CMPSC/Math 451, Numerical Computation

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Trapezoid Rule : $$\int_a^b f(x)\,dx \approx h\left[\frac{1}{2}f(x_0) + \sum_{i=1}^{n-1} f(x_i) + \frac{1}{2}f(x_n)\right]$$

Example 1: Let $f(x) = \sqrt{x^2+1}$, compute $I = \int_{-1}^{1} f(x)\,dx$ by Trapezoid rule with $n = 10$.

Answer. We can set up the data

i	x_i	f_i
0	-1	1.4142136
1	-0.8	1.2806248
2	-0.6	1.1661904
3	-0.4	1.077033
4	-0.2	1.0198039
5	0	1.0
6	0.2	1.0198039
7	0.4	1.077033
8	0.6	1.1661904
9	0.8	1.2806248
10	1	1.4142136

Here $h = 2/10 = 0.2$.

By the formula, we get

$$T = h\left[(f_0 + f_{10})/2 + \sum_{i=1}^{9} f_i\right] = 2.3003035.$$

Sample codes for Trapezoid Rule in Matlab.

Let $f(x) = x^2 + \sin(x)$. It cam be defined in file "`func.m`" as:

```
function v=func(x)
    v=x.^2 + sin(x);
end
```

In the following script, the integral value is stored in the variable '`T`'.

```
h=(b-a)/n;  x=[a:h:b];
T = (func(a)+func(b))/2;
for i=2:1:n,  T = T + func(x(i)); end
T = T*h;
```

Or, one may use directly the Matlab vector function '`sum`', and the code could be very short:

```
h=(b-a)/n;
x=[a+h:h:b-h]; % inner points
T = ((func(a)+func(b))/2 + sum(func(x)))*h;
```

Numerical integration: Introduction

Problem Description:
Given a function $f(x)$, defined on an interval $[a, b]$, we want to find an approximation to the integral

$$I(f) = \int_a^b f(x)\, dx\,.$$

Main ideas:

- Cut up $[a, b]$ into smaller sub-intervals;
- In each sub-interval, find a polynomial $p_i(x) \approx f(x)$;
- Integrate $p_i(x)$ on each sub-interval, and sum them up.

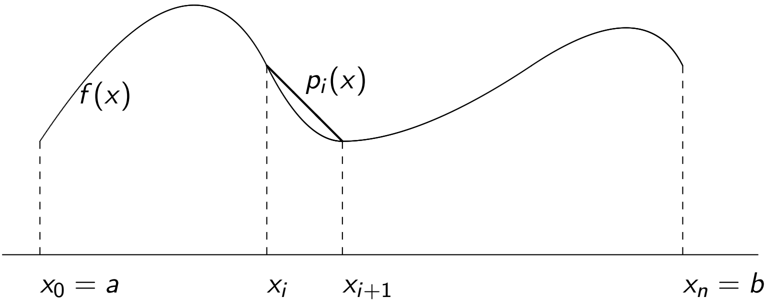
Trapezoid rule

The grid: We cut up $[a, b]$ into n sub-intervals:

$$x_0 = a, \quad x_i < x_{i+1}, \quad x_n = b$$

On $[x_i, x_{i+1}]$, approximate $f(x)$ by a linear polynomial p_i:

$$p_i(x_i) = f(x_i), \qquad p_i(x_{i+1}) = f(x_{i+1}).$$



On each sub-interval, the integral of p_i equals to the area of a trapezium:

$$\int_{x_i}^{x_{i+1}} p_i(x)\,dx = \frac{1}{2}(f(x_i) + f(x_{i+1}))(x_{i+1} - x_i).$$

Now, we use

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \approx \int_{x_i}^{x_{i+1}} p_i(x)\,dx = \frac{1}{2}\left(f(x_{i+1}) + f(x_i)\right)\left(x_{i+1} - x_i\right),$$

and we sum up all the sub-intervals

$$\begin{aligned}\int_a^b f(x)\,dx &= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\,dx \approx \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} p_i(x)\,dx \\ &= \sum_{i=0}^{n-1} \frac{1}{2}\left(f(x_{i+1}) + f(x_i)\right)\left(x_{i+1} - x_i\right)\end{aligned}$$

Uniform Grid

$$h = \frac{b-a}{n}, \qquad x_{i+1} - x_i = h.$$

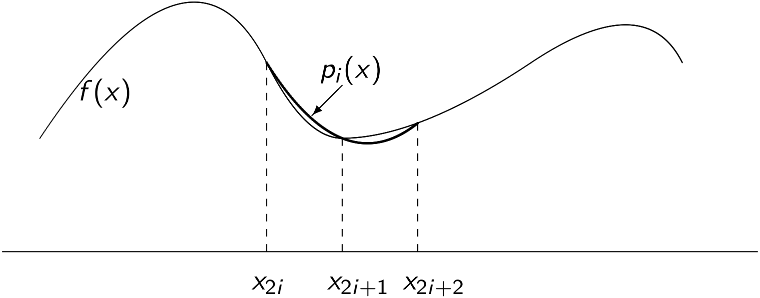
$$\begin{aligned}
\int_a^b f(x)\,dx &\approx \sum_{i=0}^{n-1} \frac{h}{2}\left(f(x_i) + f(x_{i+1})\right) \\
&= \frac{h}{2}\left[(f(x_0)+f(x_1)) + (f(x_1)+f(x_2)) + \cdots + (f(x_{n-1})+f(x_n))\right] \\
&= \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right] \\
&= \underbrace{h\left[\frac{1}{2}(f(x_0)+f(x_n)) + \sum_{i=1}^{n-1} f(x_i)\right]}_{T(f;h)}
\end{aligned}$$

Simpson's rule

We now explorer possibility of using higher order polynomials.
We cut up $[a, b]$ into $2n$ equal sub-intervals

$$x_0 = a, \quad x_{2n} = b, \quad h = \frac{b-a}{2n}, \quad x_{i+1} - x_i = h$$

On $[x_{2i}, x_{2i+2}]$, interpolates $f(x)$ at the points $x_{2i}, x_{2i+1}, x_{2i+2}$ with a quadratic polynomial $p_i(x)$.



Note that in each sub-interval there is a point in the interior.

Lagrange form for $p_i(x)$:

$$\begin{aligned} p_i(x) &= f(x_{2i})\frac{(x-x_{2i+1})(x-x_{2i+2})}{(x_{2i}-x_{2i+1})(x_{2i}-x_{2i+2})} + f(x_{2i+1})\frac{(x-x_{2i})(x-x_{2i+2})}{(x_{2i+1}-x_{2i})(x_{2i+1}-x_{2i+2})} \\ &\quad + f(x_{2i+2})\frac{(x-x_{2i})(x-x_{2i+1})}{(x_{2i+2}-x_{2i})(x_{2i+2}-x_{2i+1})} \end{aligned}$$

With uniform nodes, this becomes

$$\begin{aligned} p_i(x) &= \frac{1}{2h^2} f(x_{2i})(x-x_{2i+1})(x-x_{2i+2}) - \frac{1}{h^2} f(x_{2i+1})(x-x_{2i})(x-x_{2i+2}) \\ &\quad + \frac{1}{2h^2} f(x_{2i+2})(x-x_{2i})(x-x_{2i+1}) \end{aligned}$$

We work out the integrals (try to fill in the details yourself!)

$$
\begin{aligned}
I_1 &= \int_{x_{2i}}^{x_{2i+2}} (x - x_{2i+1})(x - x_{2i+2})\, dx = \frac{2}{3} h^3, \\
I_2 &= \int_{x_{2i}}^{x_{2i+2}} -(x - x_{2i})(x - x_{2i+2})\, dx = \frac{4}{3} h^3, \\
I_3 &= \int_{x_{2i}}^{x_{2i+2}} (x - x_{2i})(x - x_{2i+1})\, dx = \frac{2}{3} h^3,
\end{aligned}
$$

Then

$$
\begin{aligned}
\int_{x_{2i}}^{x_{2i+2}} p_i(x)\, dx &= \frac{1}{2h^2} f(x_{2i}) \cdot I_1 + \frac{1}{h^2} f(x_{2i+1}) \cdot I_2 + \frac{1}{2h^2} f(x_{2i+2}) \cdot I_3 \\
&= \frac{1}{2h^2} f(x_{2i}) \frac{2}{3} h^3 + \frac{1}{h^2} f(x_{2i+1}) \frac{4}{3} h^3 + \frac{1}{2h^2} f(x_{2i+2}) \frac{2}{3} h^3 \\
&= \frac{h}{3} \left[f(x_{2i}) + 4 f(x_{2i+1}) + f(x_{2i+2}) \right] .
\end{aligned}
$$

We now sum them up

$$
\begin{aligned}
\int_a^b f(x)\,dx \quad \approx \quad S(f;h) \;&=\; \sum_{i=0}^{n-1} \int_{x_{2i}}^{x_{2i+2}} p_i(x)\,dx \\
&=\; \frac{h}{3} \sum_{i=0}^{n-1} \left[f(x_{2i}) + 4f(x_{2i+1}) + f(x_{2i+2}) \right].
\end{aligned}
$$

$$
\begin{array}{ccccc}
 & & \boxed{\begin{array}{c}1\\1\end{array}} = 2 & 4 & 1 \\
1 & 4 & & & \\
\hline
x_{2i-2} & x_{2i-1} & x_{2i} & x_{2i+1} & x_{2i+2}
\end{array}
$$

Simpson's Rule:

$$
S(f;h) = \frac{h}{3} \left[f(x_0) + 4\sum_{i=1}^{n} f(x_{2i-1}) + 2\sum_{i=1}^{n-1} f(x_{2i}) + f(x_{2n}) \right]
$$

Error estimates for Trapezoid rule.

We define the error:

$$E_T(f;h) \doteq I(f) - T(f;h) = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} [f(x) - p_i(x)]\, dx = \sum_{i=0}^{n-1} E_{T,i}(f;h),$$

where $E_{T,i}(f;h)$ is the error on each sub-interval

$$E_{T,i}(f;h) = \int_{x_i}^{x_{i+1}} [f(x) - p_i(x)]\, dx, \qquad (i = 0, 1, \cdots, n-1)$$

Error bound with polynomial interpolation:

$$f(x) - p_i(x) = \frac{1}{2} f''(\xi_i)(x - x_i)(x - x_{i+1}), \qquad (x_i < \xi_i < x_{i+1})$$

Error estimate on each sub-interval:

$$E_{T,i}(f;h) \;=\; \frac{1}{2} f''(\xi_i) \int_{x_i}^{x_{i+1}} (x - x_i)(x - x_{i+1})\, dx \;=\; -\frac{1}{12} h^3 f''(\xi_i).$$

(You may work out the details of the integral!)

The total error is:

$$
\begin{aligned}
E_T(f;h) &= \sum_{i=0}^{n-1} E_{T,i}(f;h) = \sum_{i=0}^{n-1} -\frac{1}{12}h^3 f''(\xi_i) \\
&= -\frac{1}{12}h^3 \underbrace{\left[\sum_{i=0}^{n-1} f''(\xi_i)\right] \cdot \frac{1}{n}}_{=f''(\xi)} \cdot \underbrace{\frac{b-a}{h}}_{=n}
\end{aligned}
$$

which gives

$$
E_T(f;h) = -\frac{b-a}{12}h^2 f''(\xi), \qquad \xi \in (a,b).
$$

Error bound

$$
|E_T(f;h)| \le \frac{b-a}{12}h^2 \max_{x\in(a,b)} \left|f''(x)\right| .
$$

Example 2. Consider function $f(x) = e^x$, and the integral $I(f) = \int_0^2 e^x\,dx$. What is the minimum number of points to be used in the trapezoid rule to ensure en error $\le 0.5 \times 10^{-4}$?

Answer. We have

$$f'(x) = e^x, \quad f''(x) = e^x, \quad a = 0, \quad b = 2, \qquad \max_{x \in (a,b)} \left| f''(x) \right| = e^2.$$

By error bound, it is sufficient to require

$$\begin{aligned} & |E_T(f;h)| \le \frac{1}{6} h^2 e^2 \le 0.5 \times 10^{-4} \\ \Rightarrow \quad & h^2 \le 0.5 \times 10^{-4} \times 6 \times e^{-2} \approx 4.06 \times 10^{-5} \\ \Rightarrow \quad & \frac{2}{n} = h \le \sqrt{4.06 \times 10^{-5}} = 0.0064 \\ \Rightarrow \quad & n \ge \frac{2}{0.0064} \approx 313.8 \end{aligned}$$

We need at least 314 points.

Romberg Algorithm

Given $T(f;h)$, $T(f;h/2)$, compute

$$U(h) = T(f;h/2) + \frac{T(f;h/2) - T(f;h)}{2^2 - 1}$$

then

$$I(f) = U(h) + \tilde{a}_4 h^4 + \tilde{a}_6 h^6 + \cdots$$

We can iterate this idea. Assume we have computed $U(h), U(h/2)$,

$$\begin{aligned} (3) \quad I(f) &= U(h) + \tilde{a}_4 h^4 + \tilde{a}_6 h^6 + \cdots \\ (4) \quad I(f) &= U(h/2) + \tilde{a}_4 (h/2)^4 + \tilde{a}_6 (h/2)^6 + \cdots \end{aligned}$$

Cancel the leading error term: $(4) \times 2^4 - (3)$

$$(2^4 - 1) I(f) = 2^4 U(h/2) - U(h) + \tilde{a}_6' h^6 + \cdots$$

Let

$$V(h) = \frac{2^4 U(h/2) - U(h)}{2^4 - 1} = U(h/2) + \frac{U(h/2) - U(h)}{2^4 - 1}.$$

Then

$$I(f) = V(h) + \tilde{a}_6' h^6 + \cdots \qquad \text{6th order approximation}$$

So $V(h)$ is even better than $U(h)$.

One can keep doing this several layers, until desired accuracy is reached.

This gives the **Romberg Algorithm**

Romberg Algorithm

Set $H = b - a$, define:

$$
\begin{aligned}
R(0,0) &= T(f;H) = \frac{H}{2}(f(a) + f(b)) \\
R(1,0) &= T(f;H/2) \\
R(2,0) &= T(f;H/(2^2)) \\
&\vdots \\
R(n,0) &= T(f;H/(2^n))
\end{aligned}
$$

Romberg triangle

$$
\begin{tikzcd}
R(0,0) \arrow[dr] & & & & \\
R(1,0) \arrow[r] \arrow[dr] & R(1,1) \arrow[dr] & & & \\
R(2,0) \arrow[r] \arrow[dr] & R(2,1) \arrow[r] \arrow[dr] & R(2,2) \arrow[dr] & & \\
R(3,0) \arrow[r] \arrow[d, dash, dashed] & R(3,1) \arrow[r] \arrow[d, dash, dashed] & R(3,2) \arrow[r] \arrow[d, dash, dashed] & {} & \\
R(n,0) & R(n,1) & R(n,3) \arrow[rr, dash, dashed] & & R(n,n)
\end{tikzcd}
$$

The entry $R(n, m)$ is computed as

$$R(n, m) = R(n, m-1) + \frac{R(n, m-1) - R(n-1, m-1)}{2^{2m} - 1}$$

Accuracy:

$$I(f) = R(n, m) + \mathcal{O}(h^{2(m+1)}), \qquad h = \frac{H}{2^m}.$$

Algorithm can be done either column-by-column or row-by-row.

Romberg algorithm pseudo-code, using column-by-column

$R =$romberg(f, a, b, n)

$R = n \times n$ matrix

$h = b - a$; $R(1,1) = [f(a) + f(b)] * h/2$;

for $i = 1$ to $n - 1$ do   % 1st column recursive trapezoid

$R(i+1,1) = R(i,1)/2$; $h = h/2$;

for $k = 1$ to 2^{i-1} do

$R(i+1,1) = R(i+1,1) + h * f(a + (2k-1)h)$

end

end

for $j = 2$ to n do   % 2 to n column

for $i = j$ to n do

$R(i,j) = R(i,j-1) + \frac{1}{4^{j-1}-1}\left[R(i,j-1) - R(i-1,j-1)\right]$

end

end

Richardson Extrapolation

Given $T(f;h), T(f;h/2), T(f;h/4), \cdots$, a sequence of approximations by Trapezoid rule with different values of h.

Idea: One could combine these numbers in particular ways to get much higher order approximations.

The particular form of the eventual algorithm depends on the detailed error formula.

One can show: If $f^{(n)}$ exists and is bounded, the error for trapezoid rule satisfies the Euler MacLaurin's formula

$$E(f;h) = I(f) - T(f;h) = a_2 h^2 + a_4 h^4 + a_6 h^6 + \cdots + a_n h^n$$

Here a_n depends on the derivatives $f^{(n)}$.

Proof can be achieved by Talor series.

Error formula: $E(f;h) = I(f) - T(f;h) = a_2h^2 + a_4h^4 + a_6h^6 + \cdots + a_nh^n$

When we half the grid size h, the error formula becomes

$$E(f;\frac{h}{2}) = I(f) - T(f;\frac{h}{2}) = a_2(\frac{h}{2})^2 + a_4(\frac{h}{2})^4 + a_6(\frac{h}{2})^6 + \cdots + a_n(\frac{h}{2})^n$$

$$\begin{aligned}
(1) \quad I(f) &= T(f;h) + a_2h^2 + a_4h^4 + a_6h^6 + \cdots \\
(2) \quad I(f) &= T(f;\frac{h}{2}) + a_2(\frac{h}{2})^2 + a_4(\frac{h}{2})^4 + a_6(\frac{h}{2})^6 + \cdots + a_n(\frac{h}{2})^n
\end{aligned}$$

The goal: cancel the leading error term to get a higher order approximation. Multiplying (2) by 2^2 and subtract (1), we get

$$\begin{aligned}
(2^2 - 1) \cdot I(f) &= 2^2 \cdot T(f;h/2) - T(f;h) + a_4'h^4 + a_6'h^6 + \cdots \\
\Rightarrow I(f) &= \underbrace{\frac{4}{3}T(f;h/2) - \frac{1}{3}T(f;h)}_{U(h)} + \tilde{a}_4h^4 + \tilde{a}_6h^6 + \cdots
\end{aligned}$$

A 4th order approximation:

$$U(h) = \frac{4}{3} T(f; h/2) - \frac{1}{3} T(f; h) = \frac{2^2 T(f; h/2) - T(f; h)}{2^2 - 1}$$

This idea is called the *Richardson extrapolation*.

We do not have to stop here. One can go into many levels of this manipulation! $\Rightarrow$ Romberg Algorithm

Simpson's Rule: $$S(f;h) = \frac{h}{3}\left[f(x_0) + 4\sum_{i=1}^{n} f(x_{2i-1}) + 2\sum_{i=1}^{n-1} f(x_{2i}) + f(x_{2n})\right]$$

Example 3: Let $f(x) = \sqrt{x^2+1}$, and compute $I = \int_{-1}^{1} f(x)\,dx$ by Simpson's rule with $n = 5$, i.e. with $2n+1 = 11$ points.

Answer. We can set up the data (same as in Example 1):

i	x_i	f_i
0	-1	1.4142136
1	-0.8	1.2806248
2	-0.6	1.1661904
3	-0.4	1.077033
4	-0.2	1.0198039
5	0	1.0
6	0.2	1.0198039
7	0.4	1.077033
8	0.6	1.1661904
9	0.8	1.2806248
10	1	1.4142136

Here $h = 2/10 = 0.2$.

$$\begin{aligned} S(f;0.2) &= \frac{h}{3}[f_0 + 4(f_1 + f_3 + f_5 + f_7 + f_9) \\ &\quad +2(f_2 + f_4 + f_6 + f_8) + f_{10}] \\ &= 2.2955778. \end{aligned}$$

Question to ponder:
This value is somewhat smaller than the number we get with trapezoid rule, and it is actually more accurate. Could you intuitively explain that for this particular example?

Sample codes: Let a, b, n be given, and let the function 'func' be defined.

To find the integral with Simpson's rule, one could possibly follow the following algorithm:

```
h=(b-a)/2/n;
xodd=[a+h:2*h:b-h]; % x_i with odd indices
xeven=[a+2*h:2*h:b-2*h];  % x_i with even indices
S=(h/3)*(func(a)+4*sum(func(xodd))+2*sum(func(xeven))+func(b));
```

Error Estimate for Simpson's Rule.

The basic error on each sub-interval is

$$E_{S,i}(f;h) = -\frac{1}{90}h^5 f^{(4)}(\xi_i), \qquad \xi_i \in (x_{2i}, x_{2i+2}). \tag{1}$$

(See lecture notes or textbook for the proof.)
Then, the total error is

$$E_S(f;h) = I(f) - S(f;h) = -\frac{1}{90}h^5 \sum_{i=0}^{n-1} f^{(4)}(\xi_i)\frac{1}{n}\cdot\frac{b-a}{2h} = -\frac{b-a}{180}h^4 f^{(4)}(\xi),$$

This gives us the error bound

$$|E_S(f;h)| \le \frac{b-a}{180}h^4 \max_{x\in(a,b)} \left| f^{(4)}(x) \right|.$$

Example 4. With $f(x) = e^x$ defined on $[0, 2]$, use Simpson's rule to compute $\int_0^2 f(x)\,dx$. In order to achieve an error $\leq 0.5 \times 10^{-4}$, how many points must we take?

Answer. We have

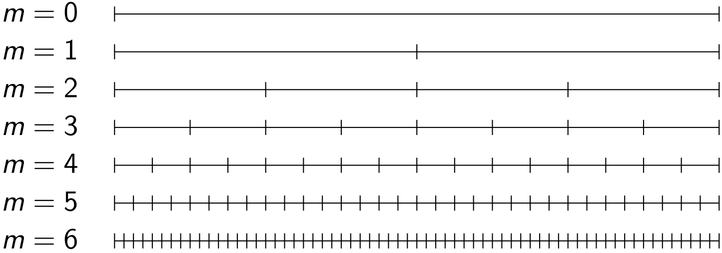
$$\begin{aligned} |E_S(f;h)| &\leq \frac{2}{180} h^4 e^2 \leq 0.5 \times 10^{-4} \\ \Rightarrow \quad & h^4 \leq 45/e^2 \times 10^{-4} \times = 6.09 \times 10^{-4} \\ \Rightarrow \quad & h \leq 0.1571 \\ \Rightarrow \quad & n = \frac{b-a}{2h} = 6.36 \approx 7 \end{aligned}$$

We need at least $2n + 1 = 15$ points.

Recall: With trapezoid rule, we need at least 314 points. The Simpson's rule uses much fewer points.

Recursive trapezoid rule; composite schemes

Divide $[a, b]$ into 2^m equal sub-intervals.



$$h_m = \frac{b-a}{2^m}, \qquad h_{m+1} = \frac{1}{2} h_m$$

Trapezoid rule:

$$
\begin{aligned}
T(f;h_m) &= h_m \cdot \left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{i=1}^{2^m-1} f(a+ih_m)\right] \\
T(f;h_{m+1}) &= h_{m+1} \cdot \left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{i=1}^{2^{m+1}-1} f(a+ih_{m+1})\right]
\end{aligned}
$$

We can re-arrange the terms in $T(f;h_{m+1})$:

$$
\begin{aligned}
T(f;h_{m+1}) &= \frac{h_m}{2}\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{i=1}^{2^m-1} f(a+ih_m) \right. \\
&\qquad \left. + \sum_{i=0}^{2^m-1} f(a+(2i+1)h_{m+1})\right] \\
&= \frac{1}{2}T(f;h_m) + h_{m+1}\sum_{i=0}^{2^m-1} f(a+(2i+1)h_{m+1})
\end{aligned}
$$

Advantages:

1. One can keep the computation for a level m. If this turns out to be not accurate enough, then add one more level to get better approximation. $\Rightarrow$ flexibility.
2. This formula allows us to compute a sequence of approximations to a define integral using the trapezoid rule without re-evaluating the integrand at points where it has already been evaluated. $\Rightarrow$ efficiency.

Question: A similar recursive algorithm could be defined using Simpson's rule. Would you like to try it?

Useful for the next topic: Romberg Algorithm.