}{2}}\right]_0^1 \quad (2)$$
$$= 2 + \frac{2}{3} + \frac{1}{5} + \frac{1}{21} + \frac{1}{108}$$
$$= 2.9235450.$$

We can then add up these two parts,

$$\int_0^1 \frac{e^x}{\sqrt{x}}\,dx \approx 0.0017691 + 2.9235450 = 2.9253141\ .$$