ON AN EXPANSION OF THE REMAINDER IN THE GAUSSIAN QUADRATURE FORMULA*

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1. *Introduction.* The Gaussian quadrature formula

$$\int_0^1 f(x)dx = A_1 f(x_1) + A_2 f(x_2) + \cdots + A_n f(x_n), \tag{1}$$

in which $x_1, x_2, \cdots, x_n$ are roots of Legendre's polynomial

$$P_n(x) = \frac{d^n x^n (x-1)^n}{dx^n},$$

and

$$A_i = \int_0^1 \frac{P_n(x)}{(x - x_i)P_n'(x_i)} dx, \quad (i = 1, 2, \cdots, n),$$

is exact in case $f(x)$ is an arbitrary polynomial of degree not exceeding $2n-1$. Otherwise the formula (1) is only approximate, and the difference between its left and right hand sides represents the error or remainder term which will be denoted in what follows by R_n. The expression of this remainder, obtained, if I am not mistaken, for the first time by A. A. Markoff in 1884, is well known. In this article I shall prove that the remainder in the Gaussian formula can be expanded into a series possessing all the properties of the classical Euler-Maclaurin expansion. This is a noteworthy fact, equally important from the theoretical and from the practical point of view.

2. *Expression of R_n.* In what follows we shall adopt E. Nörlund's definition of the Bernoullian polynomial $B_n(x)$ of order n; and we shall define the periodic function $\overline{B}_n(x)$ by the equations

$$\overline{B}_n(x) = B_n(x), \text{ for } 0 \leqq x < 1;$$

$$\overline{B}_n(x+1) = \overline{B}_n(x), \text{ for all } x.$$

With these notations, we have, for $0 \leqq \theta \leqq 1$,

* Presented to the Society, June 20, 1934.

$$f(\theta) = \int_0^1 f(x)dx + \sum_{s=1}^{2n} \frac{B_s(\theta)}{s!}\{f^{(s-1)}(1) - f^{(s-1)}(0)\}$$
$$- \int_0^1 \frac{\overline{B}_{2n}(\theta - t)}{(2n)!} f^{(2n)}(t)dt.$$

Taking here $\theta = x_1, x_2, \cdots, x_n$, multiplying the resulting equations by $A_1, A_2, \cdots, A_n$, and adding them, we get

$$\sum_{i=1}^{n} A_i f(x_i) = \int_0^1 f(x)dx$$
$$+ \frac{1}{(2n)!}\sum_{i=1}^{n} A_i B_{2n}(x_i)\{f^{(2n-1)}(1) - f^{(2n-1)}(0)\} \tag{2}$$
$$- \int_0^1 \frac{f^{(2n)}(t)}{(2n)!} \sum_{i=1}^{n} A_i \overline{B}_{2n}(x_i - t)dt,$$

since for $s = 1, 2, \cdots, 2n-1$,

$$\sum_{i=1}^{n} A_i B_s(x_i) = \int_0^1 B_s(x)dx = 0.$$

For brevity, we shall use the notations

$$\overline{B}_p(\theta - t) - B_p(\theta) = F_p(\theta, t), \qquad \sum_{i=1}^{n} A_i F_p(x_i, t) = G_p(t).$$

Then equation (2) yields

$$R_n = \frac{1}{(2n)!}\int_0^1 G_{2n}(t) f^{(2n)}(t)dt. \tag{3}$$

3. *The Function* $G_p(t)$. It follows immediately from the definition of the function $G_p(t)$ that $G_p(0) = G_p(1) = 0$. Moreover

$$G_{2s}(1 - t) = G_{2s}(t), \qquad G_{2s-1}(1 - t) = - G_{2s-1}(t). \tag{4}$$

The proof of these relations essentially depends upon the fact that the numbers $x_1, x_2, \cdots, x_n$ are symmetrically located with respect to $\frac{1}{2}$, so that, if these numbers are arranged in increasing order, $x_{n-i+1} = 1 - x_i$ and at the same time $A_{n-i+1} = A_i$. We have

$$G_p(1-t) = \sum_{i=1}^{n} A_i\{\overline{B}_p(x_i+t) - B_p(x_i)\}$$

$$= \sum_{i=1}^{n} A_{n-i+1}\{\overline{B}_p(x_{n-i+1}+t) - B_p(x_{n-i+1})\}$$

$$= \sum_{i=1}^{n} A_i\{\overline{B}_p(1+t-x_i) - B_p(1-x_i)\} = (-1)^p G_p(t),$$

which amounts to the two relations written above.

Similarly,

$$\sum_{i=1}^{n} A_i B_{2s-1}(x_i) = \sum_{i=1}^{n} A_{n-i+1} B_{2s-1}(x_{n-i+1}) = \sum_{i=1}^{n} A_i B_{2s-1}(1-x_i)$$

$$= -\sum_{i=1}^{n} A_i B_{2s-1}(x_i),$$

whence

$$\sum_{i=1}^{n} A_i B_{2s-1}(x_i) = 0,$$

so that $G_{2s-1}(t)$ can be written in the simple form

$$G_{2s-1}(t) = \sum_{i=1}^{n} A_i \overline{B}_{2s-1}(x_i - t).$$

Since

$$\overline{B}_n'(x) = n\overline{B}_{n-1}(x),$$

it follows from the last expression for $G_{2s-1}(t)$ that

$$(5)\qquad \begin{aligned} G_{2s}'(t) &= -2s\,G_{2s-1}(t),\\ G_{2s}''(t) &= 2s(2s-1)\left[G_{2s-2}(t) + \sum_{i=1}^{n} A_i B_{2s-2}(x_i)\right]. \end{aligned}$$

Furthermore

$$(6)\qquad G_{2s+1}''(t) = 2s(2s+1)G_{2s-1}(t).$$

4. *Sign of* $G_{2s}(t)$. Our main purpose is to show that, for $s \geqq n$, functions $G_{2s}(t)$ do not change sign in the interval $0<t<1$. To this end let β_s and α_s represent the number of distinct roots of the equations $G_{2s}(t)=0$ and $G_{2s-1}(t)=0$ in the interval $0<t<1$, respectively. The second of the relations (4) shows that

$G_{2s-1}(1/2)=0$; hence $\alpha_s \geqq 1$. It follows from the first of the relations (5) and Rolle's theorem that $\beta_s+1 \leqq \alpha_s$, because $G_{2s}(0) = G_{2s}(1)=0$. Again, using (6) and applying Rolle's theorem twice, we get $\alpha_s \leqq \alpha_{s-1}$, so that, for $s \geqq n$, $\beta_s+1 \leqq \alpha_n$. But if $0 \leqq t \leqq 1$, we have

$$\begin{aligned} G_{2n-1}(t) &= \sum_{i=1}^{n} A_i \overline{B}_{2n-1}(x_i - t) \\ &= \sum_{i=1}^{n} A_i B_{2n-1}(x_i - t) + (2n-1) \sum_{x_i \leq t} A_i (x_i - t)^{2n-2}, \end{aligned}$$

where the second sum in the right member contains only terms in which $x_i \leqq t$. On the other hand, we have

$$\begin{aligned} \sum_{i=1}^{n} A_i B_{2n-1}(x_i - t) &= \int_0^1 B_{2n-1}(x - t)dx \\ &= \frac{1}{2n}\{B_{2n}(1-t) - B_{2n}(-t)\} = -t^{2n-1}, \end{aligned}$$

because $B_{2n-1}(x-t)$ is a polynomial in x of degree $2n-1$. It follows that $G_{2n-1}(t)$ differs only by a constant factor from the function

$$R_0(t) = \frac{t^{2n-1}}{2n-1} - \sum_{x_i \leq t} A_i(x_i - t)^{2n-2},$$

which represents the remainder in the Gaussian formula applied to the function defined by the equations

$$\begin{aligned} f(x) &= (x-t)^{2n-2}, && \text{if } x \leqq t, \\ f(x) &= 0, && \text{if } x > t. \end{aligned}$$

5. *Fundamental Lemma. The equation* $R_0(t)=0$ *has one and only one root in the interval* $0<t<1$.

PROOF. Let

$$R_k(t) = \frac{(-1)^k t^{2n-k-1}}{2n-k-1} - \sum_{x_i \leqq t} A_i(x_i - t)^{2n-k-2}$$

for $k=0, 1, 2, \cdots, 2n-2$. The functions $R_0(t), R_1(t), \cdots, R_{2n-3}(t)$ are evidently continuous, but

$$R_{2n-2}(t) = t - \sum_{x_i \leq t} A_i$$

is discontinuous at $x_1, x_2, \cdots, x_n$. By the fundamental property of the Gaussian formula, $R_k(1) = R_k(0) = 0$. On the other hand, $R_k'(t) = -(2n-k-2)R_{k+1}(t)$, for $k = 0, 1, 2, \cdots, 2n-3$. Hence, if N_k is the number of distinct roots of the equation $R_k(t) = 0$, we shall have, by Rolle's theorem, $N_k + 1 \leqq N_{k+1}$ for $k = 0, 1, 2, \cdots, 2n-4$. Hence $N_{2n-3} \geqq N_0 + 2n - 3$. But $N_{2n-3}+1$ cannot exceed the number of variations of sign of $R_{2n-2}(t)$ when t increases from 0 to 1. Let this number be denoted by N_{2n-2}. Then first, $N_0 + 2n - 2 \leqq N_{2n-2}$; and, second, $N_{2n-2} \leqq 2n-1$. For, $R_{2n-2}(t)$ can change sign not more than once in each of the $n-1$ intervals (x_i, x_{i+1}), $(i = 1, 2, \cdots, n-1)$, and also possibly at $t = x_1, x_2, \cdots, x_n$. Since $N_0 = \alpha_k \geqq 1$, the inequality $N_0 + 2n - 2 \leqq 2n - 1$ shows that $N_0 = \alpha_n = 1$.

6. *Expansion of* R_n. Since $\alpha_n = 1$, the inequality $\beta_s + 1 \leqq \alpha_n = 1$ established for $s \geqq n$ shows that $\beta_s = 0$, that is, $G_{2s}(t)$ *does not change its sign in the interval* $0 < t < 1$, if $s \geqq n$. After this fundamental point has been established, it suffices to use the formula

$$G_{2s}''(t) = 2s(2s-1)\left[G_{2s-2}(t) + \sum_{i=1}^{n} A_i B_{2s-2}(x_i)\right],$$

and to apply repeatedly integration by parts to the integral in (3) in order to arrive at the following expansion of R_n:

$$R_n = \sum_{s=0}^{k-1} c_s \{f^{(2n+2s-1)}(1) - f^{(2n+2s-1)}(0)\} + c_k f^{(2n+2k)}(\xi), \tag{7}$$

where

$$c_s = -\frac{1}{(2n+2s)!}\sum_{i=1}^{n} A_i B_{2n+2s}(x_i) = -\frac{\gamma_{2n+2s}}{(2n+2s)!},$$

and where ξ is an unknown number between 0 and 1. To show that the expansion (7) possesses all the properties of the Euler-Maclaurin expansion, it suffices to prove that numbers $\gamma_{2n}, \gamma_{2n+2}, \gamma_{2n+4}, \cdots$ alternate in sign. To this end, we remark first that

$$\int_0^1 G_{2n+2s}(t)dt = -\gamma_{2n+2s},$$

and, second, that the sign of $G_{2n+2s}(t)$ in the interval $(0, 1)$ is the same as the sign of

$$G''_{2n+2s}(0) = (2n + 2s)(2n + 2s - 1)\gamma_{2n+2s-2}.$$

Hence γ_{2n+2s} and $\gamma_{2n+2s-2}$ have opposite signs, which was to be proved.

The coefficient c_0 is positive. For, since for small values of t the derivative $G'_{2n}(t)$ is greater than 0, $G_{2n}(t)$ will be positive for $0<t<1$; hence $\gamma_{2n}<0$ and $c_0>0$. Thus in general $(-1)^s c_s>0$. The expansion (7) is especially useful in numerical applications when all derivatives of an even order $\geqq 2n$ have the same sign in $(0, 1)$. For then, if we retain a certain number of terms in (7), the error in R_n will in absolute value be less than the first neglected term and will have the same sign as this term.

7. *Values of* c_n. The simplest way of finding the general expressions of $c_0, c_1, c_2, \cdots$ consists in taking in the Gaussian formula successively $f(x)=P_nP_n$, P_nP_{n+2}, P_nP_{n+4}, $\cdots$. Then $c_0, c_1, c_2, \cdots$ are one by one determined by a set of linear equations. While this method is theoretically simple, nevertheless the actual calculation is very laborious. Here are the expressions of c_0, c_1, c_2:

$$c_0=\left\{\frac{1\cdot 2\cdot 3 \cdots n}{(n+1)(n+2)\cdots 2n}\right\}^2 \frac{1}{(2n+1)!},$$

$$c_1=-\frac{n(4n^2+5n-2)}{24(n+1)(2n-1)(2n+3)}c_0,$$

$$c_2=\frac{n(112n^6+384n^5-151n^4-1184n^3-105n^2+635n-156)}{2880(n+1)(n+2)(2n-3)(2n-1)^2(2n+3)(2n+5)}c_0.$$

For particular values of n approximate values of the following coefficients $c_3, c_4, \cdots$ can be found without excessive labor by another method.

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