Numerical Analysis and Computing

Lecture Notes #8

— Numerical Differentiation and Integration —

Composite Numerical Integration; Romberg Integration

Adaptive Quadrature

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Outline

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 $\mathbf{3.17143}$ (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 $\mathbf{0.26570}$. (0.50%) Improvement by a factor of 10!

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^2	err/h^3	err/h^4
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

Extending the table...

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

Clearly, the **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 err/h^5 column seems to grow.

This is **numerical evidence** that the composite Simpson's rule has a convergence rate of $\mathcal{O}\left(h^4\right)$. *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 $x_j = a + jh$, $j = 0, 1, \ldots, n$, we have

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

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

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

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

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

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

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

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

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

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 $\mathbf{h^4}$ — **Convergence Rate** $\mathcal{O}\left(h^4\right)$.

Composite Simpson's Rule — Summary

Theorem (Composite Simpson's Rule)

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

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

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

Composite Simpson's Rule — Algorithm

Algorithm (Composite Simpson's Rule)

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

[1] $h = (b - a)/n$

[2] `ENDPTS = f(a)+f(b)`
`ODDPTS = 0`
`EVENPTS = 0`

[3] `FOR` $i = 1, \ldots, n-1$ — (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)

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

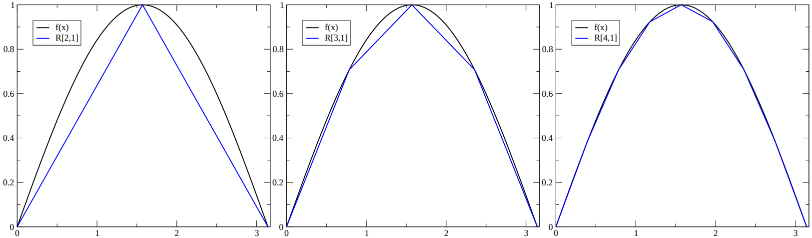
and **Richardson Extrapolation**.

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 $\mathcal{O}(\mathbf{h^2})$ 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:

$$
\begin{aligned}
R_{1,1} &= \tfrac{h_1}{2}\left[f(a)+f(b)\right] \\
R_{2,1} &= \tfrac{h_2}{2}\left[f(a)+2f(a+h_2)+f(b)\right] \\
&= \tfrac{(b-a)}{4}\left[f(a)+f(b)+2f(a+h_2)\right] \\
&= \tfrac{1}{2}\left[R_{1,1}+h_1 f(a+h_2)\right] \\
&\vdots \\
R_{k,1} &= \underbrace{\frac{1}{2}\left[R_{k-1,1}+h_{k-1}\sum_{i=1}^{2^{k-2}} f(a+(2i-1)h_k)\right]}_{\textbf{Update formula, using previous value + new points}}
\end{aligned}
$$

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 to consecutive entries $R_{k-1,1}$ and $R_{k,1}$ to form a higher order approximation $R_{k,2}$ of the integral.

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

$R_{k,1}$ — $\mathcal{O}\left(h^2\right)$	$R_{k,2}$
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 $\mathcal{O}(\mathbf{h^4})$.

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

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

Extrapolate, yet again...

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

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

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

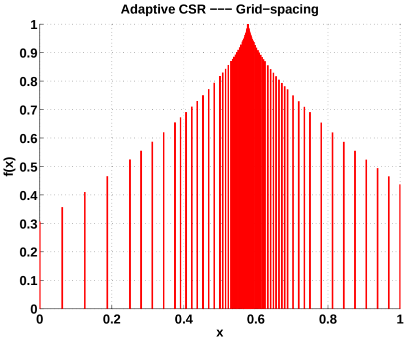
$R_{k,1}$ — $\mathcal{O}\left(h^2\right)$	$R_{k,2}$ — $\mathcal{O}\left(h^4\right)$	$R_{k,3}$ — $\mathcal{O}\left(h^6\right)$	$R_{k,4}$ — $\mathcal{O}\left(h^8\right)$
0			
1.570796326794897	2.094395102393195		
1.896118897937040	2.004559754984421	1.998570731823836	
1.974231601945551	2.000269169948388	1.999983130945986	2.000005549979671
1.993570343772340	2.000016591047935	1.999999752454572	2.000000016288042
1.998393360970145	2.000001033369413	1.999999996190845	2.000000000059674
1.999598388640037	2.000000064530001	1.999999999940707	2.000000000000229

Code Outline for Romberg Quadrature (Example)

Code (Romberg Quadrature)

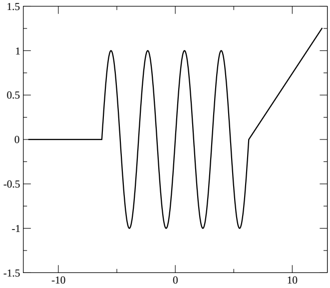
```
% Romberg Integration for sin(x) over [0,pi]
a = 0; b = pi; % The Endpoints
R = zeros(7,7);
R(1,1) = (b - a)/2 * (sin(a) + sin(b));
for k = 2 : 7
  h = (b - a)/2^(k-1);
  R(k,1)=1/2 * (R(k - 1, 1) + 2 * h * ∑(sin(a + (2 * (1 : (2^(k-2))) - 1) * h)));
end
for j = 2 : 7
  for k = j : 7
   R(k,j) =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

Adaptive


Adaptive CSR --- Grid−spacing
f(x)
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.2
0.4
0.6
0.8
1

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:

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

where

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

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

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

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

$$E(f; h_2, \mu_2) = \frac{1}{16}\left(\frac{h_1^5}{90} f^{(4)}(\mu_2)\right) = \frac{1}{16} E(f; h_1, \mu_{\mathbf{2}}).$$

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

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

Now use the assumption $f^{(4)}(\mu_1) \approx f^{(4)}(\mu_2)$ (and replace μ_1 and μ_2 by μ):

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

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

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

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

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

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 $S(f;\, a, b)$!!!

We will apply Simpson's rule to

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

Here,

$$\mathbb{S}_1(\sin(x);\, 0, \pi/2) = S(\sin(x);\, 0, \pi/2)$$

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

$$\mathbb{S}_2(\sin(x);\, 0, \pi/2) = S(\sin(x);\, 0, \pi/4) + S(\sin(x);\, \pi/4, \pi/2)$$

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

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???

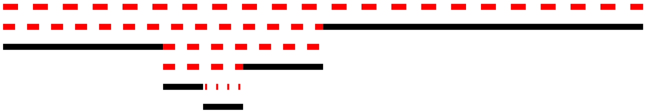
We want to approximate $\mathcal{I} = \int_a^b f(x)\,dx$ with an error less than ϵ (a specified tolerance).

[1] Compute the two approximations
$\mathbb{S}_1(f(x);\, a, b) = S(f(x);\, a, b)$, and
$\mathbb{S}_2(f(x);\, a, b) = S(f(x);\, a, \frac{a+b}{2}) + S(f(x);\, \frac{a+b}{2}, b)$.

[2] Estimate the error, if the estimate is less than ϵ, 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	ϵ	$[\mathbf{a}, \mathbf{b}]$
2	$\epsilon/2$	$[\mathbf{a}, \mathbf{a} + \frac{\mathbf{b}-\mathbf{a}}{2}]$ $\quad$ $[\mathbf{a} + (\mathbf{b} - \mathbf{a})/2, \mathbf{b}]$
3	$\epsilon/4$	$[\mathbf{a}, \mathbf{a} + \frac{\mathbf{b}-\mathbf{a}}{4}]$ $\quad$ $[\mathbf{a} + \frac{\mathbf{b}-\mathbf{a}}{4}, \mathbf{a} + \frac{\mathbf{b}-\mathbf{a}}{2}]$
$\vdots$		

Adaptive Quadrature, Interval Refinement Example #2

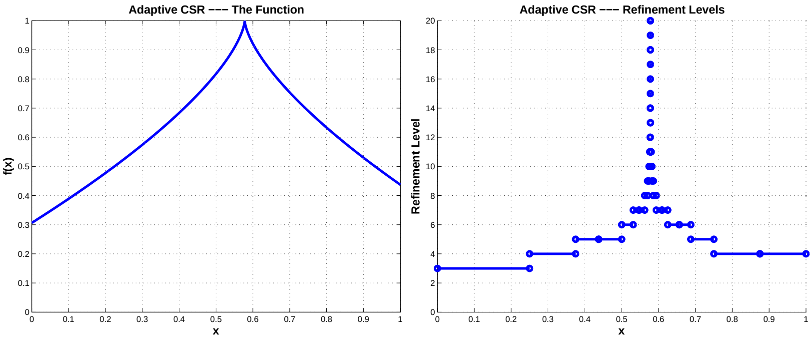


Figure: Application of adaptive CSR to the function $f(x) = 1 - \sqrt[3]{(x - \frac{\pi}{2e})^2}$. Here, we have required that the estimated error be less than 10^{-6}. The left panel shows the function, and the right panel shows the number of refinement levels needed to reach the desired accuracy. At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