Numerical Integration

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Consider a function $f(x)$ for which $\int_a^b f(x)dx$ is to be found numerically. Either the function $f(x)$ will be given explicitly or the function will be given at some tabular points, say $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$, where $y_j = f(x_j)$. If the function is given explicitly, divide the interval $[a, b]$ into n parts with a spacing h. For this, take $h = \frac{b-a}{n}$. Now define $x_0 = a, x_1 = x_0 + h, x_0 + 2h, \ldots, x_0 + nh = b$ and $y_j = f(x_j)$.

1 Newton-Cote's Formula

Recall the newtons forward interpolation formula for $f(x)$:

$$f(x) \approx y_0 + \frac{\Delta y_0}{1!}u + \frac{\Delta^2 y_0}{2!}u(u-1) + \frac{\Delta^3 y_0}{3!}u(u-1)(u-2) + \ldots,$$

where $u = \frac{x-x_0}{h}$ and $h = \frac{b-a}{n}$, the spacing.

We need to find $\int_{x_0}^{x_n} f(x)dx$. Note that when x moves from x_0 to x_n, u moves from 0 to n. Also $dx = h\,du$. Thus $\int_{x_0}^{x_n} f(x)dx = \int_0^n f(x_0 + uh)hdu$ and so

$$\begin{aligned}
\int_{x_0}^{x_n} f(x)dx &= \int_0^n (y_0 + \frac{\Delta y_0}{1!}u + \frac{\Delta^2 y_0}{2!}u(u-1) + \frac{\Delta^3 y_0}{3!}u(u-1)(u-2) + \ldots)hdu \\
&= h\left(y_0 u + \frac{\Delta y_0}{1!}\frac{u^2}{2} + \frac{\Delta^2 y_0}{2!}(\frac{u^3}{3} - \frac{u^2}{2}) + \ldots\right)_0^n. \\
&= nh\left(y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \ldots\right).
\end{aligned}$$

This is called the Newton-Cote's formula. For any fixed n, we develop a method for integration.

1.1 Trapezoidal Rule

Taking $n = 1$ in Newton-Cote's formula, we get

$$\begin{aligned}
\int_{x_0}^{x_1} f(x)dx &= h(y_0 + \frac{1}{2}\Delta y_0) \\
&= \frac{h}{2}(2y_0 + (y_1 - y_0)) \\
&= \frac{h}{2}(y_0 + y_1) \\
&= \text{area of a trapezoid having heights } y_0 \text{ and } y_1 \text{ and width } h
\end{aligned}$$

Similarly

$$\begin{aligned}
\int_{x_1}^{x_2} f(x)dx &= \frac{h}{2}(y_1 + y_2) \\
\cdots\cdots & \quad \cdots\cdots \\
\int_{x_{n-1}}^{x_n} f(x)dx &= \frac{h}{2}(y_{n-1} + y_n)
\end{aligned}$$

Hence

$$\begin{aligned}
\int_{x_0}^{x_n} f(x)dx &= \frac{h}{2}(y_0 + y_1 + y_1 + y_2 + y_2 + y_3 + \ldots + y_{n-1} + y_n) \\
&= \frac{h}{2}(y_0 + 2(y_1 + y_2 + y_3 + \ldots + y_{n-1}) + y_n)
\end{aligned}$$

Procedure:

- If $f(x)$ is given explicitly, then divide the given interval $[a,b]$ to n equal parts, taking $h=\frac{b-a}{n}$. Call $x_0=a, x_1=x_0+h, x_2=x_0+2h, \ldots, x_n=x_0+nh$. Find the corresponding images $y_0, y_1, \ldots, y_n$.

  $*$ If $f(x)$ is given as data points, then no need of this step; just find h.

- Use $\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx = \frac{h}{2}\left(y_0 + 2[y_1+y_2+y_3+\ldots+y_{n-1}]+y_n\right).$

Problems:

1. Calculate $\int_1^4 f(x)dx$ where $f(x)$ is given at

x:	1	1.5	2	2.5	3	3.5	4
f(x):	2	4.875	10	18.125	30	46.375	68

   Solution: Note that $h=0.5$ here. Now from trapezoidal rule,

$$\int_1^4 f(x)dx = \frac{0.5}{2}\left(2+2[4.875+10+18.125+30+46.375]+68\right) = 72.1875.$$

2. Evaluate $\int_0^{0.4} e^x dx$ numerically.

   Solution: Taking $n=4$, we get $h=\frac{0.4-0}{4}=0.1$. The data needed in tabular form

x:	0	0.1	0.2	0.3	0.4
f(x):	e^0	$e^{0.1}$	$e^{0.2}$	$e^{0.3}$	$e^{0.4}$

   Now from trapezoidal rule,

$$\int_0^{0.4} f(x)dx = \frac{0.1}{2}\left(1+2[e^{0.1}+e^{0.2}+e^{0.3}]+e^{0.4}\right) = 0.492234.$$

   Note: From actual integration, we get the exact value as 0.491825. So error of integration is -0.0004.

1.2 The Simpson's One-Third Rule

Taking $n=2$ in Newton-Cote's formula, we get

$$\begin{aligned}
\int_{x_0}^{x_2} f(x)dx &= 2h\left(y_0+\frac{2}{2}\Delta y_0+\frac{2(4-3)}{12}\Delta^2 y_0\right)\\
&= 2h\left(y_0+(y_1-y_0)+\frac{1}{6}(y_2-2y_1+y_0)\right)\\
&= \frac{h}{3}(y_0+4y_1+y_2)
\end{aligned}$$

Similarly

$$\begin{aligned}
\int_{x_2}^{x_4} f(x)dx &= \frac{h}{3}(y_2+4y_3+y_4)\\
\ldots\ldots & \quad \ldots\ldots\\
\int_{x_{n-2}}^{x_n} f(x)dx &= \frac{h}{3}(y_{n-2}+4y_{n-1}+y_n)
\end{aligned}$$

Note that n must be an even number. So one should divide the interval to an even number of parts. Hence

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{3}\left(y_0+4[y_1+y_3+y_5+\ldots+y_{n-1}]+2[y_2+y_4+\ldots+y_{n-2}]+y_n\right)$$

Procedure:

- If $f(x)$ is given explicitly, then divide the given interval $[a, b]$ to an even number of equal parts (n), taking $h = \frac{b-a}{n}$. Call $x_0 = a, x_1 = x_0 + h, x_2 = x_0 + 2h, \ldots, x_n = x_0 + nh$. Find the corresponding images $y_0, y_1, \ldots, y_n$.

  $*$ If $f(x)$ is given as data points, then no need of this step; just find h.

- Use $\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx = \frac{h}{3}\left(y_0 + 4[y_1 + y_3 + y_5 + \ldots + y_{n-1}] + 2[y_2 + y_4 + \ldots + y_{n-2}] + y_n\right)$

Problems:

1. Calculate $\int_1^4 f(x)dx$ where $f(x)$ is given at

x:	1	1.5	2	2.5	3	3.5	4
f(x):	2	4.875	10	18.125	30	46.375	68

Solution: Note that $h = 0.5$ here. Now from Simpson's rule,

$$\int_1^4 f(x)dx = \frac{0.5}{2}\left(2 + 4[4.875 + 18.125 + 46.375] + 2[10 + 30] + 68\right) = 71.25$$

2. Evaluate $\int_0^{0.4} e^x dx$ numerically.

Solution: Taking $n = 4$, we get $h = \frac{0.4-0}{4} = 0.1$. The data needed in tabular form

x:	0	0.1	0.2	0.3	0.4
f(x):	e^0	$e^{0.1}$	$e^{0.2}$	$e^{0.3}$	$e^{0.4}$

Now from Simpson's rule,

$$\int_0^{0.4} f(x)dx = \frac{0.1}{3}\left(1 + 4[e^{0.1} + e^{0.3}] + 2[e^{0.2}] + e^{0.4}\right) = 0.491825.$$

Note: From actual integration, we get the exact value as 0.491825. So error of integration is 0 here.

2 Quadrature Formula (for n=2)

First we consider a function $F(x)$ whose integral is to be found from -1 to 1. i.e., we need $\int_{-1}^{1} F(x)dx$.

We assume that the integral value is equal to the area of two rectangles with heights u_1, u_2 and widths c_1, c_2 respectively, where u_1 and u_2 are points between -1 and 1, which (and also c_1, c_2) are to be found.

$$\int_{-1}^{1} F(x)dx = c_1F(u_1) + c_2F(u_2) \tag{1}$$

To find c_1, c_2, u_1, u_2, we approximate $F(x)$ using a cubic polynomial. That is,

$$F(x) \approx a_0 + a_1x + a_2x^2 + a_3x^3 \tag{2}$$

Then

$$F(u_1) = a_0 + a_1u_1 + a_2{u_1}^2 + a_3{u_1}^3 \tag{3}$$
$$F(u_2) = a_0 + a_1u_2 + a_2{u_2}^2 + a_3{u_2}^3 \tag{4}$$

Substituting (2) in RHS of (1), we get

$$\int_{-1}^{1} F(x)dx = \int_{-1}^{1} a_0 + a_1x + a_2x^2 + a_3x^3dx = 2a_0 + \frac{2}{3}a_2 \tag{5}$$

From (1), (3) and (4), we get

$$\int_{-1}^{1} F(x)dx = c_1F(u_1) + c_2F(u_2) = c_1(a_0 + a_1u_1 + a_2{u_1}^2 + a_3{u_1}^3) + c_2(a_0 + a_1u_2 + a_2{u_2}^2 + a_3{u_2}^3)$$
$$= (c_1 + c_2)a_0 + (c_1u_1 + c_2u_2)a_1 + (c_1{u_1}^2 + c_2{u_2}^2)a_2 + (c_1{u_1}^3 + c_2{u_2}^3)a_3 \tag{6}$$

Equating (5) and (6), we get four equations:

$$c_1 + c_2 = 2 \tag{7}$$
$$c_1u_1 + c_2u_2 = 0 \tag{8}$$
$$c_1{u_1}^2 + c_2{u_2}^2 = \frac{2}{3} \tag{9}$$
$$c_1{u_1}^3 + c_2{u_2}^3 = 0 \tag{10}$$

Now (8) and (10) gives

$$\frac{c_1}{c_2} = -\frac{u_2}{u_1} \tag{11}$$
$$\frac{c_1}{c_2} = -\frac{u_2^3}{u_1^3} \tag{12}$$

Equating (11) and (12), we get

$$u_1^3u_2 - u_1u_2^3 = 0 \tag{13}$$

Since $u_1 = 0$, $u_2 = 0$ and $u_1 = u_2$ are not admissible, the only option is $u_1 = -u_2$ satisfying (13).

Substituting $u_1 = -u_2$ in (8), we have $c_1 = c_2$, which in (7) gives

$$c_1 = c_2 = 1.$$

Substituting in (9), we get $u_1 = \frac{1}{\sqrt{3}}$ and $u_2 = -\frac{1}{\sqrt{3}}$. Thus

$$\boxed{\int_{-1}^{1} F(x)dx = F\left(\frac{1}{\sqrt{3}}\right) + F\left(-\frac{1}{\sqrt{3}}\right)}$$

Note that any definite integral $\displaystyle\int_a^b f(x)dx$ can be easily converted to an integral of the form $\displaystyle\int_{-1}^{1} F(u)du$ by using the following transformation:
Take

$$u = \frac{2x - b - a}{b - a} \text{ and so } x = \frac{1}{2}[a + b + (b - a)u].$$

Now when x moves from a to b, u moves from -1 to 1.
Also,

$$du = \frac{2}{b - a}dx \text{ or } dx = \frac{b - a}{2}du.$$

Then

$$\int_a^b f(x)dx = \int_{-1}^{1} f(\frac{1}{2}[a + b + (b - a)u])\frac{b - a}{2}du.$$

Call $F(u) = f(\frac{1}{2}[a + b + (b - a)u])\frac{b-a}{2}$. Thus

$$\boxed{\int_a^b f(x)dx = \int_{-1}^{1} F(u)du = F\left(\frac{1}{\sqrt{3}}\right) + F\left(-\frac{1}{\sqrt{3}}\right)}$$

Note:
$f(x)$ should be given explicitly for applying this method.

Procedure:

1. Convert the given interval of integration $[a, b]$ to $[-1, 1]$ by the transformation $u = \frac{2x-b-a}{b-a}$.
2. Define $F(u) = \frac{b-a}{2} f(\frac{1}{2}[a + b + (b - a)u])$.
3. Use $\displaystyle\int_a^b f(x)dx = \int_{-1}^{1} F(u)du = F\left(\frac{1}{\sqrt{3}}\right) + F\left(-\frac{1}{\sqrt{3}}\right)$

Problems:

1. Find $\int_0^{0.4} e^x dx$ numerically.
   Solution: Put $u = \frac{2x-0.4}{0.4} = 5x - 1 \Rightarrow x = 0.2(1+u)$. Then $dx = \frac{0.4}{2} du = 0.2du$.
   Now

$$\begin{aligned}\int_0^{0.4} e^x dx &= \int_{-1}^{1} e^{0.2(1+u)} 0.2du \\ &= 0.2[e^{0.2(1+\frac{1}{\sqrt{3}})} + e^{0.2(1-\frac{1}{\sqrt{3}})}] \\ &= 0.2[e^{0.3155} + e^{0.08452}] \\ &= 0.49182.\end{aligned}$$

3 Errors in Numerical Integration

3.1 Error in Trapezoidal Rule

The error in Trapezoidal rule is given by

$$E_T = \int_{x_0}^{x_1} ydx - \frac{h}{2}(y_0 + y_1).$$

Suppose that $F(x)$ is the antiderivative of $y = f(x)$. That is $F'(x) = f(x)$. Then

$$\begin{aligned}\int_{x_0}^{x_1} ydx &= F(x_1) - F(x_0) = F(x_0 + h) - F(x_0) \\ &= F(x_0) + \frac{h}{1!} F'(x_0) + \frac{h^2}{2!} F''(x_0) + \ldots - F(x_0) \\ &= \frac{h}{1!} y_0 + \frac{h^2}{2!} {y_0}' + \frac{h^3}{3!} {y_0}'' + \ldots,\end{aligned}$$

by applying Taylor series expansion. Substituting this in E_T,

$$\begin{aligned}E_T &= \frac{h}{1!} y_0 + \frac{h^2}{2!} {y_0}' + \frac{h^3}{3!} {y_0}'' + \ldots - \frac{h}{2}(y_0 + y_1) \\ &= \frac{h}{1!} y_0 + \frac{h^2}{2!} {y_0}' + \frac{h^3}{3!} {y_0}'' + \ldots - \frac{h}{2}\left(y_0 + \left(y_0 + \frac{h}{1!} y_0 + \frac{h^2}{2!} {y_0}' + \frac{h^3}{3!} {y_0}'' + \ldots\right)\right) \\ &= -\frac{h^3}{12} {y_0}'' + \ldots\end{aligned}$$

Since h is very small, we can say that E_T is approximately equal to $-\frac{h^3}{12} y''(\zeta)$ for some $x_0 < \zeta < x_1$.

Now since $\int_a^b ydx = \int_{x_0}^{x_1} ydx + \int_{x_1}^{x_2} ydx + \ldots \int_{x_{n-1}}^{x_n} ydx$, we have

$$\begin{aligned}E_T &= -\frac{h^3}{12} \left(y''(\zeta_1) + y''(\zeta_2) + \ldots + y''(\zeta_n)\right) \\ &\approx -\frac{h^3}{12} n\, y''(\zeta), \text{ for some } a < \zeta < b. \\ &= -\frac{h^2}{12} (b-a)\, y''(\zeta)\end{aligned}$$

3.2 Error in Simpson's Rule

The error in Simpson's rule is given by

$$E_S = \int_{x_0}^{x_2} ydx - \frac{h}{3}(y_0 + 4\, y_1 + y_2).$$

Suppose that $F(x)$ is the antiderivative of $y = f(x)$. That is $F'(x) = f(x)$. Then

$$\begin{aligned}
\int_{x_0}^{x_2} y dx &= F(x_2) - F(x_0) = F(x_0 + 2h) - F(x_0) \\
&= F(x_0) + \frac{2h}{1!} F'(x_0) + \frac{(2h)^2}{2!} F''(x_0) + \ldots - F(x_0) \\
&= \frac{2h}{1!} y_0 + \frac{4h^2}{2!} {y_0}' + \frac{8h^3}{3!} {y_0}'' + \ldots,
\end{aligned}$$

by applying Taylor series expansion. Substituting this in E_S,

$$\begin{aligned}
E_S &= \frac{2h}{1!} y_0 + \frac{4h^2}{2!} {y_0}' + \frac{8h^3}{3!} {y_0}'' + \ldots - \frac{h}{3}(y_0 + 4y_1 + y_2) \\
&= \frac{2h}{1!} y_0 + \frac{4h^2}{2!} {y_0}' + \frac{8h^3}{3!} {y_0}'' + \ldots \\
&\quad - \frac{h}{3}\left(y_0 + 4\left(y_0 + \frac{h}{1!} y_0 + \frac{h^2}{2!} {y_0}' + \frac{h^3}{3!} {y_0}'' + \ldots\right) + (y_0 + 2h\,{y_0}' + \ldots)\right) \\
&= -\frac{h^5}{90} {y_0}'''' + \ldots
\end{aligned}$$

Since h is very small, we can say that E_S is approximately equal to $-\frac{h^5}{90} y''''(\zeta)$ for some $x_0 < \zeta < x_2$.

Now since $\int_a^b y dx = \int_{x_0}^{x_2} y dx + \int_{x_2}^{x_4} y dx + \ldots \int_{x_{n-2}}^{x_n} y dx$, we have

$$\begin{aligned}
E_S &= -\frac{h^5}{90}\left(y''''(\zeta_1) + y''''(\zeta_2) + \ldots + y''''(\zeta_{\frac{n}{2}})\right) \\
&\approx -\frac{h^5}{90}\frac{n}{2} y''''(\zeta), \text{ for some } a < \zeta < b. \\
&= -\frac{h^4}{180}(b-a)\, y''''(\zeta).
\end{aligned}$$