Appendix 1

Numerical methods

§ A.0 *Introduction*

In Chapter 10, the methods of *interpolation* and *extrapolation* were invoked in the description of a numerical system for internal ballistics. These are approximation methods that are very widely used in numerical analysis, but in the spirit of not requiring the reader to consult another book to understand what is being discussed in this book, a short explanation of these methods is given here

§ A.1 *Integration by Extrapolation*

Extrapolation is to estimate an unknown value based on extending a known sequence of values or facts beyond the range over which they have been evaluated.

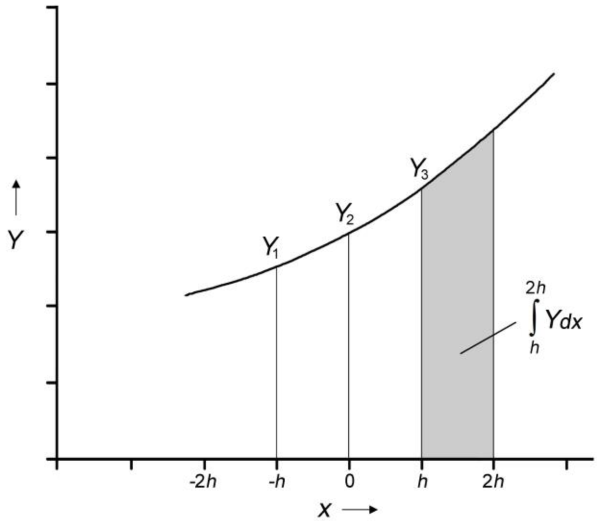

Fig. A.1 *A set of data exists for values of Y at regularly spaced values of x up to the value Y_3. The integral of Ydx is required beyond the known data set.*

Suppose there is a set of data with values Y which has been assessed as a function of x. Values of Y are only known up to Y_3 so some approximation of how Y varies beyond Y_3 is required so that the integration from $x = h$ to $x = 2h$ can be realised.

Suppose that the variation of Y with x is smooth enough that over the distance $2h$ it appears to be well approximated by a quadratic function such that,

$$Y = ax^2 + bx + c \qquad \text{A.1}$$

where a, b and c are constants. As there are three constants, their values may be determined from the values of Y for three values of x. As is often the case in sets of experimental data, the values of x are regularly spaced.

To find an expression for the integral, a similar approach is used as for the well known Simpson's Rule.

It is convenient to set the origin such that the x value for Y_2 is zero and no generality is lost in so doing. Three equations may now be written.

$$\begin{aligned} Y_1 &= ah^2 - bh + c \\ Y_2 &= c \\ Y_3 &= ah^2 + bh + c \end{aligned} \qquad \text{A.2}$$

And with a little manipulation the constants can be expressed in terms of Y,

$$\begin{aligned} ah^2 &= \frac{1}{2}Y_1 - Y_2 + \frac{1}{2}Y_3 \\ bh &= -\frac{3}{2}Y_1 + 2Y_2 - \frac{3}{2}Y_3 \\ c &= Y_2 \end{aligned} \qquad \text{A.3}$$

The integral of Y from h to $2h$ can now be written as,

$$\int_h^{2h} Y dx = \left[\frac{ax^3}{3} + \frac{bx^2}{2} + cx\right]_h^{2h} = h\left[\frac{7}{3}ah^2 + \frac{3}{2}bh + c\right] \qquad \text{A.4}$$

Substituting now for ah^2, bh and c from above, the integral can finally be rendered in terms of the known values of Y_1, Y_2 and Y_3

$$\int_h^{2h} Y dx = \frac{h}{12}\left(5Y_1 - 16Y_2 + 23Y_3\right) \qquad \text{A.5}$$

Since the integral contains terms in x^3, the error in the integral by assuming a quadratic fit to the data points will be in the unknown x^4 terms so the error in the integral then goes as h^4. This is termed as a "forth order" extrapolation.

Similarly, the integration from $x = 0$ to $x = h$ can be expressed as,

$$\int_0^h Y dx = \frac{h}{12}\left(-Y_1 + 8Y_2 + 5Y_3\right) \qquad \text{A.6}$$

though this should strictly termed an interpolation as the values of Y at $x = 0$ and $x = h$ are known.

§ A.2 *Interpolation*

Interpolation is the mathematical procedure to obtain a value or values between two points having prescribed values. As above, data sets often come as values of Y spaced at regular intervals of x. For example, powder companies will often publish spot values of vivacity for a particular powder given for values of Z (the fraction of propellant burnt) from 0 to 1 at one-tenth increment intervals. For this data to be useful it is necessary to be able to estimate vivacity values between those given. Where there is no analytic form for the way in which data points Y will vary as x, it necessary to resort to a method of reasonably estimating what the values of Y would be for intermediate values of x.

The usual approach is to assume that the unknown function Y with x will vary smoothly between three consecutive data points Y_1, Y_2 and Y_3 such that a quadratic form through the three points will satisfactorily represent the data between the points. It can be argued that if a higher order polynomial is needed, then the sample interval in x is too large. Thus, for the example above where it is defined that the x value at Y_2 value is zero, then the constants a, b and c can be written in terms of Y as,

$$\begin{aligned} a &= \frac{1}{h^2}\left[\frac{1}{2}Y_1 - Y_2 + \frac{1}{2}Y_3\right] \\ b &= \frac{1}{h}\left[-\frac{3}{2}Y_1 + 2Y_2 - \frac{3}{2}Y_3\right] \\ c &= Y_2 \end{aligned} \qquad \text{A.7}$$

and the equation $Y = ax^2 + bx + c$ can now be solved for any value of x. Such solutions would be deemed valid between $x = -h$ and x = h as this is the region where the constants were evaluated. For values of x beyond $x = -h$ and x = h another three sequential given values of Y should be chosen such that the required value of Y is within their range.

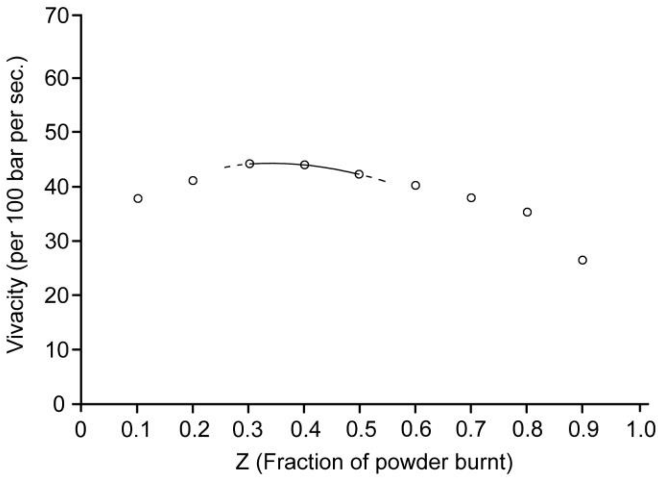

Fig. A.2 *Spot vivacity data for IMR4350 powder for one-tenth increment values of* Z *the fraction of powder mass burnt. A quadratic fit is shown between the data points* Z = 0.3 *to* Z = 0.5.

Of course, though the x origin was put at the x value at Y_2 in this case, it could be more convenient in any particular circumstance to place the origin at the x value for Y_1 or Y_3 and a similar procedure could be followed to obtain the constants a, b and c in terms of Y_1, Y_2 and Y_3