Natural Sciences Tripos Part IB
Numerical Methods

Model answers to some questions

6.1 Roots of an integrated quantity

Consider the integral

$$F(x) = \int_a^x f(\xi)\, d\xi,$$

where $f(x)$ is an easily evaluated function.

(a) Show how $F(x)$ may be calculated from $f(x)$ for some arbitrary value of x using the Trapezium Rule with the interval $[a,x]$ subdivided into $n-1$ subintervals.

(b) Derive the error term in this approximation and show how Romberg Integration may be used to improve the accuracy of the solution given estimates of $F(x)$ obtained from $n-1$ and $2n-1$ subintervals. Show that this estimate is equivalent to calculating the integral using Simpson's Rule.

(c) Suppose we wish to find the value of x such that $F(x) = 1$. Using the Newton-Raphson method, predict the location of the root using a single iteration. You may assume $F(x)$ is a monotonically increasing function of x from $x = a$ to the neighbourhood of the root $x = x^*$. Why is this assumption important?

(d) Describe how the second and subsequent iterations may be calculated. Discuss how precisely the integral $F(x)$ should be evaluated for each iteration and suggest an appropriate method for achieving this.

Answer:

(a) Let $G_n(x)$ be our approximation to $F(x)$ using the Trapezium Rule with n-1 subintervals each of a size $\Delta\xi=(x-a)/(n-1)$. [Suggestion: draw a sketch of some function f(x) showing how $G_n(x)$ is obtained using the Trapezium Rule. You may wish to state the integral from ξ to $\xi+\Delta\xi$ and then sum for the compound rule, or simply quote the compound rule as here] Then

$$G_n(x) = \frac{\Delta\xi}{2}\left[f(a) + 2f(a+\Delta\xi) + 2f(a+2\Delta\xi) + \ldots + 2f(x-\Delta\xi) + f(x) \right]$$

(b) To obtain the error in $G_n(x)$, consider first the error in one of the subintervals from ξ to $\xi+\Delta\xi$, say, using a Taylor Series expansion of f we can see

$$\int_{\xi}^{\xi+\Delta\xi} f(\xi')d\xi' = \int_0^{\Delta\xi}\left[f(\xi) + \Delta\xi f'(\xi) + \frac{\Delta\xi^2}{2} f''(\xi) + \frac{\Delta\xi^3}{6} f'''(\xi) + O(\Delta\xi^4) \right] d\xi'$$

$$= \Delta\xi f(\xi) + \frac{\Delta\xi^2}{2} f'(\xi) + \frac{\Delta\xi^3}{6} f''(\xi) + \frac{\Delta\xi^4}{24} f'''(\xi) + O(\Delta\xi^5)$$

Comparing this with the Trapezium Rule approximation for this step

$$\int_{\xi}^{\xi+\Delta\xi} f(\xi')\mathrm{d}\xi' \approx \frac{\Delta\xi}{2}\left[f(\xi)+f(\xi+\Delta\xi)\right]$$

$$\approx \frac{\Delta\xi}{2}\left[f(\xi)+f(\xi)+\Delta\xi f'(\xi)+\frac{\Delta\xi^2}{2}f''(\xi)+\frac{\Delta\xi^3}{6}f'''(\xi)+O(\Delta\xi^4)\right]$$

shows the error in the Trapezium Rule approximation to be

$$\frac{\Delta\xi^3}{12}f''(\xi)+O(\Delta\xi^4)$$

In the interval $[a,x]$ there are n-1 errors of this order ($\Delta\xi^3$), so the total error is $O((n-1)\Delta\xi^3) = (x-a)O(\Delta\xi^2)$.

For Romberg integration we try to cancel the leading order term in the expression for the error by using two integrations, one with a step size $\Delta\xi$ and the second with half this step size. We may thus write

$$F(x) = G_n(x) + c\Delta\xi^2 + O(\Delta\xi^3)$$

for some constant c. Similarly, we may use $2n$-1 subintervals, each of size $\Delta\xi/2$ to obtain

$$F(x) = G_{2n}(x) + c\Delta\xi^2/4 + O(\Delta\xi^3).$$

Eliminating the error term between these two equations gives

$$F(x) = [4G_{2n}(x) - G_n(x)]/3 + O(\Delta\xi^3).$$

Substituting in the Trapezium Rule approximations G_n and G_{2n} gives

$$G_{Rombert,2n} = \frac{1}{3}\Big[4\tfrac{1}{2}\Delta\xi\big(f(a)+2f(a+\tfrac{1}{2}\Delta\xi)+2f(a+\Delta\xi)+2f(a+\tfrac{3}{2}\Delta\xi)+\ldots+2f(x-\Delta\xi)+2f(x-\tfrac{1}{2}\Delta\xi)+f(x)\big)$$
$$-\Delta\xi\big(f(a)+2f(a+\Delta\xi)+\ldots+2f(x-\Delta\xi)+f(x)\big)\Big]$$
$$=\frac{\Delta\xi}{3}\left[f(a)+2f(a+\tfrac{1}{2}\Delta\xi)+4f(a+\Delta\xi)+2f(a+\tfrac{3}{2}\Delta\xi)+\ldots+4f(x-\Delta\xi)+2f(x-\tfrac{1}{2}\Delta\xi)+f(x)\right]$$

which is simply Simpson's Rule.

(c) Want to find $x=x^*$ such that $F(x^*) = 1$. Write $H(x) = F(x)-1$ and look for $H(x) = 0$ using Newton-Raphson algorithm:

$$x_{n+1} = x_n - \frac{H(x_n)}{H'(x_n)}$$
$$= x_n - \frac{F(x_n)-1}{f(x_n)}$$

The Newton Raphson algorithm will converge provided H' is nonzero in the neighbourhood of the root. This condition corresponds to $F(x)$ either increasing or decreasing monotonically with x. Given we are after $F(x) = 1$ and, by definininition, $F(a) = 0$, we therefore require $f(x)>0$, corresponding to $F(x)$ monotonically increasing.

To obtain a first approximation to x^*, let $x_0 = a$, then

$$x_1 = x_0 - \frac{F(x_0)-1}{f(x_0)}$$
$$= a + \frac{1}{f(a)}.$$

(d) For subsequent iterations it is necessary to calculate $F(x_n)$. This could be achieved by the Trapezium or Simpson's Rules, or by some other method such as Gauss Quadrature.

There are a number of equally valid answers to this question. It would not be necessary to go into any great detail.

You could argue that the precision to which $F(x_n)$ is evaluated need only reflect the accuracy to which you currently know x^*. Since the Newton Raphson method has second order convergence ($\varepsilon_{n+1} \sim \varepsilon_n^2$), then you could argue that the Trapezium rule is all that is required as this has a similar accuracy, and choose $\Delta\xi$ as $|x_n - x_{n-1}|$ when evaluating x_{n+1}.

From a practical point the problem with the above strategy is that the complete integral would need to be re-evaluated for each new x_n. In practice it would be better to use some higher order method, such as Gauss Quadrature or Simpson's Rule to make a much more accurate estimate for some $F(x)$ and then simply add or subtract the contributions from changing x_n as the computation proceeds. If a very high accuracy is required, it may be desirable to recalculate the full $F(x)$ with a finer $\Delta\xi$ when the process gets very close to the final root.

6.2 Shooting

Consider the second order ordinary differential equation

$$\frac{d^2y}{dx^2} = f\left(x, y, \frac{dy}{dx}\right)$$

with boundary conditions $y = y_a$ at $x = x_a$ and $y = y_b$ at $x = x_b$.

(a) Show how this equation may be rewritten as a system of two first order ordinary differential equations.

(b) Show how the Euler method may be used to step this system from $x = x_a$ to $x = x_b$, using n steps, if we assume a knowledge of dy/dx at $x = x_a$. Derive an expression for the truncation error for each step in this process.

(c) Describe how the Euler method may be combined with a root finding algorithm to determine the value of dy/dx at $x = x_a$ required to satisfy our boundary condition at $x = x_b$.

(d) Taking $f(x,y,dy/dx) = y$, $(x_a,y_a) = (0,1)$ and using initial guesses of $dy/dx = 0$ and $dy/dx = -1$ at $x = x_a$, use the Linear Interpolation method to calculate an improved estimate for dy/dx at $x = x_a$ given the other boundary condition $(x_a,y_a) = (1,1/2)$. Formulate your solution using two steps between x_0 and x_1 (*i.e.* $\Delta x = 1/2$).

Answer

(a) Let $Y = dy/dx$, then we may write

$$\frac{dY}{dx} = f(x, y, Y), \qquad \frac{dy}{dx} = Y \, .$$

(b) Let $\Delta x = (x_b - x_a)/n$ and discretise the interval such that $x_i = x_a + i\Delta x$ with the corresponding y and Y values denoted as y_i and Y_i respectively. Using the explicit Euler method we may write

$$Y_{i+1} = Y_i + f(x_i,y_i,Y_i)\Delta x,$$
$$y_{i+1} = y_i + Y_i.$$

We set $y_0 = y_a$ and $Y_0 = dy/dx$ at $x = x_a$.

The Euler method is obtained from the Taylor Series expansion for the value of y at $x = x_{i+1}$ about the point x_i:

$$y_{i+1} = y_i + \Delta x \frac{\mathrm{d}y}{\mathrm{d}x} + \frac{\Delta x^2}{2}\frac{\mathrm{d}^2 y}{\mathrm{d}^2 x} + \frac{\Delta x^3}{6}\frac{\mathrm{d}^3 y}{\mathrm{d}^3 x} + O\left(\Delta x^4\right).$$

Hence the error goes like Δx^2 for a first order equation.

(c) This is effectively the Shooting Method. The basic algorithm could be constructed as follows if you choose to use the secant method. Note that we wish to solve $g(Y_0) = Y_n^{(m)} - y_b = 0$ where $Y_n^{(m)}$ is the value of Y_n obtained assuming a particular value of $Y_0 = Y_0^{(m)}$.

1.Make two initial guess $Y_0 = Y_0^{(0)}$ and $Y_0 = Y^{(1)}$.
2.Use the Euler method to calculate Y_n for $Y_0 = Y_0^{(0)}$ to obtain $Y_n^{(0)}$.
3.Use the Euler method to calculate Y_n for $Y_0 = Y_0^{(1)}$ to obtain $Y_n^{(1)}$.
4.Predict a new initial guess $Y_0 = Y_0^{(2)}$ using the secant method:

$$Y_0^{(2)} = Y_0^{(1)} - \frac{Y_0^{(1)} - Y_0^{(0)}}{Y_n^{(1)} - Y_n^{(0)}}\left[Y_n^{(1)} - y_b\right].$$

5.Replace $Y_0^{(0)} \leftarrow Y_0^{(1)}$, $Y_n^{(0)} \leftarrow Y_n^{(1)}$ and $Y_0^{(1)} \leftarrow Y_0^{(2)}$.
6.If tolerance not satisfied, repeat from step 3

The convergence could be tested either from $|Y_0^{(1)} - Y_0^{(0)}|$ or $Y_n^{(1)} - y_b$. The linear interpolation and bisection methods may be expressed similarly. Newton Raphson method would be more difficult as

(d) For the first step we have

$$Y_1 = Y_0 + y_0\Delta x$$

$$y_1 = y_0 + Y_0\Delta x$$

The second step is then

$$\begin{aligned} Y_2 &= Y_1 + y_1\Delta x \\ &= Y_0 + y_0\Delta x + (y_0 + Y_0\Delta x)\Delta x \\ &= Y_0(1 + \Delta x^2) + 2y_0\Delta x \end{aligned}$$

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For $Y_0 = Y_0^{(0)} = 0$, this predicts $y_b = y_2 = 5/4$. Similarly for $Y_0 = Y_0^{(1)} = -1$, this predicts $y_b = y_2 = 1/4$.

We require $y_b = 1/2$. Defining $f(Y_0) = y_2 - 1/2$, the linear interpolation method gives an improved estimate $Y_0 = Y_0^{(2)}$ as

$$\begin{aligned} Y_0^{(2)} &= Y_0^{(0)} - \frac{Y_0^{(1)} - Y_0^{(0)}}{f\left(Y_0^{(1)}\right) - f\left(Y_0^{(0)}\right)} f\left(Y_0^{(0)}\right) \\ &= 0 - \frac{-1-0}{-\frac{1}{4} - \frac{3}{4}}\frac{3}{4} \\ &= -\frac{3}{4} \end{aligned}$$

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