Numerical Analysis **Solutions for sheet 6**

Lagrange polynomial interpolation, integration rules and Romberg

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1. (a) Just have to use the formula in the notes, and $x_0 = 0$, $x_1 = 1$, $x_2 = 2$ with $f(x_0) = 1$, $f(x_1) = 2$, $f(x_2) = 4$. We get

$$P_2(x) = \frac{(x-1)(x-2)}{(-1)(-2)}1 + \frac{(x-0)(x-2)}{(1)(-1)}2 + \frac{(x-0)(x-1)}{(2)(1)}4.$$

Simplifying gives

$$P_2(x) = \frac{1}{2}(x-1)(x-2) - 2x(x-2) + 2x(x-1) = \frac{x^2}{2} + \frac{x}{2} + 1.$$

(b) The error is defined (see notes) by

$$|f(x) - P_2(x)| = \frac{1}{6}|f'''(\xi)||x(x-1)(x-2)|$$

for some $\xi \in (0, 2)$. First, from $f(x) = 2^x$, we have $f'(x) = \ln(2)2^x$, and so $f'''(\xi) = (\ln(2))^3 2^\xi$. The maximum value of $|f'''(\xi)|$ for $\xi \in (0, 2)$ is therefore $4(\ln(2))^3$. Also, we need to find a bound on the second term $|x(x-1)(x-2)|$ and this requires

$$\frac{d}{dx}\left(x(x-1)(x-2)\right) = 0$$

which gives

$$3x^2 - 6x + 2 = 0.$$

Solving gives $3(x-1)^2 - 1 = 0$ and so $x = 1 \pm 1/\sqrt{3}$ at which

$$x(x-1)(x-2) = \pm\left(1 \pm 1/\sqrt{3}\right)\frac{1}{\sqrt{3}}\left(-1 \pm 1/\sqrt{3}\right) = \pm\frac{1}{\sqrt{3}}\left(\frac{1}{3} - 1\right) = \mp\frac{2}{3\sqrt{3}}.$$

We conclude, therefore, that $|x(x-1)(x-2)| < 2/3\sqrt{3}$. Putting everything together, we have that

$$|f(x) - P_2(x)| \le \frac{1}{6} \times 4(\ln(2))^3 \times \frac{2}{3\sqrt{3}} \approx 0.085.$$

(c) We can actually do this two ways. We can integrate $P_2(x)$ found in part (a) over $0 < x < 2$; or we can use the Simpson rule, where $h = 1$, to give

$$I \approx \frac{1}{3}[1 + 4 \times 2 + 4] = \frac{13}{3} \approx 4.333333$$

The actual value is easily found since if the derivative of 2^x is $\ln(2)2^x$ then the integral of 2^x is $2^x/\ln(2)$ and so $I = 3/\ln(2) \approx 4.328085$. The numerical error is -0.0052482. According to the error formula given in Simpson's rule, the error will be bounded by

$$\frac{h^5}{90}|f^{(iv)}(\xi)|$$

for some $\xi \in (0,2)$. Here $h=1$, $f^{(iv)}(\xi) = (\ln(2))^4 2^\xi \le 4(\ln(2))^4$ since $\xi \in (0,2)$. So the error in the integral should be bounded by

$$\frac{4(\ln(2))^4}{90} \approx 0.01025933.$$

Our computed error (-0.0052482) is below (about half) of this bound.

(d) Composite Simpson with $n=2$ so that $h=1/2$. This means we need to evaluate $f(0)=1$, $f(1/2)=\sqrt{2}$, $f(1)=2$, $f(3/2)=2\sqrt{2}$ and $f(2)=4$ in Simpson's rule:

$$I \approx \frac{1/2}{3}\left(1+4\times\sqrt{2}+2\times 2+4\times 2\sqrt{2}+4\right) = \frac{1}{6}\left(9+12\sqrt{2}\right) \approx 4.328427.$$

This has an error of 0.0003420 compared to the exact value. Since the error is $O(h^4)$ we expect this error to be about 1/16th of 0.005282 ... which it is !

(e) We know that composite Simpson has error $O(h^4)$ and can be expanded in a power series with leading term $O(h^4)$ (since Simpson is one Romberg step applied to Trapezium rule which itself has a power series error). I.e.

$$I = S(h) + a_4 h^4 + \ldots$$

where I is the exact value and $I(h)$ is Simpson with step size h. Then

$$I = S(h/2) + a_4 h^4/16 + \ldots$$

which means

$$I = \frac{16S(h/2) - S(h)}{15} + O(h^6)$$

using the usual methods. In this problem $S(1) = 4.3333\ldots$ and $S(1/2) = 4.328427$ so $I \approx 4.328099$ should be better. The exact value is $3/\ln(2) = 4.328085$.

2. (a) Standard integral: $I = \left[4\tan^{-1}(x)\right]_0^1 = \pi$.

(b) Using the formula for the composite trapeziodal scheme we have

$$T_1 = \frac{4}{2}\left[1 + \frac{1}{1+1^2}\right] = 3$$

then, $n=2$ and $h=1/2$

$$T_2 = \frac{4}{4}\left[1 + 2\times\frac{1}{1+(\frac{1}{2})^2} + \frac{1}{1+1^2}\right] = \frac{31}{10} = 3.1$$

and then, $n=4$, $h=1/4$

$$T_4 = \frac{4}{8}\left[1 + 2\times\frac{1}{1+(\frac{1}{4})^2} + 2\times\frac{1}{1+(\frac{1}{2})^2} + 2\times\frac{1}{1+(\frac{3}{4})^2} + \frac{1}{1+1^2}\right] \approx 3.1311764$$

So we are getting closer to π as we expect.

(c) OK, so we have

$$T_n^{(1)} = (4T_n - T_{n/2})/3$$

which means

$$T_2^{(1)} = (4T_2 - T_1)/3 = 3.1333333$$

and

$$T_4^{(1)} = (4T_4 - T_2)/3 = 3.1415686.$$

Then, at the next step the Romberg iterates are defined by

$$T_n^{(2)} = (16T_n^{(1)} - T_{n/2}^{(1)})/15$$

which we can only use with $n = 4$ to give

$$T_4^{(2)} = (16T_4^{(1)} - T_2^{(1)})/15 = 3.1421176.$$

We may wonder why $T_4^{(2)}$ is not as good as $T_4^{(1)}$. It's just that $T_4^{(1)}$ is, by accident, closer to π than it should be.

(d) With $n = 2$, $h = 1/2$, Simpsons rule is

$$S_2 = \frac{4 \times \frac{1}{2}}{3}\left[1 + 4\frac{1}{1 + (\frac{1}{2})^2} + \frac{1}{1 + 1^2}\right] = 3.1333333$$

which is the same as $T_2^{(1)}$. This was demonstrated in the lectures, that one step of Romberg gives you Simpson.

Similarly, we find $S_4 = 3.1415686$ either by using the Simpson formula directly or by equating to $T_4^{(1)}$.

3. The composite trapezoidal rule for approximating the integral $\int_a^b f(x)\,\mathrm{d}x$ is based on a subdivision of the interval $[a, b]$ into n equal subintervals. The approximation has the form

$$T_n = \frac{h}{2}[f_0 + 2f_1 + 2f_2 + 2f_3 + 2f_4 + \ldots + 2f_{n-1} + f_n]$$

where $h = (b - a)/n$, $f_j = f(x_j)$ and $x_j = a + jh$.

We have the iteration rules: $T_n^{(1)} = (4T_n - T_{n/2})/3$ and $T_n^{(2)} = (16T_n^{(1)} - T_{n/2}^{(1)})/15$. We apply this to the first example which has the solution

$$\int_0^1 \sin(x)\,\mathrm{d}x = 1 - \cos(1) = 0.4596976941$$

The last approximation $T_4^{(2)}$ is quite good considering that only up to 4 subdivisions were used. For the second example we obtain

$$\int_0^1 x\ln(x)\,\mathrm{d}x = \left[\frac{x^2}{2}\ln(x) - \frac{x^2}{4}\right]_0^1 = -0.25.$$

n	T_n	$T_n^{(1)}$	$T_n^{(2)}$
1	0.4207354924		
2	0.4500805155	0.4598621899	
4	0.4573009376	0.4597077449	0.4596974486

n	T_n	$T_n^{(1)}$	$T_n^{(2)}$
1	−0.0000000000		
2	−0.1732867951	−0.2310490602	
4	−0.2272271837	−0.2452073133	−0.2461511968

The approximation is clearly worse than in the first case. I don't expect you to know the reason, but the higher derivatives $f^{(n)}(x)$ for $n \geq 2$ diverge at $x = 0$ and this has the consequence of not being able to assume that the trapezoidal rule has an error which can be expressed as an even power series in h, which is the foundation of the Romberg method.

4. We insert a general quadratic polynomial $x(t) = \alpha t^2 + \beta t + \gamma$ into the formula

$$\int_{-1}^{1} x(t)\,\mathrm{d}t = a\,x(-1/3) + b\,x(0) + c\,x(1/3).$$

On the left-hand side we obtain

$$\int_{-1}^{1} [\alpha t^2 + \beta t + \gamma]\,\mathrm{d}t = \left[\frac{1}{3}\alpha t^3 + \frac{1}{2}\beta t^2 + \gamma t\right]_{-1}^{1} = \frac{2}{3}\alpha + 2\gamma,$$

and on the right-hand side the result is

$$a\left[\frac{\alpha}{9} - \frac{\beta}{3} + \gamma\right] + b\gamma + c\left[\frac{\alpha}{9} + \frac{\beta}{3} + \gamma\right] = \alpha\frac{a+c}{9} + \beta\frac{c-a}{3} + \gamma(a+b+c).$$

We compare the coefficients of α, β and γ on both sides of the equation and obtain

$$\frac{a+c}{9} = \frac{2}{3}, \quad \frac{c-a}{3} = 0, \quad a+b+c = 2 \qquad \Longrightarrow \qquad a = c = 3, \quad b = -4.$$

The resulting approximation formula is

$$\int_{-1}^{1} x(t)\,\mathrm{d}t \approx 3\,x(-1/3) - 4\,x(0) + 3\,x(1/3).$$

This formula is also exact for any odd function satisfying $x(-t) = -x(t)$ because then one obtains zero on both sides of the equation (note that $x(0) = 0$ if $x(t)$ is odd).

5. (a) The difficulty is the log-singularity at $x = 0$, which means we cannot use $x_0 = 0$ as an evaulation point. The solution could be the following:

$$\begin{aligned}\int_0^1 \ln(\sin(x))\,dx &= \int_0^1 \ln(\sin(x)) - \ln(x)\,dx + \int_0^1 \ln(x)\,dx \\ &= \int_0^1 \ln(\sin(x)/x)\,dx + [x\ln(x) - x]_0^1 \\ &= \int_0^1 \ln(\sin(x)/x)\,dx - 1\end{aligned}$$

Now we can use $x_0 = 0$ as an integration point since as $x \to 0$ the integrand tends to $\ln(1) = 0$.

(b) The problem here is that the range of integration is infinite. The solution is to map $[1, \infty)$ to a finite interval via a mapping. Let's choose, for example, $t = 1/x$. Then $dx = (-1/t^2)dt$ and we get

$$\int_1^\infty \frac{1}{1+x^2}\,dx = \int_1^0 \frac{-1}{t^2}\frac{1}{1+1/t^2}\,dt = \int_0^1 \frac{1}{1+t^2}\,dt.$$

(c) The problem here is the singularity at $x = 1$ which means we cannot use $x_n = 1$ as an end point. We could either do something like in part (a) and subtract of the singularity and add it back on or we could make a substitution. For example, $x = \sin\theta$, gives

$$\int_0^1 \frac{\mathrm{e}^x}{\sqrt{1-x^2}}\,dx = \int_0^{\pi/2} \mathrm{e}^{\sin\theta}\,d\theta.$$

(d) So this is a semi-infinite integral, but simply doing $x = \pi/t$ to map it to a finite integral as in part (b) is not good enough because the result involves an integrand with $\sin(\pi/t)$ which becomes increasingly oscillatory as $t \to 0$. So it's the oscillations that are the problem here, but they also provide us with an opportunity since $\sin(x + n\pi) = (-1)^n \sin x$. Thus we map the intervals $n\pi < x < (n+1)\pi$ to the interval $\pi < x < 2\pi$ to give

$$\int_\pi^\infty \frac{\sin x}{x}\,dx = \int_\pi^{2\pi} \sin x \left(\frac{1}{x} - \frac{1}{x+\pi} + \frac{1}{x+2\pi} - \dots\right) dx.$$

We can write this as

$$\int_\pi^{2\pi} g(x)\sin x\,dx$$

which we can deal with using regular integration rules like trapezoidal or Simpson in which $g(x) = \sum_{n=0}^{\infty} \frac{\pi}{(x+2n\pi)(x+(2n+1)\pi)}$ can be approximated numerically by truncating the infinite sum.

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