Part II

NUMERICAL MATHEMATICS

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QUADRATURE FORMULAE ON HALF-INFINITE INTERVALS*

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Abstract.

We develop two classes of quadrature rules for integrals extended over the positive real axis, assuming given algebraic behavior of the integrand at the origin and at infinity. Both rules are expressible in terms of Gauss-Jacobi quadratures. Numerical examples are given comparing these rules among themselves and with recently developed quadrature formulae based on Bernstein-type operators.

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1. Introduction.

For integrals extended over the whole real line, whose integrands go to zero like $|x|^{-\beta}$ when $|x| \to \infty$, special (symmetric) quadrature rules have been developed by W. M. Harper [6] and S. Haber [5] some time ago that integrate exactly the product of $(1 + x^2)^{-\beta/2}$ with certain rational functions. Here we treat in a similar spirit integrals over the half-infinite interval $[0, \infty)$ and integrands that have an algebraic singularity at the origin of type x^α, $\alpha > -1$, and behave like $x^{-\beta}$, $\beta > 1$, as $x \to \infty$. We develop two types of quadrature formulae – one having maximum polynomial degree of exactness, the other maximum "rational" degree of exactness. The former, already considered by R. Kumar and M. K. Jain [7], are subject to a severe limitation on the number of quadrature points allowed, whereas the latter are free from any such limitation. We show that both types of formulae can be reduced to Gaussian quadratures relative to appropriate Jacobi weight functions, and hence can be generated by standard mathematical software. Numerical examples are given, comparing these quadrature rules among themselves, and also with alternative rules based on Bernstein-type operators, recently developed by B. Della Vecchia [3].

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2. Formulae of maximum algebraic degree of exactness.

The object in this section is to find a quadrature formula

$$\int_0^\infty f(x)\frac{x^\alpha}{(1+x)^\beta}\,dx = \sum_{k=1}^n a_k f(x_k) + r_n(f) \tag{2.1}$$

of Gaussian type, that is, such that $r_n(f) = 0$ whenever $f \in \boldsymbol{P}_{2n-1}$, the class of polynomials of degree $\leq 2n - 1$. To assure integrability, one has to assume that

$$\alpha > -1, \quad 2n < \beta - \alpha. \tag{2.2}$$

Thus, the formula (2.1) will be applicable only if $\beta > 0$ is relatively large.

The requirement that (2.1) be exact for $f(x) = x^\lambda$, $\lambda = 0, 1, \ldots, 2n - 1$, translates, via the transformation of variables

$$\frac{1-x}{1+x} = t, \quad x = \frac{1-t}{1+t}, \tag{2.3}$$

into the condition that

$$\int_{-1}^1 \left[\frac{1-t}{1+t}\right]^{\lambda+\alpha} \left[\frac{1+t}{2}\right]^\beta \frac{2dt}{(1+t)^2} = \sum_{k=1}^n a_k x_k^\lambda, \quad \lambda = 0, 1, \ldots, 2n-1,$$

or, equivalently, that

$$\int_{-1}^1 (1-t)^\lambda (1+t)^{2n-1-\lambda} \cdot (1-t)^\alpha (1+t)^{\beta-\alpha-2n-1} dt \tag{2.4}$$

$$= 2^{\beta-1} \sum_{k=1}^n [a_k(1+t_k)^{1-2n}] \cdot (1-t_k)^\lambda (1+t_k)^{2n-1-\lambda}, \quad \lambda = 0, 1, \ldots, 2n-1.$$

Here we have set, in conformity with (2.3),

$$\frac{1-x_k}{1+x_k} = t_k, \quad x_k = \frac{1-t_k}{1+t_k}. \tag{2.5}$$

Since $\{(1-t)^\lambda(1+t)^{2n-1-\lambda}: \lambda = 0, 1, \ldots, 2n-1\}$ forms a basis in $\boldsymbol{P}_{2n-1}$, it follows from (2.4) that

$$t_k = \tau_k^J, \quad 2^{\beta-1}(1+t_k)^{1-2n} a_k = \omega_k^J, \quad k = 1, 2, \ldots, n, \tag{2.6}$$

where

$$\tau_k^J = \tau_k^{(n)}(\alpha, \beta - \alpha - 2n - 1), \quad \omega_k^J = \omega_k^{(n)}(\alpha, \beta - \alpha - 2n - 1) \tag{2.7}$$

are the n-point Gaussian nodes and weights relative to the Jacobi weight function with parameters α and $\beta - \alpha - 2n - 1$. Note, by assumption (2.2), that both parameters are larger than -1, as required by the theory of Gauss-Jacobi quadrature. (This is not the case with another relationship to Jacobi polynomials, noted in [7, Eq. (12)], which involves parameters $-\beta$ and α.) Thus, combining (2.5) and (2.6), we obtain

$$x_k = \frac{1-\tau_k^J}{1+\tau_k^J}, \quad a_k = \frac{(1+\tau_k^J)^{2n-1}}{2^{\beta-1}}\omega_k^J, \quad k = 1, 2, \ldots, n, \tag{2.8}$$

for the desired abscissae and weights in the quadrature formula (2.1).

3. Formulae of maximum "rational" degree of exactness.

For a more viable alternative to (2.1), not subject to the second condition in (2.2), we now require the quadrature rule

$$\int_0^\infty f(x)x^\alpha\,dx = \sum_{k=1}^n A_k f(X_k) + R_n(f) \tag{3.1}$$

to be exact (i.e., $R_n(f) = 0$) whenever

$$f(x) = \frac{1}{(1+x)^{\beta+\lambda}}, \quad \lambda = 0, 1, \ldots, 2n-1. \tag{3.2}$$

Here the only assumptions needed for integrability are

$$\alpha > -1, \quad \beta - \alpha > 1. \tag{3.3}$$

In the case $\alpha = 0$, $\beta = 2$, such a quadrature rule has already been suggested in [8, p. 52]; see also [2, pp. 225–226].

It is easy to see that exactness of (3.1) for the "rational" functions (3.2) is equivalent to

$$\int_0^\infty \frac{g(x)x^\alpha}{(1+x)^{\beta+2n-1}}\,dx = \sum_{k=1}^n A_k \frac{g(X_k)}{(1+X_k)^{\beta+2n-1}} \tag{3.4}$$

for

$$g(x) = x^\lambda, \quad \lambda = 0, 1, \ldots, 2n-1. \tag{3.5}$$

Indeed, putting $f(x) = g(x)/(1+x)^{\beta+2n-1}$ in (3.1), our exactness requirement implies (3.4) for $g(x) = (1+x)^{2n-\lambda-1}$, $\lambda = 0, 1, \ldots, 2n-1$, which is equivalent to (3.4), (3.5). Conversely, if (3.4), (3.5) holds, it suffices to put $g(x) = (1+x)^{2n-\lambda-1}$ in (3.4) to get exactness of (3.1) for (3.2).

Now using again the transformation of variables (2.3), and

$$\frac{1-X_k}{1+X_k} = T_k, \quad X_k = \frac{1-T_k}{1+T_k} \tag{3.6}$$

in place of (2.5), we get from (3.4), (3.5)

$$\int_{-1}^{1}\left[\frac{1-t}{1+t}\right]^{\lambda+\alpha}\left[\frac{1+t}{2}\right]^{\beta+2n-1}\frac{2}{(1+t)^2}\,dt$$

$$=\sum_{k=1}^{n}A_k\frac{X_k^\lambda}{(1+X_k)^{\beta+2n-1}},\quad \lambda=0,1,\ldots,2n-1,$$

that is,

$$\int_{-1}^{1}(1-t)^\lambda(1+t)^{2n-1-\lambda}\cdot(1-t)^\alpha(1+t)^{\beta-\alpha-2}dt$$

$$=\sum_{k=1}^{n}\tfrac{1}{2}A_k(1+T_k)^\beta\cdot(1-T_k)^\lambda(1+T_k)^{2n-1-\lambda},\quad \lambda=0,1,\ldots,2n-1.$$

As before in §2, this implies

(3.7) $$T_k=T_k^J,\quad \tfrac{1}{2}A_k(1+T_k)^\beta=\Omega_k^J,$$

where

(3.8) $$T_k^J=\tau_k^{(n)}(\alpha,\beta-\alpha-2),\quad \Omega_k^J=\omega_k^{(n)}(\alpha,\beta-\alpha-2)$$

are the n-point Jacobi nodes and weights corresponding to parameters α and $\beta-\alpha-2$. Hence, in (3.1),

(3.9) $$X_k=\frac{1-T_k^J}{1+T_k^J},\quad A_k=\frac{2\Omega_k^J}{(1+T_k^J)^\beta}.$$

In contrast to the quadrature rule of §2, it is now meaningful to discuss convergence of the rule (3.1) as $n\to\infty$. To do this, let R_n^J denote the remainder term in the Gauss-Jacobi formula with parameters α and $\beta-\alpha-2$,

(3.10) $$\int_{-1}^{1}g(t)(1-t)^\alpha(1+t)^{\beta-\alpha-2}dt=\sum_{k=1}^{n}\Omega_k^J g(T_k^J)+R_n^J(g).$$

Then an easy calculation shows that the remainder R_n in (3.1) is given by

(3.11) $$R_n(f)=2R_n^J(h),\quad h(t)=(1+t)^{-\beta}f\left[\frac{1-t}{1+t}\right].$$

Now typically,

(3.12) $$f(x)=(1+x)^{-\beta}F(x),$$

where F is a "nice" function. In this case,

(3.13) $$h(t)=2^{-\beta}F\left[\frac{1-t}{1+t}\right],\quad -1<t<1.$$

Therefore, convergence $R_n^J(h)\to 0$ in (3.10), hence $R_n(f)\to 0$ in (3.1), is assured if h in (3.13) is continuous – in fact, bounded Riemann-integrable – on the interval $[-1, 1]$, i.e., F is continuous on the closed interval $[0, \infty]$. Moreover, if $h(t)$ is analytic in a disk $|t| < r$, where $r > 1$, hence F analytic outside the disk with center at $-\frac{r^2+1}{r^2-1}$ and radius $\frac{2r}{r^2-1}$, then convergence is exponentially fast, the rate of convergence being larger the larger $r > 1$ (cf. [4, Eq. (A.1)].

It is also possible to combine the two approaches in §§2–3 and seek a quadrature formula

$$\int_0^\infty f(x)\frac{x^\alpha}{(1+x)^\beta}\,dx = \sum_{k=1}^n b_k f(y_k) + s_n(f) \tag{3.14}$$

for which, given an integer m with $0 \le m < 2n$, one has $s_n(f) = 0$ whenever

$$f(x) = \begin{cases} x^\lambda, & \lambda = 0, 1, \ldots, 2n - m - 1, \\ \dfrac{1}{(1+x)^{\lambda+1}}, & \lambda = 0, 1, \ldots, m - 1. \end{cases} \tag{3.15}$$

Here one needs to assume $\alpha > -1$ and $2n < \beta - \alpha + m$. To construct such formulae, however, seems to require different techniques (the solution of nonlinear equations), and we will not pursue this further. Note that the limit cases $m = 0$ and $m = 2n - 1$ correspond to the quadrature rules (2.1) and (3.1), respectively.

4. Formulae based on Bernstein-type operators.

The linear positive operator of Bernstein type,

$$(L_n f)(x) = (1+x)^{-n}\sum_{k=0}^n \binom{n}{k} x^k f\left[\frac{k}{n-k+1}\right], \tag{4.1}$$

was introduced by G. Bleimann, P. L. Butzer and L. Hahn [1] for approximating continuous functions on $[0, \infty)$, and was used by B. Della Vecchia [3] to construct a quadrature rule which is exact for the function $(1 + x)^{-\beta}$, $\beta > 1$. Slightly generalizing her approach, we integrate $(L_n g)(x) \cdot x^\alpha(1 + x)^{-\beta}$ from 0 to ∞, where $g(x) = f(x)(1 + x)^\beta$, to get a quadrature rule for $\int_0^\infty x^\alpha f(x)dx$. This rule is again exact when f is the function $(1 + x)^{-\beta}$, since it then takes the form $\int_0^\infty (L_n 1)(x) \cdot x^\alpha(1 + x)^{-\beta}dx = \int_0^\infty x^\alpha(1 + x)^{-\beta}dx$. As before, we assume that

$$\alpha > -1, \quad \beta - \alpha > 1. \tag{4.2}$$

To conform with the formulae obtained in the previous sections, we replace n in (4.1) by $n - 1$, and denote the quadrature nodes by

$$\xi_k = \frac{k-1}{n-k+1}, \quad k = 1, 2, \ldots, n. \tag{4.3}$$

The quadrature rule then becomes

$$\text{(4.4)} \qquad \int_0^\infty x^\alpha f(x)dx = \sum_{k=1}^n \alpha_k f(\xi_k) + \rho_n(f),$$

$$\alpha_k = \binom{n-1}{k-1}\left[\frac{n}{n-k+1}\right]^\beta \frac{\Gamma(n+\beta-\alpha-k-1)}{\Gamma(n+\beta-1)}\Gamma(\alpha+k).$$

The weights α_k are easily generated recursively by

$$\text{(4.5)} \qquad \alpha_1 = \frac{\Gamma(n+\beta-\alpha-2)}{\Gamma(n+\beta-1)}\Gamma(\alpha+1),$$

$$\alpha_k = \frac{1+\dfrac{\alpha}{k-1}}{1+\dfrac{\beta-\alpha-2}{n-k+1}}\left[\frac{n-k+2}{n-k+1}\right]^\beta \alpha_{k-1}, \quad k = 2,3,\ldots,n,$$

where, for large n, one first computes $\ln \alpha_1$, and then α_1 by exponentiation, to avoid machine overflow.

The principal virtue of the quadrature rule (4.4) seems to be its simplicity and explicit form, its major drawback slow convergence. Known error estimates (for $\alpha = 0$) due to B. Della Vecchia [3] indeed exhibit a convergence order of $O(n^{-1})$ at best, and so do our examples in §5.

5. Examples.

In this section we illustrate the performance of the three quadrature schemes of §§2–4 on a number of examples. All computations were carried out in double precision (ca. 29 decimal digits) on the Cyber 205.

EXAMPLE 1. $\displaystyle\int_0^\infty \frac{x^{1/2}\tanh x}{(1+x)^{12.5}}dx = .0034038896750456956178704228 5.$

Here $\alpha = \frac{1}{2}$, $\beta = 12.5$, so that by (2.2) the Gauss formula (2.1) exists only for $n = 1(1)5$. The associated relative errors are shown in the second column of Table 5.1. (Integers in parentheses denote decimal exponents.)

TABLE 5.1. *Relative errors of the quadrature rules* (2.1), (3.1), (4.4) *for Example* 1.

n	(2.1)	n	(3.1)	n	(3.1)	n	(4.4)
1	2.79(−2)	5	1.38(−6)	30	1.06(−21)	200	2.12(−3)
2	2.35(−3)	10	5.08(−11)	35	2.10(−23)	400	1.06(−3)
3	1.64(−4)	15	2.63(−15)	40	3.32(−25)	800	5.26(−4)
4	9.14(−5)	20	7.98(−18)	45	1.10(−26)	1600	2.62(−4)
5	3.91(−5)	25	1.94(−19)	—	—	3200	1.31(−4)

Since $F(x) = \tanh x$ (cf. (3.12)) is continuous on the closed interval $[0, \infty]$, the quadrature formula (3.1) converges as $n \to \infty$, and Table 5.1 shows a rather satisfactory speed of convergence. The numerical value of the integral shown above indeed is the numerical limit observed as (3.1) is applied with increasing values of n.

As expected, the quadrature rule (4.4) based on a Bernstein-type operator converges rather slowly, with order $O(n^{-1})$, as is evident from the last column of Table 5.1. Applying the ε-algorithm to the first 200 approximations reduces the error by only one decimal order of accuracy.

We have repeated Example 1 with $\alpha = 0$, $\beta = 1.1$ and obtained similar results for (3.1) except that convergence is considerably slower. It now takes $n = 120$ in (3.1) to get a 16S value 9.539866086478899 for the integral; the smallest error in (4.4) is 3.57(−5) (for $n = 3200$).

EXAMPLE 2. $I(r) = \displaystyle\int_0^\infty \frac{x^{-1/2}}{(x - c_r)^4 - d_r^4} \frac{dx}{(1 + x)^{12.5}}$, where $c_r = -(r^2 + 1)/(r^2 - 1)$, $d_r = 2r/(r^2 - 1)$, $r > 1$.

This example is chosen to illustrate how the rate of convergence of (3.1) depends on the analyticity properties of the function F in (3.12), that is, in our case, of the function

$$F(x) = \frac{1}{(x - c_r)^4 - d_r^4}. \tag{5.1}$$

This function has exactly four poles, respectively at $c_r \pm d_r$ and $c_r \pm id_r$, so that F is analytic outside the circle with center at c_r and radius d_r ($< |c_r|$). According to the discussion following Eq. (3.13), the rate of convergence of (3.1) should therefore increase with r. This is confirmed in Table 5.2, where comparison is made also with the other two quadrature schemes, (2.1) and (4.4). Table 5.3 gives the exact values of $I(r)$ to 26 significant digits, as determined by the quadrature rule (3.1).

TABLE 5.2. *Relative errors of* (2.1), (3.1), (4.4) *for Example* 2 *with* $r = 1.1, 1.5, 2, 5$.

r	n	(2.1)	n	(3.1)	n	(4.4)	r	n	(2.1)	n	(3.1)	n	(4.4)
1.1	1	2.38(−1)	10	1.49(−5)	100	2.89(−2)	2.0	1	3.31(−2)	6	1.53(−9)	100	3.49(−3)
	2	9.90(−2)	20	1.48(−9)	200	1.46(−2)		2	3.44(−3)	9	2.85(−13)	200	1.75(−3)
	3	5.54(−2)	30	1.80(−13)	400	7.31(−3)		3	7.49(−4)	12	6.85(−17)	400	8.79(−4)
	4	3.80(−2)	40	2.33(−17)	800	3.66(−3)		4	2.76(−4)	15	1.88(−20)	800	4.40(−4)
	5	3.06(−2)	50	3.10(−21)	1600	1.83(−3)		5	1.56(−4)	18	5.57(−24)	1600	2.20(−4)
	6	2.86(−2)	60	4.23(−25)	3200	9.17(−4)		6	1.30(−4)	21	2.89(−27)	3200	1.10(−4)
1.5	1	5.45(−2)	5	1.80(−6)	100	5.65(−3)	5.0	1	2.81(−2)	2	3.00(−5)	100	3.03(−3)
	2	9.05(−3)	10	4.76(−11)	200	2.84(−3)		2	1.90(−3)	4	5.76(−10)	200	1.52(−3)
	3	2.75(−3)	15	2.02(−15)	400	1.43(−3)		3	2.67(−4)	6	2.83(−14)	400	7.60(−4)
	4	1.27(−3)	20	1.03(−19)	800	7.14(−4)		4	7.02(−5)	8	1.33(−18)	800	3.81(−4)
	5	8.15(−4)	25	5.70(−24)	1600	3.57(−4)		5	3.22(−5)	10	7.22(−23)	1600	1.90(−4)
	6	7.06(−4)	30	1.28(−27)	3200	1.79(−4)		6	2.50(−5)	12	6.05(−27)	3200	9.52(−5)

TABLE 5.3. *Exact values of the integral in Example* 2.

r	$I(r)$
1.1	.001563427651576028654644642 88
1.5	.034607310891759677936581232 4
2.0	.098427460167752436964227875
5.0	.333873596349519021032797704

EXAMPLE 3. $\displaystyle\int_0^\infty \frac{x^{-1/2}}{(1+x)^{5/4}} e^{-x}\cos x\,dx = 1.1378118633993858829455828.$

The function $F(x) = e^{-x}\cos x$ of this example is no longer analytic at ∞, as was the case in Example 2, and the singularities at $x = 0$ and $x = -1$ are more severe than those in Example 1. These are probably the reasons why (3.1) now converges much more slowly than in the previous examples. The relative errors of (3.1), along with those of (4.4), are shown in Table 5.4.

TABLE 5.4. *Relative errors of* (3.1), (4.4) *for Example* 3.

n	(3.1)	n	(4.4)
40	8.34(−9)	100	7.40(−3)
80	9.90(−14)	200	3.69(−3)
120	8.94(−17)	400	1.85(−3)
160	3.04(−20)	800	9.23(−4)
200	6.99(−23)	1600	4.61(−4)
240	8.60(−26)	3200	2.31(−4)

Since $\alpha = -\frac{1}{2}$, $\beta = \frac{5}{4}$, the second inequality in (2.2) is violated for $n \geq 1$, so that there are no Gaussian rules (2.1) for this example.

EXAMPLE 4. $\displaystyle I(\omega) = \frac{\pi}{\omega}\int_0^\infty \frac{x^{-1/2}}{(1+x)^{5/4}} \frac{dx}{1+\omega^2(x-1)^2}, \quad \omega > 0.$

The function

$$F(x) = \frac{\pi}{\omega}\frac{1}{1+\omega^2(x-1)^2} \tag{5.2}$$

in this example has poles at $x = 1 \pm i/\omega$, which approach the point 1 on the real axis as $\omega \to \infty$. (The function is normalized to have unit integral over the whole real line; since it has a sharp peak at $x = 1$ when ω is large, it may be thought of as an approximation to the Dirac delta function centered at 1.) Naturally, our quadrature rule (3.1) will have increasing difficulty converging, as ω becomes large. This can be seen from the relative errors displayed in Table 5.5. Strangely enough, the convergence of (4.4) – slow, to be sure – is relatively unaffected by the value of ω and indeed accelerates a little bit as ω increases! The true answers for $\omega = .5, 1, 2.5, 5$, furnished by (3.1) for n sufficiently large, are shown in Table 5.6.

TABLE 5.5. *Relative errors of* (3.1), (4.4) *for Example* 4.

ω	n	(3.1)	n	(4.4)	ω	n	(3.1)	n	(4.4)
.5	10	4.97(−6)	100	4.22(−3)	2.5	30	1.02(−5)	100	2.07(−3)
	20	1.49(−10)	200	2.10(−3)		60	3.63(−11)	200	1.03(−3)
	30	9.75(−15)	400	1.05(−3)		90	1.58(−15)	400	5.16(−4)
	40	3.55(−19)	800	5.24(−4)		120	1.71(−20)	800	2.58(−4)
	50	1.03(−23)	1600	2.62(−4)		150	7.43(−26)	1600	1.29(−4)
1.0	15	3.25(−6)	100	3.25(−3)	5.0	60	2.63(−6)	100	1.72(−3)
	30	2.19(−11)	200	1.62(−3)		120	7.16(−11)	200	8.58(−4)
	45	3.80(−16)	400	8.09(−4)		180	5.14(−16)	400	4.28(−4)
	60	2.96(−21)	800	4.04(−4)		240	8.14(−22)	800	2.14(−4)
	75	4.91(−27)	1600	2.02(−4)		300	2.45(−26)	1600	1.07(−4)

TABLE 5.6. *Exact values of the integral in Example* 4.

ω	$I(\omega)$
.5	10.718576182984881437538O337
1.0	3.9449597795274933486744356
2.5	.74241157786627923083242852
5.0	.182154799099070485116688565

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BIBLIOGRAPHY

[1] G. Bleimann, P. L. Butzer and L. Hahn, *A Bernstein-type operator approximating continuous functions*, Proc. Nederl. Akad. Wetensch. A 83 (= Indag. Math. 42), 1980, 255–262.
[2] P. J. Davis and P. Rabinowitz, *Methods of Numerical Integration*, 2nd ed., Academic Press. 1984.
[3] B. Della Vecchia, *Some properties of a rational operator of Bernstein type*, J. Approx. Theory, to appear.
[4] J. D. Donaldson and D. Elliott, *A unified approach to quadrature rules with asymptotic estimates of their remainders*, SIAM J. Numer. Anal. 9, 1972, 573–602.
[5] S. Haber, *A note on some quadrature formulas for the interval* $(-\infty, \infty)$, Math. Comp. 18, 1964, 313–314.
[6] W. M. Harper, *Quadrature formulas for infinite integrals*, Math. Comp. 16, 1962, 170–175.
[7] R. Kumar and M. K. Jain, *Quadrature formulas for semi-infinite integrals*, Math. Comp. 28, 1974, 499–503. [Corrigendum: ibid. 56, 1991, 407].
[8] A. H. Stroud and Don Secrest, *Gaussian Quadrature Formulas*, Prentice-Hall, Englewood Cliffs, N.J., 1966.