ZEROS OF THE HERMITE POLYNOMIALS AND WEIGHTS FOR GAUSS' MECHANICAL QUADRATURE FORMULA

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In the numerical integration of a function $f(x)$ it is very desirable to choose the set of values $\{x_i\}$ at which the function $f(x)$ is to be observed, for it is generally possible to obtain the same accuracy with fewer points when these points are especially selected. Gauss[1] gave such a proof for the case of the finite range $(-1, +1)$ and established that the "best" accuracy with n ordinates is obtained when the corresponding abscissae are the n roots of the Legendre polynomials, $P_n(x)=0$. For this case there obtains

$$\int_{-1}^{1} f(x)dx \simeq \sum_{i=1}^{n} \lambda_{i,n} f(x_{i,n}) \tag{1}$$

where the numbers $\{x_{i,n}\}$ are the zeros of $P_n(x)$ and where the numbers $\{\lambda_{i,n}\}$ are the Christoffel or Cotes numbers. Formula (1) is exact whenever $f(x)$ is a polynomial of degree $(2n-1)$ or less. Values of the zeros $\{x_{i,n}\}$ and the corresponding Christoffel numbers $\{\lambda_{i,n}\}$ for the Legendre polynomials for $n=1$ to $n=16$ have been tabulated by the Mathematical Tables Project.[2] The range of integration can be chosen to be any finite range (p, q) with suitable modification[2] of the zeros $\{x_{i,n}\}$ and the constants $\{\lambda_{i,n}\}$.

It is understood that while selection of the abscissae $\{x_{i,n}\}$ is very desirable for theoretical reasons, it may not always be practicable to measure the ordinates of $f(x)$ at these values.

For the infinite range $(-\infty, +\infty)$ a similar situation holds for the Hermite polynomials. These may be defined by the relation

$$\begin{aligned} H_n(x) &= (-1)^n e^{x^2} \frac{d^n(e^{-x^2})}{dx^n} \\ &= (2x)^n - \frac{n(n-1)}{1!}(2x)^{n-2} \\ &\quad + \frac{n(n-1)(n-2)(n-3)}{2!}(2x)^{n-4} \pm \cdots . \end{aligned} \tag{2}$$

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[1] C. F. Gauss, *Methodus nova integralium valores per approximationem inveniendi*, Werke, vol. 3, pp. 163–196.

[2] A. N. Lowan, Norman Davids and Arthur Levenson, *Table of the zeros of the Legendre polynomials of order* 1–16 *and the weight coefficients for Gauss' mechanical quadrature formula*, Bull. Amer. Math. Soc. vol. 48 (1942) pp. 739–743.

For n even, the last term is

$$(-1)^{n/2}\frac{n!}{(n/2)!}$$

and for n odd, the last term is

$$(-1)^{(n-1)/2}\frac{n!}{((n-1)/2)!}(2x).$$

These polynomials obey the recursion relations

$$H_{n+1}(x) - 2xH_n(x) + 2nH_{n-1}(x) = 0, \tag{3}$$

$$H_n'(x) = 2nH_{n-1}(x). \tag{4}$$

[Some writers, including many statisticians, prefer to use

$$h_n(x) = e^{x^2/2}\frac{d^n(e^{-x^2/2})}{dx^n} \tag{5}$$

as the defining relation for Hermite polynomials. The relation between these two sets of polynomials is given by

$$H_n(x) = (-2^{1/2})^n h_n(2^{1/2}x).] \tag{6}$$

The approximate numerical integration formula for functions $f(x)$ on the infinite range $(-\infty, +\infty)$ with the weight function $\exp(-x^2)$ is

$$\int_{-\infty}^{\infty} e^{-x^2}f(x)dx \simeq \sum_{i=1}^{n}\lambda_{i,n}f(x_{i,n}) \tag{7}$$

where the set $\{x_{i,n}\}$ is the set of roots defined by

$$H_n(x) = 0 \tag{8}$$

and where the set $\{\lambda_{i,n}\}$ is given by[3]

$$\lambda_{i,n} = \frac{\pi^{1/2}2^{n+1}n!}{[H_n'(x_{i,n})]^2}. \tag{9}$$

If $f(x)$ is a polynomial of degree $(2n-1)$ or less, integration formula (7) is exact.[4]

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[3] Gabor Szegö, *Orthogonal polynomials*, Amer. Math. Soc. Colloquium Publications, vol. 23, 1939, p. 344.

[4] Szegö, op. cit. Chapter XV.

C. Winston, *On mechanical quadrature formula involving classical orthogonal polynomials*, Ann. of Math. (2) vol. 35 (1934) pp. 658–677.

The zeros $\{X_{i,n}\}$ for the polynomials $h_n(x)$ for $n=1$ to $n=27$ have been tabulated by Smith[5] to six decimal places. The corresponding zeros $\{x_{i,n}\}$ for the Hermite polynomial $H_n(x)$ are given by

$$x_{i,n} = \frac{1}{2^{1/2}} X_{i,n}. \tag{10}$$

Newton's tangent rule was used to improve Smith's values, and the zeros $\{x_{i,n}\}$ for $n=1$ to $n=5$ are tabulated herewith to twelve decimal places and for $n=6$ to $n=10$ to nine decimal places. The set of Christoffel numbers $\{\lambda_{i,n}\}$ were calculated from relation (9).

The results were subject to the following tests:

$$\prod \text{positive roots} = \left(\frac{|\text{coefficient of either } x^0 \text{ or } x \text{ term}|}{\text{coefficient of } x^n \text{ term}}\right)^{1/2}, \tag{11}$$

$$\sum x_{i,n}^2 = \frac{n(n-1)}{2}, \tag{12}$$

$$\sum \lambda_{i,n} = \pi^{1/2}, \tag{13}$$

$$\sum \lambda_{i,n} x_{i,n}^2 = \frac{\pi^{1/2}}{2}, \tag{14}$$

where (11) and (12) are obtained from the algebraic expressions for the products of the roots and the sum of the squares of the roots and where (13) and (14) are obtained from (7) by taking $f(x)=1$ and $f(x)=x^2$ respectively. For the most part, calculations were carried to two more places than were retained.

Because of symmetry, it is convenient to tabulate the zeros of $H_3(x)$ as x_{-1}, x_0, x_1 rather than as x_1, x_2, x_3, and the zeros of $H_4(x)$ as x_{-2}, x_{-1}, x_1, x_2 rather than as x_1, x_2, x_3, x_4, with similar notation for other values of n. Since there is but slight danger of confusion, the second subscript n on the zeros and Christoffel numbers has been omitted. Because of the relations $x_{-i}=-x_i$ and $\lambda_{-i}=\lambda_i$ only values with non-negative subscripts have been tabulated.

$n=1$	$H_1(x)=2x$	
	$x_0=0.000\ 000\ 000\ 000$	$\lambda_0=1.772\ 453\ 850\ 906$
$n=2$	$H_2(x)=4x^2-2$	
	$x_1=0.707\ 106\ 781\ 187$	$\lambda_1=0.886\ 226\ 925\ 453$
$n=3$	$H_3(x)=8x^3-12x$	
	$x_0=0.000\ 000\ 000\ 000$	$\lambda_0=1.181\ 635\ 900\ 604$
	$x_1=1.224\ 744\ 871\ 392$	$\lambda_1=0.295\ 408\ 975\ 151$

[5] E. R. Smith, *Zeroes of the Hermitean polynomials*, Amer. Math. Monthly vol. 43 (1936) pp. 354–358.

$n=4$	$H^4(x)=16x^4-48x^2+12$	
	$x_1=0.524\ 647\ 623\ 275$	$\lambda_1=0.804\ 914\ 090\ 006$
	$x_2=1.650\ 680\ 123\ 886$	$\lambda_2=0.081\ 312\ 835\ 447\ 3$
$n=5$	$H_5(x)=32x^5-160x^3+120x$	
	$x_0=0.000\ 000\ 000\ 000$	$\lambda_0=0.945\ 308\ 720\ 483$
	$x_1=0.958\ 572\ 464\ 614$	$\lambda_1=0.393\ 619\ 323\ 152$
	$x_2=2.020\ 182\ 870\ 456$	$\lambda_2=0.019\ 953\ 242\ 059\ 0$
$n=6$	$H_6(x)=64x^6-480x^4+720x^2-120$	
	$x_1=0.436\ 077\ 412$	$\lambda_1=0.724\ 629\ 595$
	$x_2=1.335\ 849\ 074$	$\lambda_2=0.157\ 067\ 320$
	$x_3=2.350\ 604\ 974$	$\lambda_3=0.004\ 530\ 009\ 90$
$n=7$	$H_7(x)=128x^7-1344x^5+3360x^3-1680x$	
	$x_0=0.000\ 000\ 000$	$\lambda_0=0.810\ 264\ 618$
	$x_1=0.816\ 287\ 883$	$\lambda_1=0.425\ 607\ 253$
	$x_2=1.673\ 551\ 629$	$\lambda_2=0.054\ 515\ 582\ 8$
	$x_3=2.651\ 961\ 357$	$\lambda_3=0.000\ 971\ 781\ 258$
$n=8$	$H_8(x)=256x^8-3584x^6+13{,}440x^4-13{,}440x^2+1680$	
	$x_1=0.381\ 186\ 990$	$\lambda_1=0.661\ 147\ 013$
	$x_2=1.157\ 193\ 712$	$\lambda_2=0.207\ 802\ 326$
	$x_3=1.981\ 656\ 757$	$\lambda_3=0.017\ 077\ 983\ 0$
	$x_4=2.930\ 637\ 420$	$\lambda_4=0.000\ 199\ 604\ 071$
$n=9$	$H_9(x)=512x^9-9216x^7+48{,}384x^5-80{,}640x^3+30{,}240x$	
	$x_0=0.000\ 000\ 000$	$\lambda_0=0.720\ 235\ 216$
	$x_1=0.723\ 551\ 019$	$\lambda_1=0.432\ 651\ 559$
	$x_2=1.468\ 553\ 289$	$\lambda_2=0.088\ 474\ 527\ 4$
	$x_3=2.266\ 580\ 585$	$\lambda_3=0.004\ 943\ 624\ 28$
	$x_4=3.190\ 993\ 202$	$\lambda_4=0.000\ 039\ 606\ 977\ 4$
$n=10$	$H_{10}(x)=1024x^{10}-23{,}040x^8+161{,}280x^6-403{,}200x^4+302{,}400x^2-30{,}240$	
	$x_1=0.342\ 901\ 327$	$\lambda_1=0.610\ 862\ 634$
	$x_2=1.036\ 610\ 830$	$\lambda_2=0.240\ 138\ 611$
	$x_3=1.756\ 683\ 649$	$\lambda_3=0.033\ 874\ 394\ 5$
	$x_4=2.532\ 731\ 674$	$\lambda_4=0.001\ 343\ 645\ 77$
	$x_5=3.436\ 159\ 119$	$\lambda_5=0.000\ 007\ 640\ 432\ 86$

As an example, consider the evaluation of

$$I=\int_{-\infty}^{\infty} e^{-x^2}\cos x\,dx.$$

The known value of this integral is

$$I = \pi^{1/2}e^{-1/4} \simeq 1.380\ 388\ 447.$$

Using formula (7) to evaluate I approximately, and taking $n=8$ and making use of symmetry, there results

$$\begin{aligned} I &\simeq \sum \lambda_{i,8} \cos (x_{i,8}) \\ &= 2[(0.661\ 147\ 013)(0.928\ 223\ 702) \\ &\quad + (0.207\ 802\ 326)(0.401\ 910\ 767) \\ &\quad + (0.017\ 077\ 983\ 0)(-0.399\ 398\ 300) \\ &\quad + (0.000\ 199\ 604\ 071)(-0.977\ 831\ 340)] \\ &= 1.380\ 388\ 447 \end{aligned}$$

which agrees to nine decimal places with the actual value.

If the function $f(x)$ is expansible in a Taylor's series about the origin, estimates of the error in using (7) may be made as follows: The error (not counting rounding off error) arises from terms in the Taylor's series with powers of x greater than $(2n-1)$ when n ordinates are used. In the example above, the largest error term is that due to the x^{16} term in the expansion of $\cos x$. Since

$$\int_{-\infty}^{\infty} \frac{e^{-x^2}x^{16}}{16!}\, dx = \frac{\pi^{1/2}}{2^{16}\cdot 8!} < 2 \times 10^{-10}$$

and since the neglected terms in the cosine expansion when integrated out as above form an alternating series of decreasing absolute values, the error can be estimated as being less than 2×10^{-10}. This heuristic estimate is not the actual error in the use of integration correspondence (7), but is a sort of an order of magnitude error.

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