75.41 A "flat" function with some interesting properties and an application

The purpose of this note is to highlight some important properties of a function which plays a key rôle in the study of mathematical physics as well as in some aerodynamic applications. Although such material is normally beyond the scope of an "A" level student, the particular function in question has some interesting properties which are accessible to sixth formers, and gives practice in certain techniques of the calculus, including limits.

Furthermore, the function occurs in the study of reaction rates in physical chemistry, also studied at "A" level. Since it is important, if possible, to discuss topics in pure mathematics, e.g. calculus, that are motivated by, or connected with an application, we provide a few brief details on this topic at the end. For the purposes of a classroom discussion, the ideas as presented here can be taken in reverse, with the application providing the motivation.

Consider the function

$$f(x) = \exp(-1/x)$$

whose shape is shown in the figure, and can easily be plotted using a graphics calculator. From this we can see a number of important properties. Firstly, the function satisfies

$$f(0) = \lim_{x \to 0} \exp(-1/x) = 0$$

where $x \to 0$ means approaching 0 from the right on the real axis. Also

$$\begin{aligned} f'(0) &= \lim_{x \to 0} \frac{\exp(-1/x)}{x^2} \\ &= \lim_{X \to \infty} \frac{X^2}{\exp(X)} \\ &= \lim_{X \to \infty} \frac{2X}{\exp(X)} \\ &= \lim_{X \to \infty} \frac{2}{\exp(X)} = 0 \end{aligned}$$

where $X = 1/x$, and we have used l'Hôpital's rule twice. Similarly, $f''(0) = 0$, and all derivatives of f vanish at $x = 0$, showing that f is a "flat" function at the origin. We leave the proof of this as an exercise for the reader!

This does not mean, however, that the function is as uninteresting as this might indicate. If we attempt to determine the Maclaurin series for f we find that

$$f(x) = 0 + x.0 + \frac{x^2}{2!}.0 + \cdots$$

which clearly makes little sense, except to say that f has *no* Maclaurin series, an unusual feature of a smooth function. Essentially, since a Maclaurin series replaces/approximates a function by a polynomial, this says that f can *not* be represented in this way. This is because f decays *faster* than any power of x, as $x \to 0$, and worth pointing out to "A" level students, or left for them to investigate. We also see that

$$f(\infty) = \lim_{x \to \infty} \exp(-1/x) = 1$$

so that f has an upper bound of unity, which is not obvious from the figure.

Another interesting feature, which can be seen from the figure, is that the slope of f initially increases, until reaching a point of inflection, and then decreases. Since

$$f''(x) = (1/x^4 - 2/x^3) \exp(-1/x),$$

then $f''(x) = 0$ when $x = 1/2$.

Finally, consider the (rather unpleasant!) chemical reaction

$$CO + Cl_2 \to COCl_2,$$

where carbon monoxide (CO) reacts (under the influence of ultra-violet light) with chlorine (Cl_2) to produce carbonyl chloride or phosgene ($COCl_2$). Such a reaction proceeds at a rate which is proportional to the product of the concentrations of the reactants, which in this case are carbon monoxide and chlorine. The constant of proportionality k is known as the rate constant (or velocity constant) and is hence given by

$$\text{rate} = k[CO][Cl_2],$$

where [CO] and [Cl_2] denote the concentrations of CO and Cl_2, respectively. (Clearly, since the reactants are continually being used up it follows that the rate of reaction will steadily fall as the reaction proceeds.)

Importantly, the rate of reaction is greatly affected by temperature. The explanation for this is based on the fact that molecules must collide before they can react, and that only certain molecules having above a certain minimum amount of kinetic energy react when they collide. The energy barrier required for reaction is known as the activation energy E_A, and raising the temperature increases the proportion of molecules with kinetic energy in excess of the value of E_A, and hence the rate of reaction. The connection between the rate of reaction constant k and the absolute temperature T for a particular reaction is through the Arrhenius equation

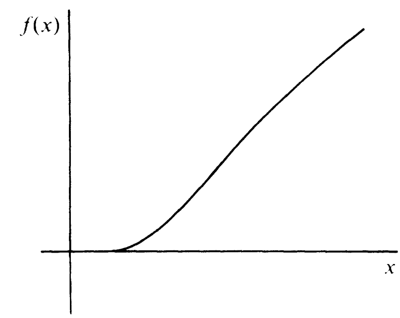
$$k = A \exp(-E_A/RT),$$

where E_A is as before, A is known as the Arrhenius factor and is a constant for a given reaction, and R is the gas constant.

We now observe that this equation contains the function in question. Hence, all the features mentioned above can be discussed in the context of the physical meaning of this expression, in particular, the exponential factor provides for the marked effect that increasing the temperature has on the proportion of high kinetic energy molecules. In order to determine more precisely the qualitative, and quantitative behaviour of this function, and hence that of k, and more importantly, to determine an approximation for small T (as a means of evaluating it), we would normally use a Maclaurin series. We have seen in this case, however, that a straightforward Maclaurin series can not be found. As an alternative, we can write

$$\exp(-E_A/RT) = \frac{1}{\exp(E_A/RT)} = \frac{1}{1 + E_A/RT + (E_A/RT)^2/2! + \cdots}$$

using the standard power series for exp. Truncation of the series on the denominator will achieve all these aims, and we leave the reader to experiment with this.



PAUL GLAISTER

Department of Mathematics, PO Box 220, University of Reading, Reading RG6 2AX

75.42 The generalised Steiner point for a triangle

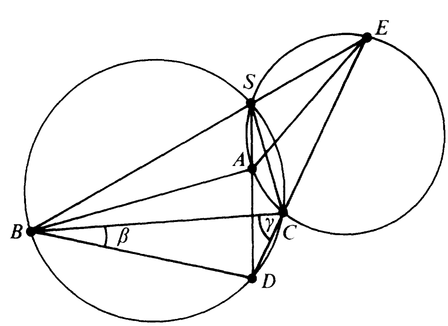


FIGURE 1.