CHAPTER 3 NUMERICAL INTEGRATION

In this Chapter, you will learn:

- the definite integral,
- three methods to do the numerical integration when the integral is complicated.
- error analysis

1. DEFINITE INTEGRAL

The *exact value* of a *definite integral* $\int_a^b f(x)dx$ can be computed only when the function $f(x)$ is integrable in finite terms.

Example 1: Find the following definite integral.

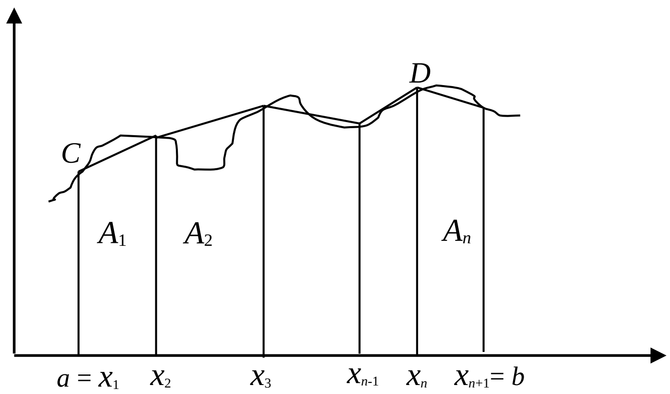
$$\int_0^2 x^2 dx = \left.\frac{x^3}{3}\right|_0^2$$
$$= \frac{2^3}{3} - \frac{0^3}{3}$$
$$= \frac{8}{3}$$

Example 2: Find the following definite integral.

$$\int_0^2 3x^2 + e^x dx =$$

The *definite integral* of a function has an interpretation as the *area under a curve*. Whenever the function $f(x)$ *cannot* be exactly integrated in finite terms or the evaluation of its integral is complicated, we can use the *numerical integration*. The numerical integrations that we are going to discuss in this chapter are *Trapezoidal rule*, *Simpson's rule* and *Romberg algorithm*.

2. TRAPEZOIDAL RULE



Let *CD* be the curve and its equation is $y = f(x)$. To evaluate $\int_a^b f(x)dx$, we subdivide the interval from *a* to *b* into *n* equal parts, so that each part is equal to $h = \frac{(b-a)}{n}$.

The area of the first trapezium, $A_1 = \frac{h}{2}[f(x_1) + f(x_2)]$

The area of the second trapezium, $A_2 = \frac{h}{2}[f(x_2) + f(x_3)]$

And the area of nth trapezium, $A_n = \frac{h}{2}[f(x_n) + f(x_{n+1})]$

Total area,

$$A_T = \int_a^b f(x)dx \approx \frac{h}{2}\{f(x_1) + f(x_{n+1}) + 2[f(x_2) + f(x_3) + \ldots + f(x_n)]\} \text{ where } x_n = a + (n-1)h, n = 1,2,..$$

The above formula is known as the *Composite Trapezoidal rule* for numerical integration.

<u>*Example 3*</u>: Dividing the range into 4 equal parts, find the approximate value of $\int_0^1 \frac{1}{1+x^2}dx$ by using *Composite Trapezoidal rule*.

$$n = 4; \quad f(x) = \frac{1}{1+x^2}; \quad h = \frac{1-0}{4} = 0.25$$

$$\begin{aligned} A_T &= \frac{0.25}{2}\{f(0) + f(1) + 2[f(0.25) + f(0.5) + f(0.75)]\} \\ &= \frac{0.25}{2}(6.262353) \\ &= 0.782794 \end{aligned}$$

Example 4: Compute an approximate value for integral given in Example 2 by using the *Composite Trapezoidal rule* with 5 points. Then compare with the actual value of the integral and find its absolute error.

Integral in Example 2: $\int_0^2 3x^2 + e^x dx$; 5 points $\Rightarrow n = 4$; $f(x) = 3x^2 + e^x$; $h = \frac{2-0}{4} = 0.5$

$$\begin{aligned} A_T &= \frac{0.5}{2}\{f(0) + f(2) + 2[f(0.5) + f(1.0) + f(1.5)]\} \\ &= \frac{0.5}{2}(59.08644) \\ &= 14.77161 \end{aligned}$$

Actual value, $I = \int_0^2 3x^2 + e^x dx =$ ____________________

Absolute Error = $|Actual\ value - Approximated\ value|$

2.1 Error Analysis

In this section, error incurred in using the *Trapezoidal rule* to estimate an integral is analyzed.

Theorem on Precision of Trapezoidal Rule
If f'' exists and is continuous on the interval $[a, b]$ and if the *Composite Trapezoidal rule* T with uniform spacing h is used to estimate the integral $I = \int_a^b f(x)dx$, then for some ζ in (a, b), $$I - T = -\frac{1}{12}(b-a)h^2 f''(\zeta) = o(h^2)$$

Proof:

Firstly, prove the theorem when $a=0, b=1$ and $h=1$. In this case, we have to show that

$$\int_0^1 f(x)dx - \frac{1}{2}[f(0)+f(1)] = -\frac{1}{12}f''(\zeta) \qquad (1)$$

Let p be the polynomial of degree 1 that interpolates f at 0 and 1. Then p is given by

$$p(x) = f(0) + [f(1) - f(0)]x$$

Hence, $\int_0^1 f(x)dx = f(0) + \frac{1}{2}[f(1) - f(0)] = \frac{1}{2}[f(0)+f(1)]$

By the following theorem,

Theorem on Interpolation Errors I
If p is the polynomial of degree at most n that interpolates f at the n + 1 distinct nodes $x_0, x_1, \ldots, x_n$ belonging to an interval $[a,b]$ and if $f^{(n+1)}$ is continuous, then for each x in $[a,b]$, there is a ξ in (a,b) for which $$f(x) - p(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi)\prod_{i=0}^{n}(x - x_i)$$

we have $(n=1, x_0=0, x_1=1)$

$$f(x) - p(x) = \frac{1}{2}f''[\xi(x)]x(x-1) \qquad (2)$$

where $\xi(x)$ depends on x in $(0,1)$. From Equation (2), it follows that

$$\int_0^1 f(x)dx - \int_0^1 p(x)dx = \frac{1}{2}\int_0^1 f''[\xi(x)]x(x-1)dx$$

That $f''[\xi(x)]$ is continuous can be proven by solving Equation (2) for $f''[\xi(x)]$ and verifying the continuity. Notice that $x(x-1)$ does not change sign in the interval $[0,1]$. Hence, by the ***Mean-Value Theorem for Integrals*** (refer to page 5), there is a point $x = s$ for which

$$\int_0^1 f''[\xi(x)]x(x-1)dx = f''[\xi(s)]\int_0^1 x(x-1)dx = -\frac{1}{6}f''(\xi)$$

By putting all these equations together, Equation (1) is obtained. From Equation (1), by making a change of variable, the ***Basic Trapezoidal rule*** with its error term is obtained.

$$\int_0^1 f(x)dx = \frac{b-a}{2}[f(a)+f(b)] - \frac{1}{12}(b-a)^3 f''(\xi) \qquad (3)$$

$$\int_0^1 f(x)dx - \frac{b-a}{2}[f(a)+f(b)] = -\frac{1}{12}(b-a)^3 f''(\xi)$$

This is the Trapezoidal rule and error term for the interval $[a,b]$ with only one subinterval, which is the entire interval. Thus, the error term is $o(h^3)$, where $h = b-a$. Here, ξ is in (a,b).

Now, let the interval $[a,b]$ be divided into n equal subintervals by points $x_0, x_1, \ldots, x_n$ with spacing h. Applying Equation (3) to subinterval $[x_i, x_{i+1}]$, we have

$$\int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}[f(x_i)+f(x_{i+1})] - \frac{1}{12}h^3 f''(\xi_i)$$

where $x_i < \xi_i < x_{i+1}$. We use this result over the interval $[a,b]$, obtaining the ***Composite Trapezoidal rule***

$$\int_a^b f(x)dx = \sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}\sum_{i=0}^{n-1}[f(x_i)+f(x_{i+1})] - \frac{h^3}{12}\sum_{i=0}^{n-1} f''(\xi_i) \qquad (4)$$

The final term in Equation (4) is the error term and it can be simplified in the following way: Since $h = \frac{b-a}{n}$, the error term for the ***Composite Trapezoidal rule*** is

$$-\frac{h^3}{12}\sum_{i=0}^{n-1} f''(\xi_i) = -\frac{b-a}{12}h^2\left[\frac{1}{n}\sum_{i=0}^{n-1} f''(\xi_i)\right] = -\frac{b-a}{12}h^2 f''(\zeta)$$

The average $\left[\frac{1}{n}\sum_{i=0}^{n-1} f''(\xi_i)\right]$ lies between the least and the greatest values of f'' on the interval (a,b). Hence, by the ***Intermediate-Value Theorem***, it is $f''(\zeta)$ for some point ζ in (a,b). This completes the proof of the error formula.

Mean-Value Theorem for Integrals	***Intermediate-Value Theorem***
Let f be continuous on $[a,b]$ and assume that g is Riemann-integrable on $[a,b]$. If $g(x) \geq 0$ on $[a,b]$, then there exists a point ξ such that $a \le \xi \le b$ and $\int_a^b f(x)g(x)dx = f(\xi)\int_a^b g(x)dx$	If the function g is continuous on an interval $[a,b]$, then for each c between $g(a)$ and $g(b)$, there is a point ξ in $[a,b]$ for which $g(\xi) = c$.

Error formula for *Trapezoidal rule*:

1. *Basic Trapezoidal rule:* $-\frac{1}{12}(b-a)^3 f''(\xi)$ for $a < \xi < b$

2. *Composite Trapezoidal rule*: $-\frac{b-a}{12}h^2 f''(\xi)$ for $a < \xi < b$

Example 5: If the *Composite Trapezoidal rule* is to be used to compute $\int_0^1 e^{-x^2}dx$ with an error of at most $\frac{1}{2}\times 10^{-4}$, how many points should be used?

> *Reminder*:
> *n* subintervals = (*n*+1) points

The error formula is $-\frac{b-a}{12}h^2 f''(\zeta)$.

$f(x) = e^{-x^2}$, $f'(x) = -2xe^{-x^2}$, $f''(x) = (4x^2-2)e^{-x^2}$

Thus, $|f''(x)| \le 2$ on the interval $[0,1]$.

$$\left|-\frac{b-a}{12}h^2 f''(\zeta)\right| = \frac{b-a}{12}h^2 f''(\zeta) = \frac{1}{12}h^2(2) = \frac{1}{6}h^2$$

To have an error of at most $\frac{1}{2}\times 10^{-4}$, we require $\frac{1}{6}h^2 \le \frac{1}{2}\times 10^{-4}$ or $h \le \sqrt{3}\times 10^{-2}$.

$h = 1/n$: so $n \ge 58$. Hence, 59 or more points will certainly produce the desired accuracy.

Example 6: How many subintervals are needed to approximate $\int_0^1 \frac{\sin x}{x}dx$ with error not to exceed $\frac{1}{2}\times 10^{-5}$ using the *Composite Trapezoidal rule*? Here, the integrand, $f(x) = x^{-1}\sin x$, is defined to be 1 when *x* is 0.

The error formula is $-\frac{b-a}{12}h^2 f''(\zeta)$.

Now, establish a bound on $f''(x)$ for *x* in the range $[0,1]$. Taking derivatives in the usual way is not satisfactory because each term contains *x* with a negative power, and it is difficult to find an upper bound on $|f''(x)|$. However using Taylor series, we have

$$f(x)=1-\frac{x^2}{3!}+\frac{x^4}{5!}-\frac{x^6}{7!}+\frac{x^8}{9!}-\ldots$$

$$f'(x)=-\frac{2x}{3!}+\frac{4x^3}{5!}-\frac{6x^5}{7!}+\frac{8x^7}{9!}-\ldots$$

$$f''(x)=-\frac{2}{3!}+\frac{3\times 4x^2}{5!}-\frac{5\times 6x^4}{7!}+\frac{7\times 8x^6}{9!}-\ldots$$

Thus, on the interval $[0,1]$, $|f''(x)|$ cannot exceed $\frac{1}{2}$ because

$$\frac{2}{3!}+\frac{3\times 4}{5!}+\frac{5\times 6}{7!}+\frac{7\times 8}{9!}+\ldots<\frac{1}{3}+\frac{1}{10}+\frac{1}{24}\left(\frac{1}{2}+\frac{1}{4}+\frac{1}{8}+\ldots\right)<\frac{1}{2}$$

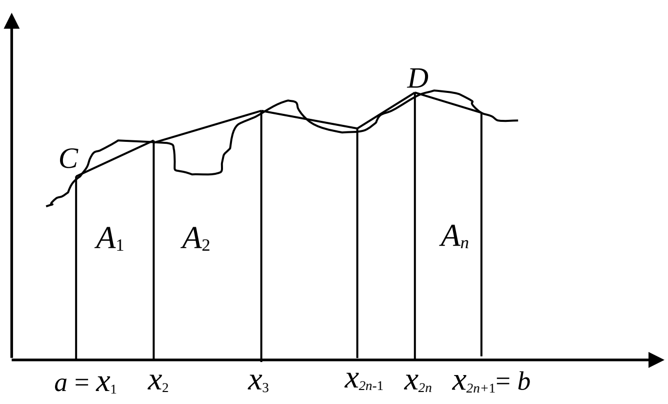
Therefore, the error term $\left|(b-a)h^2 f''(\zeta)/12\right|$ cannot exceed $h^2/24$.

$$\left|-(b-a)h^2 f''(\zeta)/12\right|=(b-a)h^2 f''(\zeta)/12=\frac{1}{12}h^2\left(\frac{1}{2}\right)=\frac{1}{24}h^2$$

To have an error of at most $\frac{1}{2}\times 10^{-5}$, we require $\frac{1}{24}h^2\le\frac{1}{2}\times 10^{-5}$ or $h\le\sqrt{1.2}\times 10^{-2}$.

$n\ge\left(1/\sqrt{1.2}\right)10^2=91.29$. This analysis shows that 92 subintervals are needed.

3. SIMPSON'S RULE



Let *CD* be the curve and its equation is $y=f(x)$. To evaluate $\int_a^b f(x)dx$, we subdivide the interval from *a* to *b* into 2*n* equal parts, so that each part is equal to $h=\frac{(b-a)}{2n}$.

By Simpson's parabolic rule,

the first area, $A_1 = \frac{1}{3}h\left[f(x_1) + 4f(x_2) + f(x_3)\right]$

the second area, $A_2 = \frac{1}{3}h\left[f(x_3) + 4f(x_4) + f(x_5)\right]$

and the n^{th} area, $A_n = \frac{1}{3}h\left[f(x_{2n-1}) + 4f(x_{2n}) + f(x_{2n+1})\right]$

Total area,

$$A_S = \int_a^b f(x)dx \approx \frac{h}{3}\left\{\begin{array}{l} f(x_1) + f(x_{2n+1}) + 4\left[f(x_2) + f(x_4) + \ldots + f(x_{2n})\right] \\ + 2\left[f(x_3) + f(x_5) + \ldots + f(x_{2n-1})\right]\end{array}\right\} \text{ where } x_n = a + (n-1)h,\ n = 1,2,..$$

Example 7: Dividing the range into 4 equal parts, find the approximate value of $\int_0^1 \frac{1}{1+x^2}dx$ by using *Simpson's rule*.

$$\begin{aligned} A_S &= \frac{1}{3}\left(\frac{1}{4}\right)\left\{f(0) + f(1) + 4\left[f(0.25) + f(0.75)\right] + 2f(0.5)\right\} \\ &= \frac{1}{12}(9.42470588) \\ &= 0.785392 \end{aligned}$$

Example 8: Compute an approximate value for integral given in Example 2 by using the *Simpson's rule* with 5 points. Then compare with the actual value of the integral and find its absolute error.

Integral in Example 2: $\int_0^2 3x^2 + e^x dx$; 5 points $\Rightarrow n = 4$; $f(x) = x^2$; $h = \frac{2-0}{4} = 0.5$

$$\begin{aligned} A_S &= \frac{1}{3}(0.5)\left\{f(0) + f(2) + 4\left[f(0.5) + f(1.5)\right] + 2\left[f(1.0)\right]\right\} \\ &= \frac{0.5}{3}(86.34726) \\ &= 14.39121 \end{aligned}$$

Actual value, $I = \int_0^2 3x^2 + e^x dx =$ ___________________

Absolute Error = $\left|Actual\ value - Approximated\ value\right|$

3.1 Error Analysis

A numerical integration rule over two equal subintervals with partition points $a = x_1, a+h$ and $a+2h = b = x_{2n+1}$ is the widely used ***Basic Simpson's rule***:

$$\int_a^{a+2h} f(x)dx \approx \frac{h}{3}[f(a)++4f(a+h)+f(a+2h)] \tag{5}$$

The error term in *Simpson's rule* can be established by using the Taylor series:

$$f(a+h) = f + hf' + \frac{1}{2!}h^2 f'' + \frac{1}{3!}h^3 f''' + \frac{1}{4!}h^4 f^{(4)} + \ldots$$

Now replacing *h* by 2*h*:

$$f(a+2h) = f + 2hf' + 2h^2 f'' + \frac{4}{3}h^3 f''' + \frac{2^4}{4!}h^4 f^{(4)} + \ldots$$

where the functions $f, f', f'',\ldots$ on the right-hand side are evaluated at *a*.

Using these two series, we obtain

$$f(a) + 4f(a+h) + f(a+2h) = 6f + 6hf' + 4h^2 f'' + 2h^3 f''' + \frac{20}{4!}h^4 f^{(4)} + \ldots$$

and thereby, we have

$$\frac{h}{3}[f(a) + 4f(a+h) + f(a+2h)] = 2hf + 2h^2 f' + \frac{4}{3}h^3 f'' + \frac{2}{3}h^4 f''' + \frac{20}{3\cdot 4!}h^5 f^{(4)} + \ldots \tag{6}$$

Hence, we have a series for the right-hand side of Equation (5). Now let's find one for the left-hand side. The Taylor series for $F(a+2h)$ is

$$F(a+2h) = F(a) + 2hF'(a) + 2h^2 F''(a) + \frac{4}{3}h^3 F'''(a) + \frac{2}{3}h^4 F^{(4)}(a) + \frac{2^5}{5!}F^{(5)}(a) + \ldots$$

Let $F(x) = \int_a^x f(t)dt$. By the Fundamental Theorem of Calculus, $F' = f$. We observe that $F(a) = 0$ and $F(a+2h)$ is the integral on the left-hand side of Equation (5). Since $F'' = f', F''' = f''$, and so on, we have

$$\int_a^{a+2h} f(x)dx = 2hf + 2h^2 f' + \frac{4}{3}h^3 f'' + \frac{2}{3}h^4 f''' + \frac{2^5}{5\cdot 4!}h^5 f^{(4)} + \ldots \tag{7}$$

Subtracting Equation (6) from Equation (7), we obtain

$$\int_a^{a+2h} f(x)dx = \frac{h}{3}[f(a)+4f(a+h)+f(a+2h)] - \frac{h^5}{90}f^{(4)} - \ldots$$

We can rewrite the ***Basic Simpson's rule*** over the interval $[a,b]$ as

$$\int_a^b f(x)dx \approx \frac{(b-a)}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$$

with error term $-\frac{1}{90}h^5 f^{(4)}(\xi)$ for some ξ in (a,b).

Suppose that the interval $[a,b]$ is subdivided into an even number of subintervals, say n, each of width $h=(b-a)/n$. Then the partition points are $x_i = a+ih$ for $0 \leq i \leq n$, where n is divisible by 2. Now from basic calculus, we have

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

Using the ***Basic Simpson's rule***, we have, for the right-hand side,

$$\approx \sum_{i=1}^{n/2}\frac{h}{3}\{f(a+2(i-1)h)+4f(a+(2i-1)h)+f(a+2ih)\}$$

$$= \frac{h}{3}\left\{f(a)+\sum_{i=1}^{(n/2)-1}f(a+2ih)+4\sum_{i=1}^{(n/2)}f(a+(2i-1)h)+\sum_{i=1}^{(n/2)-1}f(a+2ih)+f(b)\right\}$$

Thus, we obtain the ***Composite Simpson's rule*** over n (even) subintervals

$$\int_a^b f(x)dx \approx \frac{h}{3}\left\{[f(a)+f(b)]+4\sum_{i=1}^{(n/2)}f(a+(2i-1)h)+2\sum_{i=1}^{(n/2)/2}f(a+2ih)\right\} \text{ where } h=(b-a)/n.$$

The error term is $-\frac{1}{180}(b-a)h^4 f^{(4)}(\xi)$ for some ξ in (a,b).

<u>Error formula for *Simpson's rule*:</u>

1. Basic Simpson's rule: $\boxed{-\frac{1}{90}h^5 f^{(4)}(\xi) \text{ for some } \xi \text{ in } (a,b)}$

2. Composite Simpson's rule: $\boxed{-\frac{1}{180}(b-a)h^4 f^{(4)}(\xi) \text{ for some } \xi \text{ in } (a,b)}$

Example 9: Apply the *Basic Simpson's rule* to approximate $\int_1^2 \ln x dx$, and find an upper bound for the error in your approximations.

$$\begin{aligned}\int_1^2 \ln x dx &\approx \frac{h}{3}\left[f(a)+4f(a+h)+f(a+2h)\right]\\ &= \frac{0.5}{3}\left[f(1)+4f(3/2)+f(2)\right]\\ &= \frac{0.5}{3}\left[\ln 1+4\ln\frac{3}{2}+\ln 2\right]\approx 0.3858\end{aligned}$$

The error for Basic Simpson's rule is $-\frac{1}{90}h^5 f^{(4)}(\xi)$ where $1<\xi<2$. Since $f^{(4)}(x)=-\frac{6}{x^4}$, $\left|f^{(4)}(x)\right|=\left|-\frac{6}{x^4}\right|=\frac{6}{x^4}$. Thus, $\left|f^{(4)}(x)\right|\le 6$ on the interval $[1,2]$.

The error is at most $\left|-\frac{1}{90}h^5 f^{(4)}(\xi)\right|\le\frac{(0.5)^5}{90}(6)=\frac{1}{480}\approx 0.0021$

4. ROMBERG ALGORITHM

The *Romberg algorithm* produces a triangular array of numbers, all of which are numerical estimates of the definite integral $\int_a^b f(x)dx$. The array is denoted here by the notation

$n \backslash m$	0	1	2	3	$\cdots$	
0	$R(0,0)$					
1	$R(1,0)$	$R(1,1)$				
2	$R(2,0)$	$R(2,1)$	$R(2,2)$			
3	$R(3,0)$	$R(3,1)$	$R(3,2)$	$R(3,3)$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
	$R(n,0)$	$R(n,1)$	$R(n,2)$	$R(n,3)$	$\cdots$	$R(n,m)$

The first column of this table contains estimates of the integral obtained by the recursive trapezoid formula with decreasing values of the step size. Explicitly, $R(n,0)$ is the result of applying the trapezoid rule with 2^n equal subintervals. The first of them, $R(0,0)$, is obtained with just one trapezoid:

$$R(0,0)=\frac{1}{2}(b-a)[f(a)+f(b)]$$

Note that $R(n,0)$ is obtained easily from $R(n-1,0)$, that is

$$R(n,0)=\frac{1}{2}R(n-1,0)+h\sum_{k=1}^{2^{n-1}} f[a+(2k-1)h];\quad h=\frac{(b-a)}{2^n},\ n\geq 1$$

The second and successive columns in the *Romberg* array are generated by the extrapolation formula

$$R(n,m)=R(n,m-1)+\frac{1}{4^m-1}[R(n,m-1)-R(n-1,m-1)]$$

with $n\geq 1$, $m\geq 1$ and $m\leq n$.

Example 10: If $R(8,2)=8$ and $R(7,2)=1$, what is $R(8,3)$?

$$R(8,3)=R(8,2)+\frac{1}{63}[R(8,2)-R(7,2)]=\frac{73}{9}$$

Example 11: Compute $\int_0^1 \frac{1}{1+x^2}dx$ by the Romberg algorithm using 4 equal parts and show your calculations correct to SIX decimal places. Then, compare with the values obtained from the methods of Composite Trapezoidal rule (Example 3) and Simpson's rule (Example 7).

n	0	1	2	3
0	0.750000			
1	0.775000	0.783333		
2	0.782794			
3				