Numerical Analysis

by

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Chapter 7

Numerical Differentiation and Integration

Module No. 3

Gaussian Quadrature

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In the Newton-Cotes method (discussed in Module 2 of Chapter 7), the finite interval of integration $[a, b]$ is divided into n equal subintervals. That is, the arguments $x_i, i = 0, 1, 2, \ldots, n$ are known and they are equispaced. Also, all the Newton-Cotes formulae give exact result for the polynomials of degree up to n. It is mentioned that the Newton-Cotes formulae have some limitations. These formulae are not applicable for improper integrals.

This drawback can be removed by taking non-equal arguments. But, the question is *how one can choose the arguments?* That is, in this case the arguments are unknown. For this situation, one new kind of quadrature formulae are devised which give exact result for the polynomials of degree up to $2n - 1$. These methods are called **Gaussian quadrature methods**, described below.

3.1 Gaussian quadrature

The Gaussian quadrature formula is of the following form

$$\int_a^b \psi(x) f(x) dx = \sum_{i=1}^{n} w_i f(x_i) + E, \tag{3.1}$$

where x_i and w_i are respectively called nodes and weights and $\psi(x)$ is called the weight function, E is the error. Here, the weights w_i's are discrete numbers, but the weight function $\psi(x)$ is a continuous function and defined on the interval of integration $[a, b]$. In Newton-Cotes formulae, the weights w_i's were unknown but x_i's were known, while in Gaussian formulae, both are unknown. By changing the weight function $\psi(x)$ one can derived different quadrature formulae.

The fundamental theorem of Gaussian quadrature is stated below:
the optimal nodes of the n-point Gaussian quadrature formula are precisely the zeros of the orthogonal polynomial for the same interval and weight function.

Gaussian quadrature gives exact result for all polynomial up to degree $2n - 1$.

Suppose the Gaussian nodes x_i's are chosen by some way. The weights w_i's can be computed by using Lagrange's interpolating formula. Let

$$\pi(x) = \prod_{j=1}^{m} (x - x_j). \tag{3.2}$$

Then

$$\pi'(x_j) = \prod_{\substack{i=1 \\ i\neq j}}^{m} (x_j - x_i). \tag{3.3}$$

Then Lagrange's interpolating polynomial for m arguments is

$$\phi(x) = \sum_{j=1}^{m} \frac{\pi(x)}{(x-x_j)\pi'(x_j)} f(x_j) \tag{3.4}$$

for arbitrary point x.

Now, from the equation (3.1)

$$\begin{aligned}\int_a^b \phi(x)\psi(x)dx &= \int_a^b \sum_{j=1}^{m} \frac{\pi(x)\psi(x)}{(x-x_j)\pi'(x_j)} f(x_j)dx \\ &= \sum_{j=1}^{m} w_j f(x_j).\end{aligned} \tag{3.5}$$

Comparing, we get

$$w_j = \frac{1}{\pi'(x_j)} \int_a^b \frac{\pi(x)\psi(x)}{x-x_j} dx. \tag{3.6}$$

The weights w_j are sometimes called the **Christofell numbers**.

It is obvious that any finite interval $[a, b]$ can be converted to the interval $[-1, 1]$ using the following linear transformation

$$x = \frac{b-a}{2}t + \frac{b+a}{2} = qt + p, \text{ where } q = \frac{b-a}{2} \text{ and } p = \frac{b+a}{2}. \tag{3.7}$$

Then,

$$\int_a^b f(x)\, dx = \int_{-1}^{1} f(qt+p)\, q\, dt. \tag{3.8}$$

In Gaussian quadrature the limits of the integration are taken as -1 and 1, and it is possible for any finite interval shown above. Thus, we consider the following Gaussian integral

$$\int_{-1}^{1} \psi(x) f(x) dx = \sum_{i=1}^{n} w_i f(x_i) + E. \tag{3.9}$$

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Depending on the weight function $\psi(x)$ one can generate different Gaussian quadrature formulae. In this module, we consider two Gaussian quadrature formulae.

3.2 Gauss-Legendre quadrature formulae

In this formula, the weight function $\psi(x)$ is taken as 1. Then the quadrature formula is

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} w_i f(x_i) + E. \tag{3.10}$$

Here, w_i's and x_i's are $2n$ unknown parameters. Therefore, w_i's and x_i's can be determined such that the formula (3.10) gives exact result when $f(x)$ is a polynomial of degree up to $2n-1$.

Let

$$f(x) = c_0 + c_1 x + c_2 x^2 + \cdots + c_{2n-1} x^{2n-1}. \tag{3.11}$$

be a polynomial of degree $2n-1$.

Now, the left hand side of the equation (3.10) is,

$$\begin{aligned} \int_{-1}^{1} f(x)dx &= \int_{-1}^{1} [c_0 + c_1 x + c_2 x^2 + \cdots + c_{2n-1} x^{2n-1}]dx \\ &= 2c_0 + \frac{2}{3}c_2 + \frac{2}{5}c_4 + \cdots . \end{aligned} \tag{3.12}$$

When $x = x_i$, equation (3.11) becomes

$$f(x_i) = c_0 + c_1 x_i + c_2 x_i^2 + c_3 x_i^3 + \cdots + c_{2n-1} x_i^{2n-1}.$$

The right hand side of the equation (3.10) is

$$\begin{aligned}\sum_{i=1}^{n} w_i f(x_i) = & \; w_1[c_0 + c_1 x_1 + c_2 x_1^2 + \cdots + c_{2n-1} x_1^{2n-1}] \\ & + w_2[c_0 + c_1 x_2 + c_2 x_2^2 + \cdots + c_{2n-1} x_2^{2n-1}] \\ & + w_3[c_0 + c_1 x_3 + c_2 x_3^2 + \cdots + c_{2n-1} x_3^{2n-1}] \\ & + \cdots\cdots\cdots\cdots\cdots\cdots \\ & + w_n[c_0 + c_1 x_n + c_2 x_n^2 + \cdots + c_{2n-1} x_n^{2n-1}] \\ = & \; c_0(w_1 + w_2 + \cdots + w_n) + c_1(w_1 x_1 + w_2 x_2 + \cdots + w_n x_n) \\ & + c_2(w_1 x_1^2 + w_2 x_2^2 + \cdots + w_n x_n^2) + \cdots \\ & + c_{2n-1}(w_1 x_1^{2n-1} + w_2 x_2^{2n-1} + \cdots + w_n x_n^{2n-1}). \qquad (3.13)\end{aligned}$$

Hence, equation (3.10) becomes

$$\begin{aligned}& 2c_0 + \frac{2}{3}c_2 + \frac{2}{5}c_4 + \cdots \\ = & \; c_0(w_1 + w_2 + \cdots + w_n) + c_1(w_1 x_1 + w_2 x_2 + \cdots + w_n x_n) \\ & + c_2(w_1 x_1^2 + w_2 x_2^2 + \cdots + w_n x_n^2) + \cdots \\ & + c_{2n-1}(w_1 x_1^{2n-1} + w_2 x_2^{2n-1} + \cdots + w_n x_n^{2n-1}).\end{aligned}$$

Comparing both sides the coefficients of c_i's, and we obtained the following $2n$ equations:

$$\begin{aligned} w_1 + w_2 + \cdots + w_n &= 2 \\ w_1 x_1 + w_2 x_2 + \cdots + w_n x_n &= 0 \\ w_1 x_1^2 + w_2 x_2^2 + \cdots + w_n x_n^2 &= \tfrac{2}{3} \qquad (3.14) \\ \cdots\cdots\cdots\cdots\cdots\cdots & \quad \cdots \\ w_1 x_1^{2n-1} + w_2 x_2^{2n-1} + \cdots + w_n x_n^{2n-1} &= 0. \end{aligned}$$

Now, the equation (3.14) is a system of non-linear equations containing $2n$ equations and $2n$ unknowns w_i and x_i, $i = 1, 2, \ldots, n$. Let the solution of these equations be $w_i = w_i^*$ and $x_i = x_i^*, i = 1, 2, \ldots, n$.

Then the Gauss-Legendre quadrature formula is given by

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} w_i^* f(x_i^*). \qquad (3.15)$$

Unfortunately, the system of equations (3.14) is non-linear and it is very difficult to find its solution for large n. But, for lower values of n, one can find the exact solution of the system. Some particular cases are discussed below:

Case I. When $n = 1$, the Gauss-Legendre quadrature formula becomes

$$\int_{-1}^{1} f(x)dx = w_1 f(x_1)$$

and the system of equations is

$$w_1 = 2 \text{ and } w_1 x_1 = 0, \text{ i.e. } x_1 = 0.$$

Thus, for $n = 1$,

$$\int_{-1}^{1} f(x)dx = 2f(0). \tag{3.16}$$

Note the this is a very simple formula to get the value of an integration. This formula is known as 1-point Gauss-Legendre quadrature formula. It gives an approximate value of the integration and it gives exact answer when $f(x)$ is a polynomial of degree one.

Case II. When $n = 2$, then the quadrature formula reduces to

$$\int_{-1}^{1} f(x)dx = w_1 f(x_1) + w_2 f(x_2). \tag{3.17}$$

In this case, the system of equations (3.14) becomes

$$\begin{aligned} w_1 + w_2 &= 2 \\ w_1 x_1 + w_2 x_2 &= 0 \\ w_1 x_1^2 + w_2 x_2^2 &= \tfrac{2}{3} \\ w_1 x_1^3 + w_2 x_2^3 &= 0. \end{aligned} \tag{3.18}$$

The solution of these equations is $w_1 = w_2 = 1, x_1 = -1/\sqrt{3}, x_2 = 1/\sqrt{3}$. Hence, the 2-point Gauss-Legendre quadrature formula is

$$\int_{-1}^{1} f(x)dx = f(-1/\sqrt{3}) + f(1/\sqrt{3}). \tag{3.19}$$

The above system of equations can also be obtained by substituting $f(x) = 1, x, x^2$ and x^3 to the equation (3.17) successively.

This 2-point quadrature formula gives exact answer when $f(x)$ is a polynomial of degree up to three.

Case III. When $n = 3$, then the Gauss-Legendre formula becomes

$$\int_{-1}^{1} f(x)dx = w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3). \tag{3.20}$$

In this case, the system of equations containing six unknowns x_1, x_2, x_3 and w_1, w_2, w_3 is

$$\begin{aligned} w_1 + w_2 + w_3 &= 2 \\ w_1x_1 + w_2x_2 + w_3x_3 &= 0 \\ w_1x_1^2 + w_2x_2^2 + w_3x_2^3 &= \tfrac{2}{3} \\ w_1x_1^3 + w_2x_2^3 + w_3x_2^3 &= 0 \\ w_1x_1^4 + w_2x_2^4 + w_3x_2^4 &= \tfrac{2}{5} \\ w_1x_1^5 + w_2x_2^5 + w_3x_2^5 &= 0. \end{aligned}$$

This system of equations can also be obtained by substituting $f(x) = 1, x, x^2, x^3, x^4, x^5$ to the equation (3.20).

Solution of this system of equations is

$$x_1 = -\sqrt{3/5}, x_2 = 0, x_3 = \sqrt{3/5}, w_1 = 5/9, w_2 = 8/9, w_3 = 5/9.$$

Hence, in this case, the Gauss-Legendre quadrature formula is

$$\int_{-1}^{1} f(x)dx = \frac{1}{9}[5f(-\sqrt{3/5}) + 8f(0) + 5f(\sqrt{3/5})]. \tag{3.21}$$

This is known as 3-point Gauss-Legendre quadrature formula.

In this way, one can determine Gauss-Legendre quadrature formulae for higher values of n.

Note that the system of equations (3.14) is non-linear with respect to x_i's, but if x_i's are known, then this system becomes linear one.

It is very interesting that the nodes x_i's, $i = 1, 2, \ldots, n$ are the zeros of the nth degree Legendre's polynomial

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}[(x^2 - 1)^n].$$

. . . .

This is a well known orthogonal polynomial and it is obtained from the following recurrence relation:

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \tag{3.22}$$

where $P_0(x) = 1$ and $P_1(x) = x$.

Some lower order Legendre polynomials are

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= x \\ P_2(x) &= \tfrac{1}{2}(3x^2 - 1) \\ P_3(x) &= \tfrac{1}{2}(5x^3 - 3x) \\ P_4(x) &= \tfrac{1}{8}(35x^4 - 30x^2 + 3). \end{aligned} \tag{3.23}$$

It can be verified that the roots of the equation $P_n(x) = 0$ are the nodes x_i's of the n-point Gauss-Legendre quadrature formula. Finding of zeros of lower degree Gauss-Legendre polynomial is easy than finding the solution of the system of equations (3.14). For example, the roots of the equation $P_2(x) = 0$ are $\pm 1/\sqrt{3}$ and these are the nodes for 2-point Gauss-Legendre quadrature formula. Similarly, the roots of the equation $P_3(x) = 0$ are $0, \pm\sqrt{3/5}$ and these are the nodes of 3-point formula, and so on.

Again, it is proved that the weights w_i's can be determined from the following equation

$$w_i = \frac{2}{(1 - x_i^2)[P_n'(x_i)]^2}. \tag{3.24}$$

It can be shown that the error of this formula is

$$E = \frac{2^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\xi), \qquad -1 < \xi < 1. \tag{3.25}$$

The nodes and weights for some lower values of n are listed in Table 3.1.

Note 3.1 *The Gauss-Legendre quadrature generates several formulae for different values of n. These formulae are known as n-point formula, where $n = 1, 2, \ldots$.*

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n	node x_i	weight w_i	order of truncation error
2	± 0.57735027	1.00000000	$f^{(4)}(\xi)$
3	0.00000000	0.88888889	$f^{(6)}(\xi)$
	± 0.77459667	0.55555556	
4	± 0.33998104	0.65214515	$f^{(8)}(\xi)$
	± 0.86113631	0.34785485	
5	0.00000000	0.56888889	
	± 0.53846931	0.47862867	$f^{(10)}(\xi)$
	± 0.90617985	0.23692689	
6	± 0.23861919	0.46791393	
	± 0.66120939	0.36076157	$f^{(12)}(\xi)$
	± 0.93246951	0.17132449	

Table 3.1: Values of x_i and w_i for Gauss-Legendre quadrature

Example 3.1 *Find the value of* $\int_0^1 x^2 \sin x \, dx$ *by Gauss-Legendre formula for* $n = 2, 4, 6$. *Also, calculate the absolute errors.*

Solution. To apply the Gauss-Legendre formula, the limits are transferred to $-1, 1$ by substituting $x = \frac{1}{2}u(1-0) + \frac{1}{2}(1+0) = \frac{1}{2}(u+1)$.

Then,

$$I = \int_0^1 x^2 \sin x \, dx = \int_{-1}^1 \frac{1}{8}(u+1)^2 \sin\left(\frac{u+1}{2}\right) du = \frac{1}{8}\sum_{i=1}^n w_i f(u_i)$$

where $f(x_i) = (x_i + 1)^2 \sin\left(\frac{x_i+1}{2}\right)$.

For the two-point formula $(n = 2)$

$x_1 = -0.57735027, x_2 = 0.57735027, w_1 = w_2 = 1$.

Then $I = \frac{1}{8}[1 \times 0.037469207 + 1 \times 1.7650614] = 0.22531632$.

For the four-point formula $(n = 4)$

$x_1 = -0.33998104, x_2 = -0.86113631, x_3 = -x_1, x_4 = -x_2,$

$w_1 = w_3 = 0.65214515, w_2 = w_4 = 0.34785485.$

. . . .

Then,

$$\begin{aligned}
I &= \frac{1}{8}[w_1 f(x_1) + w_3 f(x_3) + w_2 f(x_2) + w_4 f(x_4)] \\
&= \frac{1}{8}[w_1\{f(x_1) + f(-x_1)\} + w_2\{f(x_2) + f(-x_2)\}] \\
&= \frac{1}{8}[0.65214515 \times (0.14116516 + 1.1149975) + 0.34785485 \times (0.0013377874 + 2.77785)] \\
&= 0.22324429.
\end{aligned}$$

For the six-point formula ($n = 6$)

$x_1 = -0.23861919, x_2 = -0.66120939, x_3 = -0.93246951, x_4 = -x_1,$

$x_5 = -x_2, x_6 = -x_3, w_1 = w_4 = 0.46791393, w_2 = w_5 = 0.36076157,$

$w_3 = w_6 = 0.17132449.$

Then,

$$\begin{aligned}
I &= \frac{1}{8}[w_1\{f(x_1) + f(-x_1)\} + w_2\{f(x_2) + f(-x_2)\} + w_3\{f(x_3) + f(-x_3)\}] \\
&= \frac{1}{8}[0.46791393 \times (0.2153945 + 0.89054879) + 0.36076157 \times (0.019350185 + 2.0375335) \\
&\quad +0.17132449 \times (0.00015395265 + 3.0725144)] \\
&= 0.22324427.
\end{aligned}$$

The exact value is 0.22324428.

The following table gives a comparison among the different Gauss-Legendre formulae.

n	Exact value	Gauss formula	Error
2	0.22324428	0.22531632	2.07×10^{-3}
4	0.22324428	0.22324429	0.01×10^{-6}
6	0.22324428	0.22324427	0.01×10^{-6}

By considering the weight function $\psi(x) = (1 - x^2)^{-1/2}$, we obtain another type of Gaussian quadrature known as Gauss-Chebyshev quadrature, discussed in next section.

3.3 Gauss-Chebyshev quadrature formulae

Gauss-Chebyshev quadrature is also known as **Chebyshev quadrature**. Its weight function is taken as $\psi(x) = (1 - x^2)^{-1/2}$. The general form of this method is

$$\int_{-1}^{1} \frac{1}{\sqrt{1 - x^2}} f(x)dx = \sum_{i=1}^{n} w_i f(x_i) + E, \qquad (3.26)$$

where E is the error.

This formula also contains $2n$ unknown parameters. So, as per Gaussian quadrature, this method gives exact answer for polynomials of degree up to $2n-1$.

For $n=3$ the equation (3.26) becomes

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x)dx = w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3). \tag{3.27}$$

Since the method gives exact value for the polynomials of degree up to $2n-1$. i.e. up to 5. Therefore, for $f(x) = 1, x, x^2, x^3, x^4, x^5$ the following equations are obtained from (3.27).

$$\begin{aligned} w_1 + w_2 + w_3 &= \pi \\ w_1x_1 + w_2x_2 + w_3x_3 &= 0 \\ w_1x_1^2 + w_2x_2^2 + w_3x_3^2 &= \tfrac{\pi}{2} \\ w_1x_1^3 + w_2x_2^3 + w_3x_3^3 &= 0 \\ w_1x_1^4 + w_2x_2^4 + w_3x_3^4 &= \tfrac{3\pi}{8} \\ w_1x_1^5 + w_2x_2^5 + w_3x_3^5 &= 0. \end{aligned}$$

Solution of this system of equations is $x_1 = \sqrt{3}/2, x_2 = 0, x_3 = -\sqrt{3}/2$, $w_1 = w_2 = w_3 = \pi/3$.

Thus the formula (3.27) becomes

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x)dx = \frac{\pi}{3}\Big[f(\sqrt{3}/2) + f(0) + f(-\sqrt{3}/2)\Big]. \tag{3.28}$$

This is known as 3-point Gauss-Chebyshev quadrature formula.

Like Gauss-Legendre quadrature formulae, many Gauss-Chebyshev quadrature formulae can be derived for different values of n.

In Gauss-Chebyshev quadrature formulae, the nodes $x_i, i = 1, 2, \ldots, n$, are the zeros of the Chebyshev polynomials

$$T_n(x) = \cos(n \cos^{-1} x). \tag{3.29}$$

That is, the nodes x_i's are given by equation

$$x_i = \cos\left(\frac{(2i-1)\pi}{2n}\right), i = 1, 2, \ldots, n. \tag{3.30}$$

. . . .

The weights w_i's are same for all values of i and these are given by

$$w_i = -\frac{\pi}{T_{n+1}(x_i)T_n'(x_i)} = \frac{\pi}{n}, \qquad i = 1, 2, \dots, n. \tag{3.31}$$

Using these results, the 1-point Gauss-Chebyshev quadrature formula is deduced below:

For $n = 1$, $x_1 = \cos\frac{\pi}{2} = 0$ and $w_1 = \pi$. That is,

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x)dx = w_1 f(x_1) = \pi f(0). \tag{3.32}$$

For $n = 2$, $x_i = \cos(2i-1)\frac{\pi}{4}$, $i = 1, 2$.

Thus,

$$x_1 = \cos\frac{\pi}{4} = \frac{1}{\sqrt{2}} \text{ and } x_2 = \cos\frac{3\pi}{4} = -\frac{1}{\sqrt{2}}.$$

The weights are $w_1 = w_2 = \dfrac{\pi}{2}$.

Thus, 2-point Gauss-Chebyshev quadrature formula is

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x)dx = w_1 f(x_1) + w_2 f(x_2) \tag{3.33}$$

$$= \frac{\pi}{2}\left[f\left(\frac{1}{\sqrt{2}}\right) + f\left(-\frac{1}{\sqrt{2}}\right)\right]. \tag{3.34}$$

The error in Gauss-Chebyshev quadrature is

$$E = \frac{2\pi}{2^{2n}(2n)!} f^{(2n)}(\xi), \qquad -1 < \xi < 1. \tag{3.35}$$

The more general Gauss-Chebyshev quadrature formula is then

$$\int_{-1}^{1} \frac{f(x)dx}{\sqrt{1-x^2}} = \frac{\pi}{n}\sum_{i=1}^{n} f\left[\cos\left\{\frac{(2i-1)}{2n}\pi\right\}\right] + \frac{2n}{2^{2n}(2n)!} f^{(2n)}(\xi). \tag{3.36}$$

In Table 3.2, the values of nodes and weights for first few Gauss-Chebyshev quadrature formulae are provided.

n	node x_i	weight w_i	order of truncation error
2	± 0.7071068	1.5707963	$f^{(4)}(\xi)$
3	0.0000000	1.0471976	
	± 0.8660254	1.0471976	$f^{(6)}(\xi)$
4	± 0.3826834	0.7853982	
	± 0.9238795	0.7853982	$f^{(8)}(\xi)$
5	0.0000000	0.6283185	
	± 0.5877853	0.6283185	$f^{(10)}(\xi)$
	± 0.9510565	0.6283185	

Table 3.2: Nodes and weights for Gauss-Chebyshev quadrature formulae

Example 3.2 *Find the value of* $\int_0^1 \frac{1}{1+x^2}\,dx$ *using Gauss-Chebyshev four-point formula.*

Solution. Let $f(x) = \frac{\sqrt{1-x^2}}{1+x^2}$. Here $x_1 = -0.3826834 = x_2$, $x_3 = -0.9238795 = -x_4$ and $w_1 = w_2 = w_3 = w_4 = 0.7853982$.

Then

$$
\begin{aligned}
I &= \int_0^1 \frac{1}{1+x^2}dx = \frac{1}{2}\int_{-1}^1 \frac{1}{1+x^2}dx = \frac{1}{2}\int_{-1}^1 \frac{f(x)}{\sqrt{1-x^2}}dx \\
&= \frac{1}{2}[w_1 f(x_1) + w_2 f(x_2) + w_3 f(x_3) + w_4 f(x_4)] \\
&= \frac{1}{2} \times 0.7853982[f(x_1) + f(x_2) + f(x_3) + f(x_4)] \\
&= \frac{1}{2} \times 0.7853982[2 \times 0.8058636 + 2 \times 0.2064594] = 0.7950767,
\end{aligned}
$$

while the exact value is $\pi/4 = 0.7853982$. Thus, the absolute error is 0.0096785.