THE NUMERICAL CALCULATION OF $\int_0^\infty x^m e^{-x} f(x)\,dx$

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The type of integral considered, $\int_0^\infty x^m e^{-x} f(x)\,dx$ $(m > 0)$, is of frequent occurrence in problems in the kinetic theory of gases and in particular is required in the paper which follows, in calculating viscosity. The result is an extension of one given by Berger*, and the analysis follows closely the discussion of Gauss's formula for approximate quadrature in Whittaker and Robinson, *The calculus of observations*; the novelty lies in the use of Sonine polynomials†, which are peculiarly well suited for the discussion of this type of integral.

The Sonine polynomial $T_m^n(x)$ is usually defined by the expansion

$$(1+s)^{-m-1}\exp\left(\frac{xs}{1+s}\right) = \sum_{n=0}^{n=\infty} \Gamma(m+n+1)\, s^n T_m^n(x),$$

but in kinetic theory it is advantageous to use the modified function‡

$$S_m^n(x) = (-1)^n T_m^n(x).$$

The following properties of the polynomials are readily established:

(i) $S_m^n(x) \equiv \dfrac{1}{n!\,\Gamma(m+1)}\left[1 - \dfrac{n}{m+1}\dfrac{x}{1!} + \dfrac{n(n-1)}{(m+1)(m+2)}\dfrac{x^2}{2!} - \cdots\right]$;

(ii) the zeros of $S_m^n(x)$ are all real and different;

(iii) $\dfrac{d}{dx} x^m S_m^n(x) = x^{m-1} S_{m-1}^n(x)$;

(iv) $\int_0^\infty x^m S_m^n(x)\, S_m^r(x)\, e^{-x} dx = 0, \quad r \neq n.$

If $f(x)$ is a function whose $2n$th differences are negligible, it can be represented by a polynomial of degree $2n-1$, or by a series of Sonine polynomials of the form

$$S_m^n(x) \sum_{r=0}^{r=n-1} A_r S_m^r(x) + \sum_{k=1}^{k=n} B_k \frac{S_m^n(x)}{x - x_k},$$

* Berger, *Nova Acta Upsaliensis* (3), 16 (1893).

† These are effectively the same polynomials as are used by Schrödinger in his well-known papers on wave mechanics under the name of generalized Laguerre polynomials; but I have preferred to follow the nomenclature and notation of earlier authors—cf. for example Whittaker and Watson, *Modern analysis*, 4th ed. (Cambridge, 1927), p. 352, ex. 8, and Bateman, *Electrical and optical wave motion* (Cambridge, 1915), 98.

‡ Cf. Burnett, *Proc. Lond. Math. Soc.* (2), 39 (1935), 385.

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where $x_1, x_2, \ldots, x_n$ are the n different real zeros of $S_m^n(x)$; so that

$$f(x_k) = B_k \left[\frac{d}{dx} S_m^n(x)\right]_{x=x_k}$$

and

$$x_k^m f(x_k) = B_k \left[\frac{d}{dx} x^m S_m^n(x)\right]_{x=x_k}$$
$$= B_k x_k^{m-1} S_{m-1}^n(x_k).$$

Now by virtue of (iv) above it follows that

$$\int_0^\infty x^m e^{-x} f(x)\, dx = \sum_{k=1}^{k=n} B_k \int_0^\infty \frac{S_m^n(x)}{x - x_k} x^m e^{-x} dx$$
$$= \sum_{k=1}^{k=n} B_k C_k x_k^{m-1} S_{m-1}^n(x_k)$$
$$= \sum_{k=1}^{k=n} C_k x_k^m f(x_k),$$

where C_k is a constant defined by

$$C_k x_k^{m-1} S_{m-1}^n(x_k) = \int_0^\infty \frac{S_m^n(x)}{x - x_k} x^m e^{-x} dx.$$

Hence, if $D_k = C_k x_k^m$, $\quad \int_0^\infty x^m e^{-x} f(x)\, dx = \sum_{k=1}^{k=n} D_k f(x_k)$.

If $n = 1$, i.e. if the second differences of $f(x)$ are negligible*,

$$S_m^1(x) = \frac{1}{\Gamma(m+1)}\left(1 - \frac{x}{m+1}\right),$$

so that

$$x_1 = m + 1$$

and

$$C_1 (m+1)^{m-1} \frac{1}{\Gamma(m)}\left(1 - \frac{m+1}{m}\right) = -\frac{1}{\Gamma(m+2)} \int_0^\infty x^m e^{-x} dx = -\frac{1}{m+1},$$

that is

$$C_1 = \frac{1}{(m+1)^m} \Gamma(m+1).$$

Hence the first approximation to the integral is

$$\Gamma(m+1) f(m+1).$$

If $n = 2$, $\quad S_m^2(x) = \frac{1}{2\Gamma(m+1)}\left[1 - \frac{2}{m+1} x + \frac{1}{(m+1)(m+2)} x^2\right]$,

and, if the zeros of this are x_1 and x_2,

$$C_1 x_1^{m-1} S_{m-1}^2(x_1) = \int_0^\infty \frac{x - x_2}{2\Gamma(m+3)} x^m e^{-x} dx = \frac{\Gamma(m+1)}{2\Gamma(m+3)} (m + 1 - x_2).$$

Similarly

$$C_2 x_2^{m-1} S_{m-1}^2(x_2) = \frac{\Gamma(m+1)}{2\Gamma(m+3)} (m + 1 - x_1).$$

* This case is trivial but is given for completeness and to illustrate the method.

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The corresponding formulae for $n = 3, 4, \ldots$ can be obtained in the same way, and need not be written out.

The cases which are of importance in kinetic theory* have $m = 2$, 3, and 4, and we give specific formulae for these with $n = 2$ and $n = 3$.

Case 1 (*a*), $m = 2$, $n = 2$. The equation determining x_1 and x_2 is

$$x^2 - 8x + 12 = 0,$$

so that $$x_1 = 2, \; x_2 = 6.$$

Also $$D_1 = C_1 x_1^2 = x_1 \frac{3 - x_2}{2(x_1^2 - 6x_1 + 6)},$$

on inserting the value of $S_{m-1}^2(x_1)$, and this gives

$$D_1 = \tfrac{3}{2}.$$

By symmetry $$D_2 = x_2 \frac{3 - x_1}{2(x_2^2 - 6x_2 + 6)} = \tfrac{1}{2}.$$

Hence $$\int_0^\infty x^2 e^{-x} f(x)\, dx = \tfrac{3}{2} f(2) + \tfrac{1}{2} f(6),$$

provided that the fourth differences of $f(x)$ are negligible.

Case 1 (*b*), $m = 2$, $n = 3$. Here x_1, x_2, x_3 are the roots of $S_2^3(x) = 0$, that is of $x^3 - 15x^2 + 60x - 60 = 0$.

These are found to be $x_1 = 1{\cdot}5173$, $x_2 = 4{\cdot}3116$, $x_3 = 9{\cdot}1711$, to 4 places of decimals. Hence

$$\begin{aligned} D_1 = C_1 x_1^2 &= \frac{x_1}{S_1^3(x_1)} \int_0^\infty \frac{S_2^3(x)}{x - x_1} x^2 e^{-x} dx \\ &= \frac{x_1}{720\, S_1^3(x_1)} \int_0^\infty (x - x_2)(x - x_3)\, x^2 e^{-x} dx \\ &= \frac{x_1}{720\, S_1^3(x_1)} \{4! - 3!(x_2 + x_3) + 2!\, x_2 x_3\}, \end{aligned}$$

and this, after substitution for $S_1^3(x_1)$ and some reduction, is found to be

$$D_1 = \frac{2}{5} \frac{x_1^2 - 11x_1 + 20}{x_1^2 - 8x_1 + 12}.$$

D_2 and D_3 are, of course, given by similar expressions in which x_1 is replaced by x_2 and x_3 respectively. The values are found to be $D_1 = 1{\cdot}0374$, $D_2 = 0{\cdot}9058$, $D_3 = 0{\cdot}0568$ to 4 places of decimals as before. Hence if the sixth differences of $f(x)$ are negligible

$$\int_0^\infty x^2 e^{-x} f(x)\, dx = 1{\cdot}0374 f(1{\cdot}5173) + 0{\cdot}9058 f(4{\cdot}3116) + 0{\cdot}0568 f(9{\cdot}1711).$$

* Cf. Chapman, *Phil. Trans. Roy. Soc.* 211 (1911), 433; Massey and Mohr, *Proc. Roy. Soc.* 141 (1933), 434.

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Case 2 (*a*), $m = 3$, $n = 2$. Here x_1 and x_2 are the roots of $x^2 - 10x + 20 = 0$, so that

$$x_1 = 5 - \sqrt{5} = 2{\cdot}763932, \quad x_2 = 5 + \sqrt{5} = 7{\cdot}236068.$$

Also
$$D_1 = x_1 \frac{4 - x_2}{40} \frac{48}{x_1^2 - 8x_1 + 12} = \frac{3x_1}{5} \frac{x_2 - 4}{4 - x_1} = \frac{12}{5} \frac{5 - x_1}{4 - x_1} = 4{\cdot}341641,$$

$$D_2 = \frac{12}{5} \frac{5 - x_2}{4 - x_2} = 1{\cdot}658359,$$

and so, neglecting fourth differences of $f(x)$,

$$\int_0^\infty x^3 e^{-x} f(x)\, dx = 4{\cdot}34164 f(2{\cdot}76393) + 1{\cdot}65836 f(7{\cdot}23607).$$

Case 2 (*b*), $m = 3$, $n = 3$. The equation determining x_1, x_2, x_3 is

$$x^3 - 18x^2 + 90x - 120 = 0,$$

from which it is found that

$$x_1 = 2{\cdot}1413, \quad x_2 = 5{\cdot}3154, \quad x_3 = 10{\cdot}5433;$$
$$D_1 = 2{\cdot}8365, \quad D_2 = 2{\cdot}9512, \quad D_3 = 0{\cdot}2124,$$

the working being similar to that in case 1 (*b*). Hence, if the sixth differences of $f(x)$ are neglected,

$$\int_0^\infty x^3 e^{-x} f(x)\, dx = 2{\cdot}8365 f(2{\cdot}1413) + 2{\cdot}9512 f(5{\cdot}3154) + 0{\cdot}2124 f(10{\cdot}5433).$$

Case 3 (*a*), $m = 4$, $n = 2$. The equation for x_1 and x_2 is

$$x^2 - 12x + 30 = 0,$$

so that
$$x_1 = 6 - \sqrt{6} = 3{\cdot}55051, \quad x_2 = 6 + \sqrt{6} = 8{\cdot}44949$$

and the values of D_1 and D_2 are found as before to be

$$D_1 = 16{\cdot}89898, \quad D_2 = 7{\cdot}10102.$$

Hence, neglecting the fourth differences of f,

$$\int_0^\infty x^4 e^{-x} f(x)\, dx = 16{\cdot}8990 f(3{\cdot}5505) + 7{\cdot}1010 f(8{\cdot}4495).$$

Case 3 (*b*), $m = 4$, $n = 3$. The equation for x is

$$x^3 - 21x^2 + 126x - 210 = 0,$$

which gives
$$x_1 = 2{\cdot}7963, \quad x_2 = 6{\cdot}3185, \quad x_3 = 11{\cdot}8852.$$

It is also found that

$$D_1 = 10{\cdot}554, \quad D_2 = 12{\cdot}453, \quad D_3 = 0{\cdot}993,$$

and so

$$\int_0^\infty x^4 e^{-x} f(x)\, dx = 10{\cdot}554 f(2{\cdot}7963) + 12{\cdot}453 f(6{\cdot}3185) + 0{\cdot}993 f(11{\cdot}8852),$$

provided that the sixth differences of $f(x)$ can be neglected.

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