NUMERICAL INTEGRATION

Basic **idea**: Replace the function by a 'closely fitting' polynomial, integrate that instead.

Following **polynomial** will do: Evaluate the function at a few values of x (so called **nodes**), fit by Lagrange interpolating polynomial.

Make the **choice** of: How many nodes, and *where*?

Trapezoidal rule (one point at each end):

Interpolating polynomial is the straight line

$$y(A)\,\frac{x-B}{A-B}+y(B)\,\frac{x-A}{B-A}$$

Integrate that instead

$$\frac{y(A)}{A-B}\int_A^B (x-B)\,dx+\frac{y(B)}{B-A}\int_A^B (x-A)\,dx$$

$$=\frac{y(A)+y(B)}{2}\cdot(B-A)$$

The resulting 'trapezoidal' rule is:

$$\int_A^B y(x)\,dx\simeq\frac{y(A)+y(B)}{2}\cdot(B-A)$$

To estimate its error, we (Taylor) expand $y(x)$ at $x\equiv x_c=\frac{A+B}{2}$, thus

$$\begin{aligned}y(x)&=y(x_c)+y'(x_c)(x-x_c)\\&+\frac{y''(x_c)}{2}(x-x_c)^2+\frac{y'''(x_c)}{6}(x-x_c)^3\\&+\frac{y^{iv}(x_c)}{24}(x-x_c)^4+\ldots\end{aligned}$$

Integrating right hand side **exactly**:

$$\begin{aligned}&y(x_c)\cdot(B-A)+y'(x_c)\frac{(x-x_c)^2}{2}\Bigg|_{x=A}^{B}\\&+\frac{y''(x_c)}{2}\,\frac{(x-x_c)^3}{3}\Bigg|_{x=A}^{B}+\frac{y'''(x_c)}{6}\,\frac{(x-x_c)^4}{4}\Bigg|_{x=A}^{B}\\&+\frac{y^{iv}(x_c)}{24}\,\frac{(x-x_c)^5}{5}\Bigg|_{x=A}^{B}\ldots\\&=y(x_c)\,h+\frac{y''(x_c)}{24}h^3+\frac{y^{iv}(x_c)}{1920}h^5+\ldots\end{aligned}$$

($h\equiv B-A$).

Using our trapezoidal rule instead yields:

$$\frac{1}{2}\left(y(x_c)+y'(x_c)\frac{h}{2}+\frac{y''(x_c)}{2}\,\frac{h^2}{4}+\frac{y'''(x_c)}{6}\,\frac{h^3}{8}+\frac{y^{iv}(x_c)}{24}\,\frac{h^4}{16}+\right.$$

$$\left.y(x_c)-y'(x_c)\frac{h}{2}+\frac{y''(x_c)}{2}\,\frac{h^2}{4}-\frac{y'''(x_c)}{6}\,\frac{h^3}{8}+\frac{y^{iv}(x_c)}{24}\,\frac{h^4}{16}\right)\cdot h=$$

$$y(x_c)\,h+\frac{y''(x_c)}{8}h^3+\frac{y^{iv}(x_c)}{384}h^5+\ldots$$

The error of the latter is thus:

$$\frac{y''(x_c)}{12}h^3 + \frac{y^{iv}(x_c)}{480}h^5 + \ldots$$

In its current form, the trapezoidal rule is too primitive, e.g. $\int_0^{\pi/2} \sin x\, dx$ (= 1 exact) would yield $\frac{1}{2} \cdot \frac{\pi}{2} = 0.785$ (off by 21.5%).

We can improve the accuracy by reducing h, i.e. subdividing (A, B) into n equal subintervals, applying trapezoidal rule to each subinterval, then adding the results.

This leads to the so called **composite rule:**

The new value of h is $\frac{B-A}{n}$, with nodes at $x_0 = A$, $x_1 = A + h$, $x_2 = A + 2h$, ..., $x_n = B$.

The composite formula:

$$\frac{y_0 + y_1}{2}h + \frac{y_1 + y_2}{2}h + \ldots + \frac{y_{n-1} + y_n}{2}h =$$
$$\frac{y_0 + 2y_1 + 2y_2 + \ldots + 2y_{n-1} + y_n}{2n} \cdot (B - A)$$

(note the weighted average of the y_i values, the endpoints taken only 'half seriously').

Its error is:

$$\frac{h^3}{12}\sum_{i=1}^{n} y''\left(\frac{x_i + x_{i-1}}{2}\right) + \ldots = \frac{h^3}{12} \cdot n y''_{av} + \ldots = h^2 \frac{B - A}{12} y''_{av} + \ldots$$

Example: Approximate $\int_0^{\pi/2} \sin x\, dx$ using $n = 1, 2, 4, 8, 16, 32$ and 64:

i	n	$\frac{\left(1+2\sum_{j=1}^{n-1}\sin\left(\frac{\pi \cdot j}{2n}\right)\right)}{2n} \cdot \frac{\pi}{2}$	error
0	1	0.7853981635	0.2146
1	2	0.948059449	0.0519
2	4	0.987115801	0.0129
3	8	0.996785172	0.0032
4	16	0.9991966805	0.0008
5	32	0.9997991945	0.0002
6	64	0.999498	0.00005

(error reduced, roughly, by 4, each step).

Romberg integration:

The error follows a regular pattern (as we have just learnt), namely: $I_0 = I + \frac{c}{4^0}$, $I_1 = I + \frac{c}{4^1}$, $I_2 = I + \frac{c}{4^2}$...., where $c = \frac{(B-A)^3}{12} y''_{av}$, and I is the exact answer.

We can eliminate this error from any two consecutive results, i.e.

$$I_i = I + \frac{c}{4^i}$$
$$I_{i+1} = I + \frac{c}{4^{i+1}}$$

by

$$J_i = \frac{4I_{i+1} - I_i}{3}$$

Example:

i	$J_i \equiv \frac{4I_{i+1}-I_i}{3}$
0	1.002279878
1	1.000134585
2	1.000008296
3	1.000000517
4	1.000000033
5	1.000000002

Errors now a lot smaller; they decrease, in each step, by roughly a factor of 16!

Continuing the idea of eliminating them, we define

$$K_i \equiv \frac{16J_{i+1} - J_i}{15}$$

The K's errors will decrease by a factor of 64, so we can improve further by

$$L_i \equiv \frac{64K_{i+1} - K_i}{63}$$

etc., until we come to the end (or the numbers no longer change).

Example:

i	J_i	$K_i = \frac{16J_{i+1}-J_i}{15}$	$L_i = \frac{64K_{i+1}-K_i}{63}$
0	1.002279878	0.9999915654	1.000000009
1	1.000134585	0.9999998774	0.9999999997
2	1.000008296	0.999999998	
3	1.000000517		

reaching the limit of Maple's accuracy (after that, the accuracy will deteriorate - we should know when to stop).