On Some Gauss and Lobatto Based Integration Formulae

By T. N. L. Patterson

1. Introduction. The economy of the Gaussian quadrature formulae for carrying out numerical integration is to some extent reduced by the fact that an increase in the order of the formulae makes no use of previous integrand evaluations. Kronrod [1] has shown how the Gauss formula of degree $2n - 1$ can be extended to one of degree $3n + 2$ by making use of the original n Gauss points and an additional set of n points. However, it is not possible to proceed further than this without using an entirely new set of points with a resulting waste of computational labor. It may be noted that due to the absence of a convenient error estimate for the Gaussian formulae it is usually necessary to carry out a quadrature using more than one order of formulae to check the convergence.

In this paper a set of integration formulae is derived based on a set of $2^r + 1$ Gauss or Lobatto points, where r is an integer. If the original points are denoted by x_j, $j = 1, 2, \cdots, (2^r + 1)$, then r subsets of points $x_{2^i(j-1)+1}$, $j = 1, 2, \cdots, (2^{r-i} + 1)$ are obtained for $i = 1, 2, \cdots, r$ by successively deleting alternate points from the preceding subset. The integration weights associated with each subset can be determined as described in Section 2. In carrying out an integration the number of points is successively increased until convergence appears satisfactory or until the number of points reaches $2^r + 1$ corresponding to the full accuracy of the Gauss or Lobatto formulae. Since each subset includes the points of the previous subset, no integrand evaluations are wasted. The degree of precision of the successive formulae are one less than the number of points used, since they are of the Newton-Cotes type. For the base formula, the Newton-Cotes weights and the base weights degenerate of course to one and the same.

The integration formulae have been derived for the basic set of 33 Gauss points ($r = 5$) as well as for the sets of 65 Gauss and Lobatto points ($r = 6$). It was considered that the 65-point Gauss and Lobatto formulae were capable of dealing with all but pathological integrands so that it was unnecessary to base the formulae on higher values of r. For example, the Gauss 65-point formula will integrate powers of x up to 154 with a relative accuracy of just less than nine decimal digits.

The Chebyshev expansion method of Clenshaw and Curtiss [2] has also the characteristic of not wasting previous integrand evaluations, and a comparison with the new formulae is therefore presented in Section 3. The Clenshaw-Curtiss quadrature formulae may be interpreted as the Newton-Cotes formulae with the abscissas $x_k = \cos(k\pi/(n - 1))$, $k = 0, 1, \cdots, n - 1$. These formulae will be referred to later as Chebyshev formulae.

2. Evaluation of the Integration Weights. The Lagrangian interpolating poly-

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nomial of degree $n - 1$ for a function $f(x)$ given at the points x_i, $i = 1, \cdots, n$, is

$$P(x) = \sum_{i=1}^{n} L_i(x) f(x_i)$$

where

$$L_i(x) = F_i(x)/F_i(x_i)$$

and

$$F_i(x) = \prod_{j=1}^{k} (x - x_j)/(x - x_i) .$$

Thus the weights of an n-point integration formula

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} \omega_i f(x_i)$$

are given by

$$\omega_i = \int_{-1}^{1} L_i(x)dx .$$

These weights can be evaluated exactly in a numerically stable fashion using a Gauss formula with $n/2$ points when n is even and $(n + 1)/2$ points when n is odd. It is to be noted that the weights for any quadrature formula, including the Gaussian and Lobatto formulae, can be calculated in this way.

If the derivatives of the integral are known as well, the Hermite interpolation formula allow the weights B_i and C_i of the formula

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} B_i f(x_i) + \sum_{i=1}^{n} C_i f'(x_i)$$

to be obtained from

$$B_i = \int_{-1}^{1} [1 - 2L_i'(x_i)(x - x_i)]L_i^2(x)dx ,$$

$$C_i = \int_{-1}^{1} (x - x_i)L_i^2(x)dx .$$

These weights can be evaluated exactly using a Gauss formula with n points. As Lanczos [3] has noted, the inclusion of the n values of the derivatives in an arbitrary point formula gives rise to an integration formula with the same integrating power as the n-point Gauss formula.

3. New Formulae. By the method of Section 2 integration formulae with 5, 9, and 17 points were derived, based on the 33 Gauss points, together with formulae with 5, 9, 17 and 33 points based on the 65 Gauss and Lobatto points. The Chebyshev formulae for 5, 9, 17, 33 and 65, were also derived for comparison. The integrand weights for the Lobatto, Gauss and Chebyshev formulae are given in Tables* M1, M2, M3 and M4. All the Gauss formulae used to evaluate the weights were obtained from Gawlik [4]. The weights associated with the 65-point Lobatto formula have been given by Rabinowitz [5] and have not been included in Table

* The letter M preceding a table number refers to the microfiche card.

M1. The 65 Gauss points and weights have not previously been tabulated and had to be calculated to derive Table M2. To assess the integrating power of the formulae each was applied to integrate powers of x higher than those which should be integrated exactly. In Figs. 1 to 4 the modulus of the fractional error (defined as the ratio of the error to the true value of the integral) committed by the various formulae is plotted against the power of x being integrated. It can be seen that the formulae based on the 33 Gauss points probably give the best overall performance. The Lobatto formulae appear to be particularly good at integrating very high powers of x. A further indication of this is evident from Table 1, which records the performance of the various formulae when integrating $\int_{-1}^{1} |x + \frac{1}{2}|^{1/2} dx$, whose integrand has a singularity in its derivatives at $x = -\frac{1}{2}$. This integrand could

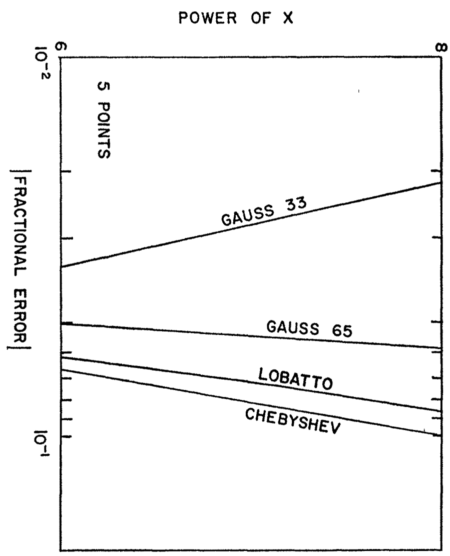

FIGURE 1

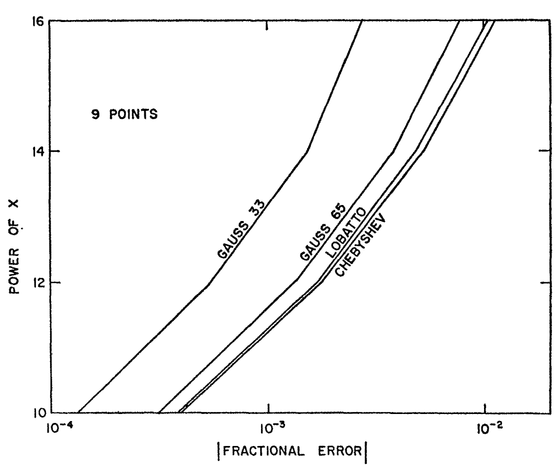

FIGURE 2

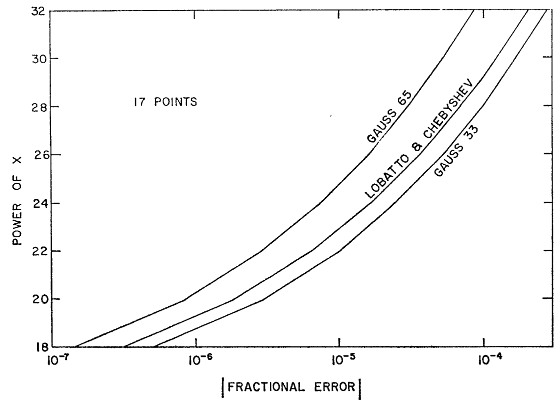

FIGURE 3

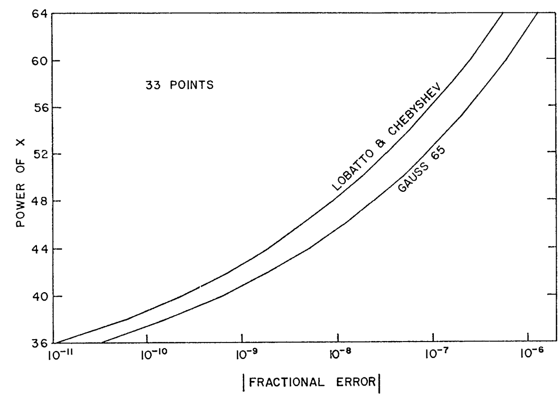

FIGURE 4

TABLE 1
Errors in Calculating $\int_{-1}^{1} |x + \frac{1}{2}|^{1/2} dx$

Basic points	*Number of points*				
	5	9	17	33	65
Gauss 65	0.0569	0.0180	0.0041	0.0029	−0.0011
Gauss 33	0.0507	0.0194	0.0011	0.0026	——
Chebyshev	0.0627	0.0160	0.0064	0.0021	−0.00078
Lobatto 65	0.0608	0.0168	0.0058	0.0025	0.00039

probably only be approximated with acceptable accuracy by a polynomial of very high degree. It would thus seem that the Lobatto based formulae may provide a useful scheme for controlling the accuracy and economy of numerical integrations.

The tables were calculated using at least thirty-digit arithmetic and are correct to all figures given. The usual checks of integration of powers were successfully applied. It is interesting to note that the weights of all the formulae are positive so that their stability is likely to be high.

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<u>Table 2. 65 point Gauss based formulae.</u>

Points $\pm x_i$	65 point weights	33 point weights	17 point weights	9 point weights	5 point weights
.99832 60870 75412 87727	.17292 58251 30025 09010(-2)	.30441 97014 58135 19556(-2)	.73735 62822 86801 97790(-2)	.21905 59827 46544 73784(-1)	.76239 00494 04943 49172(-1)
.99645 09480 61849 16305	.40215 24172 00373 63508(-2)				
.99128 52761 76801 66872	.63079 42578 97175 45363(-2)	.12805 87802 53133 18183(-1)			
.98383 98121 87034 94137	.85801 48266 88145 99187(-2)				
.97413 15398 33551 16907	.10832 67878 95979 88616(-1)	.21554 17023 26746 81730(-1)	.43066 33529 25252 75302(-1)		
.96218 27547 18055 23771	.13060 31163 99948 46348(-1)				
.94802 09281 68407 50637	.15257 91214 64483 10356(-1)	.30591 83784 97943 13089(-1)			
.93167 86282 28749 33796	.17420 42199 76702 48513(-1)				
.91319 34405 42846 28173	.19542 86583 67500 62822(-1)	.39028 72940 63504 42414(-1)	.78304 33261 43550 10842(-1)	.15344 26268 79133 89905	
.89260 78805 04738 93142	.21620 36128 49340 62864(-1)				
.86996 92949 26407 03619	.23648 12969 12872 36700(-1)	.47341 68877 12917 53856(-1)			
.84532 97528 99830 28394	.25621 50693 80377 58245(-1)				
.81874 59259 22651 45343	.27535 95408 84503 43961(-1)	.55034 08703 40153 66833(-1)	.11006 08507 67542 79078		
.79027 89574 92121 84304	.29387 08778 93106 88073(-1)				
.75999 43224 41999 78687	.31170 59038 01891 42478(-1)	.62373 70111 65072 50920(-1)			
.72796 16763 29424 67901	.32882 41967 63685 75006(-1)				
.69425 46952 13991 63355	.34518 61839 85490 58645(-1)	.69008 52916 25285 07271(-1)	.13813 41131 61540 86992	.27754 23945 21943 45091	.53361 53702 14679 86808
.65895 09061 93625 13304	.36075 42322 55652 73950(-1)				
.62213 15090 85400 24158	.37549 25344 82577 09836(-1)	.75124 39868 57990 98010(-1)			
.58388 11896 60487 31332	.38936 71920 40511 97632(-1)				
.54428 79248 62227 13854	.40234 62927 30055 33822(-1)	.80445 47555 61372 29465(-1)	.16089 11528 09167 43671		
.50344 27804 55006 88234	.41439 99841 72402 93037(-1)				
.46143 97015 69145 05770	.42550 05424 67558 02744(-1)	.85122 30703 95099 24347(-1)			
.41837 52966 23405 00927	.43562 24359 58004 86541(-1)				
.37434 86151 22066 01201	.44474 23839 50829 74463(-1)	.88927 45716 09983 70813(-1)	.17793 75985 79179 17838	.35483 50852 63219 13873	
.32946 09198 37486 40764	.45283 94102 63002 30677(-1)				
.28381 54539 02248 73061	.45989 48914 66516 96980(-1)	.91999 14597 86843 85432(-1)			
.23751 72033 46416 06857	.46589 25997 27334 98328(-1)				
.19067 26558 26142 76977	.47081 87401 04545 22276(-1)	.94144 15699 96288 41230(-1)	.18829 02646 05197 09975		
.14338 95546 98975 17113	.47466 19823 28855 03151(-1)				
.95776 65320 91975 05650(-1)	.47741 34868 12406 21588(-1)	.95501 95436 74321 64545(-1)			
.47943 46235 31718 57520(-1)	.47906 89250 04958 62041(-1)				
.0	.47961 84939 44666 18130(-1)	.95904 55119 74980 40185(-1)	.19188 35788 95248 63765	.38454 85861 22098 07363	.78029 12496 89651 56653

Table 3. 33 point Gauss based formulae.

Points ± x_i	17 point weights	9 point weights	5 point weights
.99742 46942 46455 21727	.11623 49999 61774 10637(-1)	.28210 52928 72118 72213(-1)	.85481 63137 13397 12011(-1)
.96682 29096 89992 76893	.48568 44100 19008 39306(-1)		
.90231 67677 43433 58304	.80362 29158 91677 86887(-1)	.16051 86377 65131 69293	
.80616 23562 74166 58980	.11125 28477 03219 22361		
.68173 19599 69742 78627	.13694 53995 20868 36957	.27498 26866 29756 86132	.53423 75368 55781 14693
.53338 99047 86347 64355	.15883 02328 43363 17321		
.36633 92577 48073 34107	.17431 31094 29639 89209	.34855 05608 69857 42723	
.18643 92988 27991 57234	.18441 98781 38042 26688		
.0	.18736 85995 55242 07573	.37547 51708 96084 29263	.76056 16635 45758 28208

Table 4. Chebyshev formulae.

Points x_i	65 point weights	33 point weights	17 point weights	9 point weights	5 point weights
1.	.24420 02442 00244 54132(-3)	.97751 71065 49364 26791(-3)	.39215 68627 45098 06785(-2)	.15873 01587 30158 72875(-1)	.66666 66666 66666 66667(-1)
.99879 54562 05172 39247	.23514 90675 31170 28321(-2)				
.99518 47266 72196 88840	.48314 65448 79091 24944(-2)	.93931 97962 95501 51477(-2)			
.98917 65099 64780 97339	.71926 93161 73611 44980(-2)				
.98078 52804 03230 44883	.95823 38795 28379 04172(-2)	.19234 24513 26811 49340(-1)	.37368 70263 72054 09687(-1)		
.97003 12531 94543 99239	.11923 39471 42127 71424(-1)				
.95694 03357 32208 86500	.14252 06043 23519 86494(-1)	.28457 91667 72336 89572(-1)			
.94154 40651 83020 77865	.16534 98765 72895 89616(-1)				
.92387 95325 11286 75635	.18786 52974 17957 83624(-1)	.37594 34191 40472 06247(-1)	.75482 33154 31518 34579(-1)	.14621 86492 16018 15491	
.90398 92931 23443 33166	.20986 27442 97374 33974(-1)				
.88192 12643 48355 02963	.23140 69493 43581 98810(-1)	.46262 76283 77517 49742(-1)			
.85772 86100 00272 06973	.25235 06498 17547 65960(-1)				
.83146 96123 02545 23690	.27272 25714 14683 84845(-1)	.54555 01630 39803 10377(-1)	.10890 55525 81890 93048		
.80320 75314 80644 90970	.29240 65319 74683 37588(-1)				
.77301 04533 62736 96085	.31141 29710 40676 24338(-1)	.62272 10954 52940 04280(-1)			
.74095 11253 54959 09130	.32964 54656 99763 29952(-1)				
.70710 67811 86547 52457	.34710 49818 09251 14241(-1)	.69427 57563 04354 50981(-1)	.13895 64683 66233 07393	.27936 50793 65079 36524	.53333 33333 33333 33333
.67155 89548 47018 40076	.36370 92028 66391 83230(-1)				
.63439 32841 63645 49823	.37945 45992 12848 17208(-1)	.75883 80044 13884 70666(-1)			
.59569 93044 92433 34344	.39426 98871 29560 99830(-1)				
.55557 02330 19602 22464	.40815 01340 03578 33905(-1)	.81634 81765 49385 10299(-1)	.16317 26642 81703 30291		
.51410 27441 93221 72648	.42103 33111 14181 02024(-1)				
.47139 67368 25997 64846	.43291 51496 16908 28370(-1)	.86577 53844 10274 35377(-1)			
.42755 50934 30282 09427	.44374 17923 92573 15734(-1)				
.38268 34323 65089 77175	.45351 10955 16606 72175(-1)	.90706 11286 77209 98655(-1)	.18147 37842 36493 35666	.36171 78587 20489 76161	
.33688 98533 92220 05075	.46217 66751 09255 76840(-1)				
.29028 46772 54462 36769	.46973 95904 66141 48722(-1)	.93943 24443 87687 35769(-1)			
.24298 01799 93263 88999	.47616 04450 52501 93012(-1)				
.19509 03220 16128 26787	.48144 43257 25122 03466(-1)	.96282 32594 54881 79252(-1)	.19251 38846 12925 64715		
.14673 04744 55361 75168	.48555 84485 71410 52759(-1)				
.98017 14032 95606 01975(-1)	.48851 25664 30660 93762(-1)	.97698 18820 80555 81844(-1)			
.49067 67432 74180 14236(-1)	.49028 01843 10255 52933(-1)				
	.49087 62351 49424 55850(-1)	.98178 57778 17682 96751(-1)	.19641 01258 21890 52757	.39365 07936 50793 65077	.80000 00000 00000 00000

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