Other Rules

(designing our own formulas with any number of nodes).

Example 1:

Four nodes, at A, $A+\frac{B-A}{3}$, $B-\frac{B-A}{3}$, B. Utilizing symmetry we have:

$$\begin{gathered}\left[c_e\, y(A) + c_i\, y(A+\tfrac{B-A}{3})\right.\\ \left. +c_i\, y(B-\tfrac{B-A}{3}) + c_e\, y(B)\right](B-A)\end{gathered}$$

To find c_e and c_i, we take $A=-1$ and $B=1$ ($A+\frac{B-A}{3}=-\frac{1}{3}$, $B-\frac{B-A}{3}=\frac{1}{3}$), and making the rule correct with $y(x)=1$ and $y(x)=x^2$, namely:

$$\begin{aligned}(2c_e+2c_i)\cdot 2 &= 2\\ (2c_e+2\tfrac{c_i}{9})\cdot 2 &= \tfrac{2}{3}\end{aligned}$$

which yields $c_i=\frac{3}{8}$, $c_e=\frac{1}{8}$. The resulting formula:

$$\begin{gathered}\int\limits_A^B y(x)\,dx \simeq \\ (B-A)\,\frac{y(A)+3\,y(A+\frac{B-A}{3})+3\,y(B-\frac{B-A}{3})\;+\;y(B)}{8}\end{gathered}$$

Example 2:

Three nodes, at $x_1=A+\frac{B-A}{6}$, $x_2=\frac{A+B}{2}$, $x_3=B-\frac{B-A}{6}$ (still symmetrical), so

$$(B-A)(c_s\,y_1+c_c y_2+c_s y_3)$$

Setting $A=-1$ and $B=1$ (i.e. $x_1=-\frac{2}{3}$, $x_2=0$, $x_3=\frac{2}{3}$) we get (for $y(x)=1$ and $y(x)=x^2$):

$$\begin{aligned}(2c_s+c_c)\cdot 2 &= 2\\ 2\cdot\tfrac{4}{9}\,c_s\cdot 2 &= \tfrac{2}{3}\end{aligned}$$

implying that $c_s=\frac{3}{8}$ and $c_c=\frac{2}{8}$, i.e.

$$\int\limits_A^B y(x)\,dx \simeq \frac{3\,y_1+2\,y_2+3\,y_3}{8}\,(B-A)$$

Based on Taylor expansion of $y(x)$, the error of this rule is computed by

$$\begin{aligned}&\frac{3}{8}\left(y(x_c)+y'(x_c)\frac{h}{3}+\frac{y''(x_c)}{2}\frac{h^2}{9}+\frac{y'''(x_c)}{6}\frac{h^3}{27}+\frac{y^{iv}(x_c)}{24}\frac{h^4}{81}\right.\\ &+\frac{2}{3}y(x_c)\\ &\left.+y(x_c)-y'(x_c)\frac{h}{3}+\frac{y''(x_c)}{2}\frac{h^2}{9}-\frac{y'''(x_c)}{6}\frac{h^3}{27}+\frac{y^{iv}(x_c)}{24}\frac{h^4}{81}\right)\cdot h=\end{aligned}$$

$$
\begin{aligned}
& \left(y(x_c)\,h + \frac{y''(x_c)}{24} h^3 + \frac{y^{iv}(x_c)}{2592} h^5 + ... \right) \\
& - \left(y(x_c)\,h + \frac{y''(x_c)}{24} h^3 + \frac{y^{iv}(x_c)}{1920} h^5 + ... \right) \\
= \quad & -\frac{7\,y^{iv}(x_c)}{51840}\, h^5 + ...
\end{aligned}
$$

i.e. *smaller* than that of the Simpson rule, and of the opposite sign (can we choose the points to eliminate this term entirely)?

Example 3:

We derive a formula to approximate $\int_0^3 y(x)\,dx$ assuming that only three values of $y(x)$ are known, $y(0)$, $y(1)$ and $y(3)$. The formula will have the form of

$$c_0\,y(0) + c_1\,y(1) + c_3\,y(3)$$

and has to be exact for $y(x) = 1$, $y(x) = x$ and $y(x) = x^2$, i.e.:

$$
\begin{aligned}
c_0 + c_1 + c_3 &= \int_0^3 dx = 3 \\
c_1 + 3\,c_3 &= \int_0^3 x\,dx = \frac{9}{2} \\
c_1 + 9\,c_3 &= \int_0^3 x^2\,dx = 9
\end{aligned}
$$

The last two equations can be solved for c_1 and c_3:

$$\begin{bmatrix} 9 & -3 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} \frac{9}{2} \\ 9 \end{bmatrix} \div 6 = \begin{bmatrix} \frac{9}{4} \\ \frac{3}{4} \end{bmatrix}$$

implying that $c_0 = 0$. The final rule is thus:

$$\int_0^3 y(x)\,dx \simeq \frac{9}{4}\,y(1) + \frac{3}{4}\,y(3)$$

Singular and Improper Integrals

All formulas we derived so far will fail miserably when applied to:

$$\int_0^1 \frac{\exp(x^2)}{\sqrt{x}}\,dx$$

(they all assume that the integrand, with all its derivatives, is finite).

This integrand is singular due to $\frac{1}{\sqrt{x}}$. Even though creating a problem numerically, $\frac{1}{\sqrt{x}}$ is quite easy to integrate on its own. We will **separate** it from the rest of the integrand, thus:

$$\int_0^1 \frac{y(x)}{\sqrt{x}}\,dx$$

We can now derive an approximate formula for this kind of integral in the usual fashion, i.e.:

Using $x = 0$, $\frac{1}{2}$ and 1 as our nodes, we get

$$y(x) \approx$$
$$\frac{(x-\frac{1}{2})(x-1)}{\frac{1}{2}}\,y(0) + \frac{x\,(x-1)}{-\frac{1}{4}}\,y(\tfrac{1}{2}) + \frac{x\,(x-\frac{1}{2})}{\frac{1}{2}}\,y(1)$$

Since

$$\int_0^1 \frac{(x-\frac{1}{2})(x-1)}{\sqrt{x}}\,dx = \frac{2}{5}$$
$$\int_0^1 \frac{x\,(x-1)}{\sqrt{x}}\,dx = -\frac{4}{15}$$
$$\int_0^1 \frac{x\,(x-\frac{1}{2})}{\sqrt{x}}\,dx = \frac{1}{15}$$

our integration rule reads:

$$\int_0^1 \frac{y(x)}{\sqrt{x}}\,dx \simeq \frac{12}{15}\,y(0) + \frac{16}{15}\,y(\tfrac{1}{2}) + \frac{2}{15}\,y(1)$$

Or, alternately:

$$\int_0^1 \frac{y(x)}{\sqrt{x}}\,dx \simeq c_0\,y(0) + c_{\frac{1}{2}}\,y(\tfrac{1}{2}) + c_1\,y(1)$$

(the ';weight function' $\frac{1}{\sqrt{x}}$ breaks the symmetry), we make it correct for $y(x) = 1$, x and x^2:

$$\begin{aligned} c_0 + c_{\frac{1}{2}} + c_1 &= \int_0^1 \frac{1}{\sqrt{x}}\,dx = 2 \\ \frac{1}{2}c_{\frac{1}{2}} + c_1 &= \int_0^1 \frac{x}{\sqrt{x}}\,dx = \frac{2}{3} \\ \frac{1}{4}c_{\frac{1}{2}} + c_1 &= \int_0^1 \frac{x^2}{\sqrt{x}}\,dx = \frac{2}{5} \end{aligned}$$

resulting in $c_{\frac{1}{2}} = \frac{16}{15}$, $c_1 = \frac{2}{15}$, and $c_0 = \frac{12}{15}$ (check).

Applying this rule to the original $\int_0^1 \frac{\exp(x^2)}{\sqrt{x}}\,dx$ results in $\frac{12}{15} + \frac{16}{15}\,e^{\frac{1}{4}} + \frac{2}{15}\,e =$ 2.532. This compares favorably (0.4% error) with the exact answer of 2.543.

To extend the formula to $\int_0^A \frac{y(x)}{\sqrt{x}}\,dx$, we introduce $z = A\,x$ and write

$$\begin{aligned}\int_0^A \frac{y(x)}{\sqrt{x}}\,dx &= \int_0^1 \frac{y(\frac{z}{A})}{\sqrt{\frac{z}{A}}}\,\frac{dz}{A} \\ &\simeq \sqrt{A}\cdot\left[\frac{12}{15}\,y(0) + \frac{16}{15}\,y(\tfrac{A}{2}) + \frac{2}{15}\,y(A)\right]\end{aligned}$$

Another example:

Develop a 4 point formula for approximating:

$$\int_0^\infty y(x)\exp(-x)\,dx$$

We choose $x = 0$, 1, 2 and 3 as our four nodes. The interpolating polynomial is thus

$$\begin{aligned}&\frac{(x-1)(x-2)(x-3)}{-6}\,y(0) + \frac{x\,(x-2)(x-3)}{2}\,y(1) + \\ &+\frac{x\,(x-1)(x-3)}{-2}\,y(2) + \frac{x\,(x-1)(x-2)}{6}\,y(3) = \\ &\frac{x^3-6x^2+11x-6}{-6}\,y(0) + \frac{x^3-5x^2+6x}{2}\,y(1) + \\ &+\frac{x^3-4x^2+3x}{-2}\,y(2) + \frac{x^3-3x^2+2x}{6}\,y(3)\end{aligned}$$

Multiplying by e^{-x} and integrating from 0 to ∞ yields (remember that $\int_0^\infty x^k e^{-x} dx = k!$):

$$\begin{aligned}&\frac{6-12+11-6}{-6}\,y(0) + \frac{6-10+6}{2}\,y(1) \\ &+\frac{6-8+3}{-2}\,y(2) + \frac{6-6+2}{6}\,y(3) = \\ &\tfrac{1}{6}\,y(0) + y(1) - \tfrac{1}{2}\,y(2) + \tfrac{1}{3}\,y(3)\end{aligned}$$

(our final rule). Note that one of our coefficients is negative (indication of badly chosen nodes).

Applied to $\int_0^\infty \frac{\exp(-x)}{x+2}\,dx$. our formula yields: $\frac{1}{6}\cdot\frac{1}{2} + \frac{1}{3} - \frac{1}{2}\cdot\frac{1}{4} + \frac{1}{3}\cdot\frac{1}{5} = 0.358\bar{3}$, reasonably close (0.8% error) to the exact answer of 0.3613.

The obvious questions to ask now:

Is there a better way of selecting our four nodes?

Is there a **best** way of selecting them? 'Best' in what sense?