

# Numerical Analysis and Computing

## Lecture Notes #8

— Numerical Differentiation and Integration —  
Composite Numerical Integration; Romberg Integration  
Adaptive Quadrature

Peter Blomgren,  
(blomgren.peter@gmail.com)

Department of Mathematics and Statistics  
Dynamical Systems Group  
Computational Sciences Research Center  
San Diego State University  
San Diego, CA 92182-7720

<http://terminus.sdsu.edu/>

Composite-Romberg-Adaptive

— (1/31)

## Outline

- 1 Composite Quadrature
  - Divide and Conquer; Example — Simpson's Rule
  - Generalization
  - Collecting the Error...
  - Summary, Algorithm
- 2 Romberg Quadrature
  - Applying Richardson's Extrapolation
  - Romberg Quadrature — Code Outline
- 3 Adaptive Quadrature
  - Introduction
  - Building the Adaptive CSR Scheme
  - Example...
  - Putting it Together...

Composite-Romberg-Adaptive

— (2/31)

## Divide and Conquer with Simpson's Rule

1 of 3

The exact solution:

$$\int_0^4 e^x dx = e^4 - e^0 = 53.59815$$

Simpson's Rule with  $h = 2$

$$\int_0^4 e^x dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958.$$

The error is **3.17143** (5.92%).

Divide-and-Conquer: Simpson's Rule with  $h = 1$

$$\int_0^2 e^x dx + \int_2^4 e^x dx \approx \frac{1}{3}(e^0 + 4e^1 + e^2) + \frac{1}{3}(e^2 + 4e^3 + e^4) = 53.86385$$

The error is **0.26570**. (0.50%) Improvement by a factor of 10!

Composite-Romberg-Adaptive

— (3/31)

## Divide and Conquer with Simpson's Rule

2 of 3

The exact solution:

$$\int_0^4 e^x dx = e^4 - e^0 = 53.59815$$

Divide-and-Conquer: Simpson's Rule with  $h = 1/2$

$$\int_0^1 + \int_1^2 + \int_2^3 + \int_3^4 e^x dx \approx \frac{1}{6}(e^0 + 4e^{1/2} + e^1) + \frac{1}{6}(e^1 + 4e^{3/2} + e^2) \\ + \frac{1}{6}(e^2 + 4e^{5/2} + e^3) + \frac{1}{6}(e^3 + 4e^{7/2} + e^4) = 53.61622$$

The error has been reduced to **0.01807** (0.034%).

$h$	abs-error	err/h	err/h <sup>2</sup>	err/h <sup>3</sup>	err/h <sup>4</sup>
2	3.17143	1.585715	0.792857	0.396429	0.198214
1	0.26570	0.265700	0.265700	0.265700	0.265700
1/2	0.01807	0.036140	0.072280	0.144560	0.289120

Composite-Romberg-Adaptive

— (4/31)

Extending the table...

$h$	abs-error	$\text{err}/h$	$\text{err}/h^2$	$\text{err}/h^3$	$\text{err}/h^4$	$\text{err}/h^5$
2	3.171433	1.585716	0.792858	0.396429	<b>0.198215</b>	0.099107
1	0.265696	0.265696	0.265696	0.265696	<b>0.265696</b>	0.265696
1/2	0.018071	0.036142	0.072283	0.144566	<b>0.289132</b>	0.578264
1/4	0.001155	0.004618	0.018473	0.073892	<b>0.295566</b>	1.182266
1/8	0.000073	0.000580	0.004644	0.037152	<b>0.297215</b>	2.377716
1/16	0.000004	0.000072	0.001162	0.018601	<b>0.297629</b>	4.762065

Clearly, the  $\text{err}/h^4$  column seems to converge (to a non-zero constant) as  $h \searrow 0$ . The columns to the left seem to converge to zero, and the  $\text{err}/h^5$  column seems to grow.

This is **numerical evidence** that the composite Simpson's rule has a convergence rate of  $\mathcal{O}(h^4)$ . *But, isn't Simpson's rule 5th order???*

For an even integer  $n$ : Subdivide the interval  $[a, b]$  into  $n$  subintervals, and apply Simpson's rule on each consecutive pair of sub-intervals. With  $h = (b - a)/n$  and  $x_j = a + jh$ ,  $j = 0, 1, \dots, n$ , we have

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

$$= \sum_{j=1}^{n/2} \left\{ \frac{h}{3} \left[ f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j}) \right] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\},$$

for some  $\xi_j \in [x_{2j-2}, x_{2j}]$ , if  $f \in C^4[a, b]$ .

Since all the interior "even"  $x_{2j}$  points appear twice in the sum, we can simplify the expression a bit...

$$\int_a^b f(x) dx = \frac{h}{3} \left[ f(x_0) - f(x_n) + \sum_{j=1}^{n/2} \left[ 4f(x_{2j-1}) + 2f(x_{2j}) \right] \right]$$

$$- \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

The error term is:

$$E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j), \quad \xi_j \in [x_{2j-2}, x_{2j}]$$

If  $f \in C^4[a, b]$ , the **Extreme Value Theorem** implies that  $f^{(4)}$  assumes its max and min in  $[a, b]$ . Now, since

$$\min_{x \in [a, b]} f^{(4)}(x) \leq f^{(4)}(\xi_j) \leq \max_{x \in [a, b]} f^{(4)}(x),$$

$$\left[ \frac{n}{2} \right] \min_{x \in [a, b]} f^{(4)}(x) \leq \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \left[ \frac{n}{2} \right] \max_{x \in [a, b]} f^{(4)}(x),$$

$$\min_{x \in [a, b]} f^{(4)}(x) \leq \left[ \frac{2}{n} \right] \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \max_{x \in [a, b]} f^{(4)}(x),$$

By the **Intermediate Value Theorem**  $\exists \mu \in (a, b)$  so that

$$f^{(4)}(\mu) = \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \Leftrightarrow \frac{n}{2} f^{(4)}(\mu) = \sum_{j=1}^{n/2} f^{(4)}(\xi_j)$$

We can now rewrite the error term:

$$E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) = -\frac{h^5}{180} n f^{(4)}(\mu),$$

or, since  $h = (b - a)/n \Leftrightarrow n = (b - a)/h$ , we can write

$$E(f) = -\frac{(b - a)}{180} h^4 f^{(4)}(\mu).$$

Hence **Composite Simpson's Rule** has **degree of accuracy 3** (since it is exact for polynomials up to order 3), and the error is proportional to  $h^4$  — **Convergence Rate**  $\mathcal{O}(h^4)$ .

Theorem (Composite Simpson's Rule)

Let  $f \in C^4[a, b]$ ,  $n$  be even,  $h = (b - a)/n$ , and  $x_j = a + jh$ ,  $j = 0, 1, \dots, n$ . There exists  $\mu \in (a, b)$  for which the **Composite Simpson's Rule** for  $n$  subintervals can be written with its error term as

$$\int_a^b f(x) dx = \frac{h}{3} \left[ f(a) - f(b) + \sum_{j=1}^{n/2} [4f(x_{2j-1}) + 2f(x_{2j})] \right] - \frac{(b - a)}{180} h^4 f^{(4)}(\mu).$$

**Note:**  $x_0 = a$ , and  $x_n = b$ .

Algorithm (Composite Simpson's Rule)

Given the end points  $a$  and  $b$  and an even positive integer  $n$ :

- ```
[1]  h = (b - a)/n
[2]  ENDPNTS = f(a)+f(b)
      ODDPTS = 0
      EVENPTS = 0
[3]  FOR i = 1, ..., n - 1  — (interior points)
      x = a + i * h
      if i is even: EVENPTS += f(x)
      if i is odd:  ODDPTS  += f(x)
      END
[4]  INTAPPROX = h*(ENDPTS+2*EVENPTS+4*ODDPTS)/3
```

Romberg Integration is the combination of the **Composite Trapezoidal Rule** (CTR)

$$\int_a^b f(x) dx = \frac{h}{2} \left[ f(a) + f(b) + 2 \sum_{j=1}^{n-1} f(x_j) \right] - \frac{(b - a)}{12} h^2 f''(\mu)$$

and **Richardson Extrapolation**.

Here, we know that the error term for regular Trapezoidal Rule is  $\mathcal{O}(h^3)$ . By the same argument as for Composite Simpson's Rule, this gets reduced to  $\mathcal{O}(h^2)$  for the composite version.

Let  $R_{k,1}$  denote the Composite Trapezoidal Rule with  $2^{k-1}$  sub-intervals, and  $h_k = (b-a)/2^{k-1}$ . We get:

$$R_{1,1} = \frac{h_1}{2} [f(a) + f(b)]$$

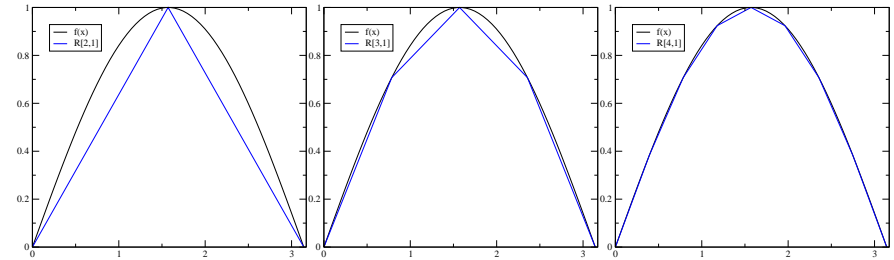
$$\begin{aligned} R_{2,1} &= \frac{h_2}{2} [f(a) + 2f(a+h_2) + f(b)] \\ &= \frac{(b-a)}{4} [f(a) + f(b) + 2f(a+h_2)] \\ &= \frac{1}{2} [R_{1,1} + h_1 f(a+h_2)] \end{aligned}$$

⋮

$$R_{k,1} = \frac{1}{2} \left[ R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k) \right]$$

Update formula, using previous value + new points

Example:  $R_{k,1}$  for  $\int_0^\pi \sin(x) dx$



| $k$ | $R_{k,1}$       |
|-----|-----------------|
| 1   | 0               |
| 2   | 1.5707963267949 |
| 3   | 1.8961188979370 |
| 4   | 1.9742316019455 |
| 5   | 1.9935703437723 |
| 6   | 1.9983933609701 |
| 7   | 1.9995983886400 |

Extrapolate using Richardson

We know that the error term is  $\mathcal{O}(h^2)$ , so in order to eliminate this term we combine consecutive entries  $R_{k-1,1}$  and  $R_{k,1}$  to form a higher order approximation  $R_{k,2}$  of the integral.

$$R_{k,2} = R_{k,1} + \frac{R_{k,1} - R_{k-1,1}}{2^2 - 1}$$

| $R_{k,1} - \mathcal{O}(h^2)$ | $R_{k,2}$     |
|------------------------------|---------------|
| 0                            | 0             |
| 1.5707963267949              | 2.09439510239 |
| 1.8961188979370              | 2.00455975498 |
| 1.9742316019455              | 2.00026916994 |
| 1.9935703437723              | 2.00001659104 |
| 1.9983933609701              | 2.00000103336 |
| 1.9995983886400              | 2.00000006453 |

Extrapolate, again...

It turns out [RALSTON-RABINOWITZ, 1978, pp. 136–140] that the complete error term for the Trapezoidal rule only has even powers of  $h$ :

$$\int_a^b f(x) = R_{k,1} - \sum_{i=1}^{\infty} E_{2i} h_k^{2i}.$$

Hence the  $R_{k,2}$  approximations have error terms that are of size  $\mathcal{O}(h^4)$ .

To get  $\mathcal{O}(h^6)$  approximations, we compute

$$R_{k,3} = R_{k,2} + \frac{R_{k,2} - R_{k-1,2}}{4^2 - 1}$$

Extrapolate, yet again...

In general, since we only have even powers of  $h$  in the error expansion:

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$$

Revisiting  $\int_0^\pi \sin(x) dx$ :

| $R_{k,1} - \mathcal{O}(h^2)$ | $R_{k,2} - \mathcal{O}(h^4)$ | $R_{k,3} - \mathcal{O}(h^6)$ | $R_{k,4} - \mathcal{O}(h^8)$ |
|------------------------------|------------------------------|------------------------------|------------------------------|
| 0                            |                              |                              |                              |
| 1.570796326794897            | 2.094395102393195            |                              |                              |
| 1.896118897937040            | 2.004559754984421            | 1.998570731823836            |                              |
| 1.974231601945551            | 2.000269169948388            | 1.999983130945986            | 2.000005549979671            |
| 1.993570343772340            | 2.000016591047935            | 1.999999752454572            | 2.000000016288042            |
| 1.998393360970145            | 2.000001033369413            | 1.999999996190845            | 2.000000000059674            |
| 1.999598388640037            | 2.000000064530001            | 1.99999999940707             | 2.000000000000229            |

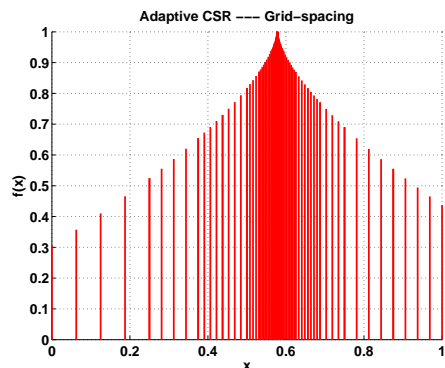
Code Outline for Romberg Quadrature (Example)

Code (Romberg Quadrature)

```
% Romberg Integration for sin(x) over [0,pi]
a = 0; b = pi; % The Endpoints
R = zeros(7,7);
R(1,1) = (b - a)/2 * (sin(a) + sin(b));
for k = 2 : 7
    h = (b - a)/2^(k-1);
    R(k,1) = 1/2 * (R(k-1,1) + 2 * h * sum(sin(a + (2 * (1 : (2^(k-2)) - 1) * h))));
end
for j = 2 : 7
    for k = j : 7
        R(k,j) = R(k,j-1) + (R(k,j-1) - R(k-1,j-1))/(4^(j-1) - 1);
    end
end
disp(R)
```

More Advanced Numerical Integration Ideas

### Adaptive

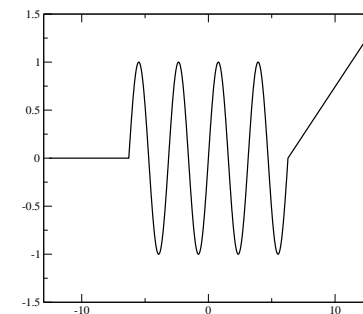


Introduction

Adaptive Quadrature

The **composite formulas** require **equally spaced nodes**.

This is not good if the function we are trying to integrate has both regions with large fluctuations, and regions with small variations.



We need many points where the function fluctuates, but few points where it is close to constant or linear.

**Idea** Cleverly predict (or measure) the amount of variation and automatically add more points where needed.

We are going to discuss this in the context of Composite Simpson's rule, but the approach can be adopted for other integration schemes.

**First** we are going to develop a way to **measure the error** — a numerical estimate of the actual error in the numerical integration. Note: just knowing the structure of the error term is not enough! (We will however use the structure of the error term in our derivation of the numerical error estimate.)

**Then** we will use the error estimate to decide whether to accept the value from CSR, or if we need to refine further (recompute with smaller  $h$ ).

**Notation — “One-step” Simpson's Rule:**

$$\int_a^b f(x) dx = S(f; a, b) - \underbrace{\frac{h_1^5}{90} f^{(4)}(\mu_1)}_{E(f; h_1, \mu_1)}, \quad \mu_1 \in (a, b),$$

where

$$S(f; a, b) = \frac{(b-a)}{6} \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right], \quad h_1 = \frac{(b-a)}{2}.$$

## Composite Simpson's Rule (CSR)

With this notation, we can write CSR with  $n = 4$ , and  $h_2 = (b-a)/4 = h_1/2$ :

$$\int_a^b f(x) dx = S(f; a, \frac{a+b}{2}) + S(f; \frac{a+b}{2}, b) - E(f; h_2, \mu_2).$$

We can squeeze out an estimate for the error by noticing that

$$E(f; h_2, \mu_2) = \frac{1}{16} \left( \frac{h_1^5}{90} f^{(4)}(\mu_2) \right) = \frac{1}{16} E(f; h_1, \mu_2).$$

Now, **assuming**  $f^{(4)}(\mu_1) \approx f^{(4)}(\mu_2)$ , we do a little bit of algebra magic with our two approximations to the integral...

Wait! Wait! Wait! — I pulled a fast one!

$$E(f; h_2, \mu_2) = \frac{1}{32} \left( \frac{h_1^5}{90} f^{(4)}(\mu_2^1) \right) + \frac{1}{32} \left( \frac{h_1^5}{90} f^{(4)}(\mu_2^2) \right)$$

where  $\mu_2^1 \in [a, \frac{a+b}{2}]$ ,  $\mu_2^2 \in [\frac{a+b}{2}, b]$ .

If  $f \in C^4[a, b]$ , then we can use our old friend, the **intermediate value theorem**:

$$\exists \mu_2 \in [\mu_2^1, \mu_2^2] \subset [a, b] : f^{(4)}(\mu_2) = \frac{f^{(4)}(\mu_2^1) + f^{(4)}(\mu_2^2)}{2}.$$

So it follows that

$$E(f; h_2, \mu_2) = \frac{1}{16} \left( \frac{h_1^5}{90} f^{(4)}(\mu_2) \right).$$

Back to the Error Estimate...

Now we have

$$S(f; a, \frac{a+b}{2}) + S(f; \frac{a+b}{2}, b) - \frac{1}{16} \left( \frac{h_1^5}{90} f^{(4)}(\mu_2) \right) \\ = S(f; a, b) - \frac{h_1^5}{90} f^{(4)}(\mu_1).$$

Now use the assumption  $f^{(4)}(\mu_1) \approx f^{(4)}(\mu_2)$  (and replace  $\mu_1$  and  $\mu_2$  by  $\mu$ ):

$$\frac{h_1^5}{90} f^{(4)}(\mu) \approx \frac{16}{15} \left[ S(f; a, b) - S(f; a, (a+b)/2) - S(f; (a+b)/2, b) \right],$$

notice that  $\frac{h_1^5}{90} f^{(4)}(\mu) = E(f; h_1, \mu) = 16E(f; h_2, \mu)$ . Hence

$$E(f; h_2, \mu) \approx \frac{1}{15} \left[ S(f; a, b) - S(f; a, (a+b)/2) - S(f; (a+b)/2, b) \right],$$

Finally, we have the error estimate in hand...

Using the estimate of  $\frac{h_1^5}{90} f^{(4)}(\mu)$ , we have

Error Estimate for CSR

$$\left| \int_a^b f(x) dx - S(f; a, (a+b)/2) - S(f; (a+b)/2, b) \right| \\ \approx \frac{1}{15} \left| S(f; a, b) - S(f; a, (a+b)/2) - S(f; (a+b)/2, b) \right|$$

**Notice!!!**  $S(f; a, (a+b)/2) + S(f; (a+b)/2, b)$  approximates  $\int_a^b f(x) dx$  **15 times better** than it agrees with the known quantity  $S(f; a, b)$ !!!

Example — Error Estimates

1 of 2

We will apply Simpson's rule to

$$\int_0^{\pi/2} \sin(x) dx = 1.$$

Here,

$$\mathbb{S}_1(\sin(x); 0, \pi/2) = S(\sin(x); 0, \pi/2) \\ = \frac{\pi}{12} \left[ \sin(0) + 4 \sin(\pi/4) + \sin(\pi/2) \right] = \frac{\pi}{12} \left[ 2\sqrt{2} + 1 \right] \\ = 1.00227987749221.$$

$$\mathbb{S}_2(\sin(x); 0, \pi/2) = S(\sin(x); 0, \pi/4) + S(\sin(x); \pi/4, \pi/2) \\ = \frac{\pi}{24} \left[ \sin(0) + 4 \sin(\pi/8) + 2 \sin(\pi/4) + 4 \sin(3\pi/8) + \sin(\pi/2) \right] \\ = 1.00013458497419.$$

Example — Error Estimates

2 of 2

The error estimate is given by

$$\frac{1}{15} \left[ \mathbb{S}_1(\sin(x); 0, \pi/2) - \mathbb{S}_2(\sin(x); 0, \pi/2) \right] \\ = \frac{1}{15} \left[ 1.00227987749221 - 1.00013458497419 \right] \\ = 0.00014301950120.$$

This is a very good approximation of the actual error, which is 0.00013458497419.

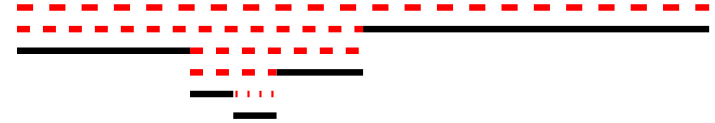
**OK, we know how to get an error estimate. How do we use this to create an adaptive integration scheme???**

## Adaptive Quadrature

We want to approximate  $\mathcal{I} = \int_a^b f(x) dx$  with an error less than  $\epsilon$  (a specified tolerance).

- [1] Compute the two approximations  $S_1(f(x); a, b) = S(f(x); a, b)$ , and  $S_2(f(x); a, b) = S(f(x); a, \frac{a+b}{2}) + S(f(x); \frac{a+b}{2}, b)$ .
- [2] Estimate the error, if the estimate is less than  $\epsilon$ , we are done. Otherwise...
- [3] Apply steps [1] and [2] recursively to the intervals  $[a, \frac{a+b}{2}]$  and  $[\frac{a+b}{2}, b]$  with tolerance  $\epsilon/2$ .

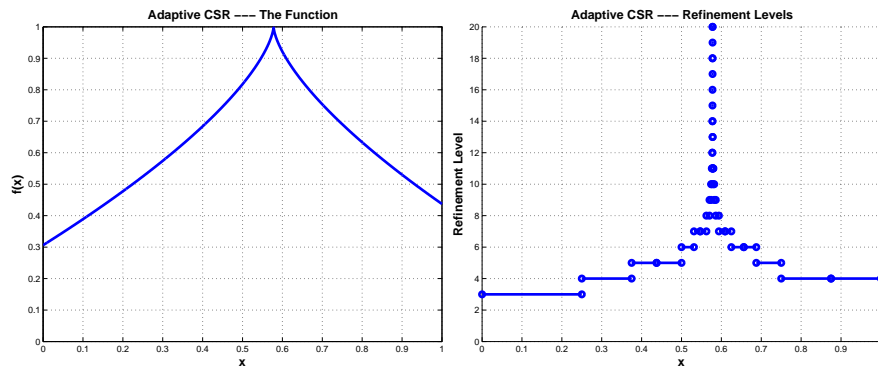
## Adaptive Quadrature, Interval Refinement Example #1



The funny figure above is supposed to illustrate a possible sub-interval refinement hierarchy. **Red** dashed lines illustrate failure to satisfy the tolerance, and **black** lines illustrate satisfied tolerance.

| level | tol          | interval                                                          |
|-------|--------------|-------------------------------------------------------------------|
| 1     | $\epsilon$   | $[a, b]$                                                          |
| 2     | $\epsilon/2$ | $[a, a + \frac{b-a}{2}]$ $[a + (b-a)/2, b]$                       |
| 3     | $\epsilon/4$ | $[a, a + \frac{b-a}{4}]$ $[a + \frac{b-a}{4}, a + \frac{b-a}{2}]$ |
| ⋮     |              |                                                                   |

## Adaptive Quadrature, Interval Refinement Example #2



**Figure:** Application of adaptive CSR to the function  $f(x) = 1 - 3\sqrt{(x - \frac{\pi}{2e})^2}$ . Here, we have required that the estimated error be less than  $10^{-6}$ . The left panel shows the function, and the right panel shows the number of refinement levels needed to reach the desired accuracy. At completion we have the value of the integral being  $0.61692712$ , with an estimated error of  $3.93 \cdot 10^{-7}$ .