MR0218014 (36 #1103) 65.55

Gautschi, Walter

Numerical quadrature in the presence of a singularity.

SIAM J. Numer. Anal. **4** 1967 357–362

This paper is concerned with the procedure of ignoring the singularity in numerical integration [P. J. Davis and P. Rabinowitz, same J. **2** (1965), 367–383; MR0195256 (33 #3459)]. The quadratures of interest use the roots of the Čebyšev polynomials of the first and second kinds, respectively, along with the weights which yield maximal polynomial precision. The singularity occurs as an endpoint of the interval of integration and the integrand is monotonic in a neighborhood of it. Convergence is shown to occur, the key step being the verification for these quadratures of conditions due to P. Rabinowitz [ibid. **4** (1967), 191–201; MR0213016 (35 #3881)].

Reviewed by *R. E. Barnhill*

MR856708 (88a:65028) 65D32

Caliò, Franca (I-MILANP); **Gautschi, Walter** (1-PURD-C); **Marchetti, Elena** (I-MILANP)

On computing Gauss-Kronrod quadrature formulae.

Math. Comp. **47** (1986), *no. 176,* 639–650, S57–S63.

The computation of Gauss-Kronrod quadrature formulae is discussed in this paper. It is well known that Gaussian quadrature formulae are nonprogressive, so that function evaluations made for a quadrature with a specific number of points or abscissae can never be reused when a formula with more points is used to confirm convergence. The Gauss-Kronrod formulae allow a given Gaussian formula to be extended from n points by a further $n+1$ points to give a degree of exactness of $3n+1$. The computation involves solving nonlinear equations for the new nodes at the extra $n+1$ points, and for new weights throughout. This work uses a direct solution of the nonlinear equations by Newton's method, but claims no comparison with other techniques. The interlacing property is used to get good initial approximations, and the condition factors in the problem are considered. A number of weight functions $w(x)$ and intervals are considered, including $w(x)=1$ on $[-1,1]$, $w(x)=\ln(1/t)$ on $[0,1]$ and $w(x)=t^{1/2}\ln(1/t)$ on $[0,1]$.

Reviewed by *G. A. Evans*

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Numer. Math., v. 48, 1986, pp. 369-382. MR0834326 (87i:33028)
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Note: This list reflects references listed in the original paper as accurately as possible with no attempt to correct errors.

MR894123 (88i:65154) 65R10 (65D30 65D32)

Gautschi, Walter (1-PURD-C); **Wimp, Jet** (1-PURD-C)

Computing the Hilbert transform of a Jacobi weight function.

BIT **27** (1987), *no. 2,* 203–215.

Summary: "We discuss the evaluation of the Hilbert transform $⨍_{-1}^{1}(t-\xi)^{-1}w^{(\alpha,\beta)}(t)dt$, $-1<\xi<1$, of the Jacobi weight function $w^{(\alpha,\beta)}(t)=(1-t)^{\alpha}(1+t)^{\beta}$ by analytic and numerical means and we also comment on the recursive computation of the quan- tities $⨍_{-1}^{1}(t-\xi)^{-1}\pi_n(t;w^{(\alpha,\beta)})w^{(\alpha,\beta)}(t)dt$, $n=0,1,2,\cdots$, where $\pi_n(\cdot\,;w^{(\alpha,\beta)})$ is the Jacobi polynomial of degree n."

Reviewed by *G. F. Miller*

MR907571 (88i:65030) 65D30
Gautschi, Walter (1-PURD-C); **Kovačević, M. A.** (YU-NIS);
Milovanović, Gradimir V. (YU-NIS)
The numerical evaluation of singular integrals with coth-kernel.
BIT **27** (1987), *no. 3,* 389–402.

For the numerical evaluation of singular integrals of the form $I(x)=\int_{-1}^{1} f(t)\coth(a(t-x))\,dt$, by subtracting out the singularity we can write $I(x)=I_1(x)+I_2(x)$, where $I_1(x)$ is a simple Cauchy-type integral that can be evaluated in closed form, and $I_2(x)$ is a more general, but ordinary, integral. This paper considers problems arising in the numerical approximation of $I_2(x)$.

The evaluation of $I_2(x)$ is complicated by the existence of complex poles of the integrand. This causes difficulties when $a\gg 1$. The authors study two methods: Gauss-Christoffel quadrature, with weights that depend on a and x, and Gauss-Legendre quadrature, with weights that are independent of these parameters. Gauss-Christoffel quadratures converge more rapidly at the expense of more work. A number of specific examples illustrate this. The paper also presents an error analysis.

Reviewed by *P. Linz*

MR960329 (89k:41035) 41A55 (65D32)

Gautschi, Walter (1-PURD-C)

Gauss-Kronrod quadrature—a survey.

Numerical methods and approximation theory, III (*Niš*, 1987), 39–66, *Univ. Niš, Niš,* 1988.

The author surveys the literature, and synthesizes earlier work on orthogonality with respect to a particular sign-variable order-dependent weight function by Stieltjes and Szegő, with that following the work of Kronrod on the extension of the n-point Gauss Legendre quadrature to a $(2n+1)$-point formula having maximum degree of exactness.

{For the entire collection see MR0960326 (89c:65007)}

Reviewed by *A. J. Rodrigues*

MR1021523 (90m:65104) 65H10 (65D32)

Gautschi, Walter (1-PURD-C); **Notaris, Sotirios E.** (1-PURD-C)

Newton's method and Gauss-Kronrod quadrature.

Numerical integration, III (Oberwolfach, 1987), 60–71, *Internat. Schriftenreihe Numer. Math.*, 85, *Birkhäuser, Basel*, 1988.

Introduction: "Gautschi, jointly with F. Calio and E. Marchetti [Math. Comp. **47** (1986), no. 176, 639–650, S57–S63; MR 88a: 65028], considered the application of Newton's method (for large nonlinear systems of equations) in the context of computing Gauss-Kronrod quadrature rules. With the equations set up in an appropriate manner, it was found that, by careful choice of initial approximations and continued monitoring of the iteration process, the method could be made to work for rules with up to 81 nodes (40 Gauss and 41 Kronrod nodes). This was documented for the Legendre weight on $[-1,1]$ (where in fact formulae with up to 161 nodes were computed) and for weight functions on $[0,1]$ involving logarithmic and algebraic singularities. Further evidence of the feasibility of Newton's method, also for Kronrod extension of Gauss-Radau and Gauss-Lobatto formulae, is contained in Notaris's thesis (1988). If one attempts, however, to repeat Kronrod extension in the manner of Patterson (1968), one discovers that Newton's method quickly deteriorates and eventually fails to converge. The purpose of this note is to shed some light on the reasons for this failure of Newton's method. One of these is the excessive magnitude of the inverse Jacobian of the nonlinear system (evaluated at the solution) which comes about because of a peculiar behavior of a certain polynomial responsible for the magnitude of this inverse. Graphical evidence is provided to underscore the phenomenon. For simplicity we consider only integrals over a finite interval (standardized by $[-1,1]$) with constant weight function."

{For the entire collection see MR1021517 (90e:65003)}

MR942152 (89f:65031) 65D32
Gautschi, Walter (1-PURD-C); **Notaris, Sotirios E.** (1-PURD)
An algebraic study of Gauss-Kronrod quadrature formulae for Jacobi weight functions.
Math. Comp. **51** (1988), *no. 183,* 231–248.

The Gauss-Kronrod quadrature formula for the nonnegative weight $w(x)$ on $[a,b]$ is an interpolatory quadrature with two types of nodes, $\{\tau_i\}_1^n$ and $\{\tau_k^*\}_1^{n+1}$, where $\{\tau_i\}_1^n$ are the Gaussian nodes for the weight $w(x)$ and $\tau_1^*,\cdots,\tau_{n+1}^*$ are then chosen to maximize the algebraic degree of precision (ADP) of the quadrature. The existence of nodes $\{\tau_k^*\}_1^{n+1}$ that assure the maximal $\mathrm{ADP}=3n+1$ is a well-known fact. They are zeros of a polynomial π_{n+1}^* characterized by an orthogonal property. The authors study numerically the questions about the reality and location of the zeros of π_{n+1}^*, as well as the positivity of the coefficients. They consider the case of the Jacobi weight function $w^{(\alpha,\beta)}(t)=(1-t)^\alpha(1+t)^\beta$, $-1<t<1$, $\alpha>-1$, $\beta>-1$, and especially the Gegenbauer weight $w_\lambda(t)=w^{(\lambda-1/2,\lambda-1/2)}(t)$, $-1<t<1$, $\lambda>-\frac{1}{2}$. A number of conjectures are suggested by the numerical results.

Reviewed by *B. Boyanov*

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Note: This list reflects references listed in the original paper as accurately as possible with no attempt to correct errors.

MR958640 (89m:65029) 65D32
Gautschi, Walter (1-PURD-C); **Rivlin, Theodore J.** (1-IBM)
A family of Gauss-Kronrod quadrature formulae.
Math. Comp. **51** (1988), *no. 184,* 749–754.

A quadrature rule $\int_{\mathbf{R}} f(t)\,d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n(f)$, where $d\sigma$ is a positive measure, is called a Gauss-Kronrod rule if $\tau_\nu = \tau_\nu^{(n)}$ are the Gaussian nodes for $d\sigma$ and the weights $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma_\mu^* = \sigma_\mu^{*(n)}$ and the nodes $\tau_\mu^* = \tau_\mu^{*(n)}$ are chosen to maximize the degree of exactness of the quadrature rule. In this paper Gauss-Kronrod rules for the measure

$$d\sigma_\gamma(t) = (1+\gamma)^2(1-t^2)^{1/2}\,dt/((1+\gamma)^2 - 4\gamma t^2),$$

with $-1 < \gamma \le 1$, are considered. It is shown that for all $n \ge 1$, the $(2n+1)$-point formula satisfies $-\infty < \tau_{n+1}^{*(n)} < \tau_n^{(n)} < \tau_n^{*(n)} < \cdots < \tau_2^{*(n)} < \tau_1^{(n)} < \tau_1^{*(n)} < \infty$ (the interlacing property) and the positivity property: $\sigma_\nu^{(n)} > 0$ for $\nu = 1, \cdots, n$, and $\sigma_\mu^{*(n)} > 0$ for $\mu = 1, \cdots, n+1$. Explicit formulae for σ_γ and σ_μ^* are given, from which the positivity is derived.

Reviewed by *Hans Strauss*

MR988057 (90d:65045) 65D32
Gautschi, Walter (1-PURD-C); **Notaris, Sotorios E. [Notaris, Sotirios E.]** (1-PURD)
Gauss-Kronrod quadrature formulae for weight functions of Bernstein-Szegő type.
J. Comput. Appl. Math. **25** (1989), *no. 2,* 199–224.

The authors study Kronrod extensions of Gaussian quadrature formulae with weight functions consisting of any one of the four Chebyshev weights divided by an arbitrary quadratic polynomial that remains positive on $[-1, 1]$. Some new results are presented.

Reviewed by *Siegfried Filippi*

MR1026373 (90m:65055) 65D32

Gautschi, W. [Gautschi, Walter]; **Notaris, S. E.**

Erratum to: "Gauss-Kronrod quadrature formulae for weight functions of Bernstein-Szegő type" [J. Comput. Appl. Math. 25 (1989), no. 2, 199–224; MR0988057 (90d:65045)].

J. Comput. Appl. Math. **27** (1989), *no. 3,* 429.

Several typographical errors are corrected.

MR1127485 (92h:65038) 65D32 (41A55)
Gautschi, Walter (1-PURD-C)
Quadrature formulae on half-infinite intervals.
BIT **31** (1991), *no. 3,* 438–446.

Two classes of quadrature rules for integrals over the interval $[0, \infty)$ are developed. It is assumed that the integrand has an algebraic singularity at the origin of type x^α, $\alpha > -1$, and behaves like $x^{-\beta}$, $\beta > 1$, as $x \to \infty$. One rule has maximum polynomial degree of exactness while the other has maximum rational degree of exactness. It is shown 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 rules among themselves and with recently developed quadrature formulae based on Bernstein-type operators.

Reviewed by *N. S. Kambo*

MR1198903 (94e:41049) 41A80 (65D32)
Gautschi, Walter (1-PURD-C)
Remainder estimates for analytic functions. (English summary)
Numerical integration (Bergen, 1991), 133–145, *NATO Adv. Sci. Inst. Ser. C Math. Phys. Sci.*, 357, *Kluwer Acad. Publ., Dordrecht*, 1992.

Contour integral representations, and estimates, for the remainder term in quadrature rules of the form

$$\int_{-1}^{1} f(t)w(t)\,dt = \sum_{k=1}^{n} w_k f(t_k) + R_n(f)$$

are considered. The function f is analytic and the weight function w is integrable over the interval $[-1,1]$. The paper is a survey of available methods. Special attention is given to Gauss-type quadrature rules and to the behaviour of the kernel function (defined as a ratio of the corresponding nth-degree orthogonal polynomial and its associated polynomial) on circular and elliptic contours.

{For the entire collection see MR1198893 (93f:65006)}

Reviewed by *John H. McCabe*

MR1202296 (93m:33018) 33E20 (82B99)

Gautschi, Walter (1-PURD-C)

On the computation of generalized Fermi-Dirac and Bose-Einstein integrals. (English summary)

Comput. Phys. Comm. **74** (1993), *no. 2,* 233–238.

Summary: "Gauss-type quadrature formulae based on rational functions are proposed to evaluate generalized Fermi-Dirac and Bose-Einstein integrals to high accuracy. The method is compared with recent quadrature methods of B. Pichon and R. P. Sagar."

MR1344614 (96k:33015) 33C45 (41A55 65D32)
Gautschi, Walter (1-PURD-C); **Notaris, Sotirios E.**
Stieltjes polynomials and related quadrature formulae for a class of weight functions. (English summary)
Math. Comp. **65** (1996), *no. 215,* 1257–1268.

Let $d\sigma$ be a nonnegative measure with support in the interval $[a,b]$, $\pi_n(\cdot)=\pi_n(\cdot;d\sigma)$ be the respective monic orthogonal polynomial of degree n, and $\pi^*_{n+1}(\cdot)=\pi^*_{n+1}(\cdot;d\sigma)$ be the corresponding monic Stieltjes polynomial of degree $n+1$, defined uniquely by the orthogonality condition $\int_a^b\pi^*_{n+1}(t)t^k\pi_n(t)d\sigma(t)=0,\ k=0,1,\cdots,n$. The authors consider a special measure $d\sigma\in\mathcal{M}_l^{(\alpha,\beta)}[a,b]$ such that the polynomials π_n satisfy the three-term recurrence relation $\pi_{n+1}(t)=(t-\alpha_n)\pi_n(t)-\beta_n\pi_{n-1}(t)$ with constant coefficients $\alpha_n=\alpha$, $\beta_n=\beta$ for $n\ge l$. In this case, they prove that $\pi^*_{n+1}(\cdot;d\sigma)$ has a very simple and useful representation $\pi^*_{n+1}(t)=\pi_{n+1}(t)-\beta\pi_{n-1}(t)$ for $n\ge 2l-1$, and the corresponding Gauss-Kronrod quadrature formula has all the desirable properties (the interlacing of nodes, their inclusion in the closed interval $[a,b]$ if in addition $a=\alpha-2\sqrt{\beta}$ and $b=\alpha+2\sqrt{\beta}$, the positivity of all weights, and the degree of exactness is at least $4n-2l+2$). Also, they prove that the interpolatory quadrature formulae based on the zeros of the Stieltjes polynomials π^*_{n+1}, $n\ge 2n-1$, have positive weights and degree of exactness $2n-1$.

Reviewed by *Gradimir V. Milovanović*

MR1442065 (98j:41034) 41A55 (44A60 65D32)

Gautschi, W. [Gautschi, Walter] (1-PURD)

Moments in quadrature problems. (English summary)

Approximation theory and applications.

Compút. Math. Appl. **33** (1997), *no. 1-2,* 105–118.

Summary: "An account is given of the role played by moments and modified moments in the construction of quadrature rules, specifically weighted Newton-Cotes and Gaussian rules. Fast and slow Lagrange interpolation algorithms, combined with Gaussian quadrature, as well as linear algebra methods based on moment equations, are described for generating Newton-Cotes formulae. The weaknesses and strengths of these methods are illustrated in concrete examples involving weight functions with and without singularities. New conjectures are formulated concerning the positivity of certain Newton-Cotes formulae for Jacobi weight functions and for the logistics weight, with numerical evidence being provided to support them. Finally, an inherent limitation is pointed out in the use of moment information to construct Gauss-type quadrature rules for the Hermite weight function on bounded or half-infinite intervals."

MR1759036 (2001d:65032) 65D30
Gander, Walter (CH-ETHZ-ISC); **Gautschi, Walter** (CH-ETHZ-ISC)
Adaptive quadrature—revisited. (English summary)
BIT **40** (2000), *no. 1,* 84–101.

This paper is a special review, dedicated to Cleve Moler's 60th birthday, which considers adaptive quadratures with particular emphasis on the choice of termination condition for the recursive procedure. Matlab is the vehicle of implementation.

The usual terminating criterion of $|I_1 - I_2| < \mathrm{tol} * |I_1|$, where I_1 and I_2 are estimates of the integral over some subinterval of the recursion, also requires $|I_1| < \eta|I|$, where I is the whole integral, and tol and η are tolerances, in order to terminate the process robustly.

The choice of η and tol, and the practical use of Simpson's rule and Lobatto's rule (with Kronrod extensions) are considered with comparisons to both IMSL and NAG library routines on Kahaner's test functions.

Reviewed by *G. A. Evans*

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(1969), pp. 483–495. MR0240981 (39 #2326)

Note: This list reflects references listed in the original paper as accurately as possible with no attempt to correct errors.

MR1854270 (2002h:65214) 65R10
Gautschi, Walter (1-PURD-C); **Waldvogel, Jörg** (CH-ETHZ-AM)
Computing the Hilbert transform of the generalized Laguerre and Hermite weight functions. (English summary)
BIT **41** (2001), *no. 3,* 490–503.

Summary: "Explicit formulae are given for the Hilbert transform $⨍_{\mathbb{R}} w(t)dt/(t-x)$, where w is either the generalized Laguerre weight function $w(t)=0$ if $t\le 0$, $w(t)=t^\alpha e^{-t}$ if $0<t<\infty$, and $\alpha>-1,\ x>0$, or the Hermite weight function $w(t)=e^{-t^2}$, $-\infty<t<\infty$, and $-\infty<x<\infty$. Furthermore, numerical methods of evaluation are discussed based on recursion, contour integration and saddle-point asymptotics, and series expansions. We also study the numerical stability of the three-term recurrence relation satisfied by the integrals $⨍_{\mathbb{R}} \pi_n(t;w)w(t)dt/(t-x)$, $n=0,1,2,\ldots$, where $\pi_n(\cdot;w)$ is the generalized Laguerre [resp. the Hermite] polynomial of degree n."

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MR2457098 (2009k:65041) 65D30 (65B10)
Gautschi, Walter (1-PURD-C)
The numerical evaluation of a challenging integral. (English summary)
Numer. Algorithms **49** (2008), *no. 1-4,* 187–194.

The author calculates the integral

$$I=\int_0^\infty t^{-1}\cos(t\ln(t))dt,$$

whose integrand is highly oscillatory, to 60 digits accuracy. His approach is obvious but interesting. In step 1, after some transformations, the author obtains the representation

$$I=\int_0^{\pi/2}\frac{\cos x}{x+u(x)}dx+\sum_{k=1}^\infty(-1)^k\int_{-\pi/2}^{\pi/2}\frac{\cos t}{t+k\,\pi+u(t+k\,\pi)}dt=$$
$$a_0+\sum_{k=1}^\infty(-1)^k\,a_k,$$

where $u(x)$ is implicitly defined by the relation $u(x)\ln[u(x)]=x$. The integration interval $(0,\infty)$ is divided into subintervals, resulting in the alternating-series representation $\sum_{k=1}^\infty(-1)^k\,a_k$, where the a_k can be calculated easily by numerical quadrature. Step 2 of the transformation described by the author consists in a convergence acceleration method for the strictly alternating series $\sum_{k=1}^\infty(-1)^k\,a_k$. A number of methods have been described in the literature for this purpose, all of which work well. The author chooses Wynn's well-known epsilon algorithm, which calculates Padé approximants and easily achieves (more than) 60 digits of accuracy (see Equation (12) of the reviewed paper).

The function $u(x)$ is calculated by Newton's method, using a suitable starting value of $u_0\approx u(x)$ which is given (for small x) by a polynomial approximation to $u(x)$ and/or (for large x) by a truncated asymptotic expansion.

The two-step acceleration process (first step: to bring the numerical problem into tractable form, e.g., into the form of an alternating series; second step: to accelerate the convergence of the resulting series by an acceleration algorithm) seems to be somewhat generally applicable. In practice, a combined transformation of two steps (another example is the so-called combined nonlinear-condensation transformation) seems to produce the most favourable results—iterative procedures have traditionally received less attention—because the "acceleration potential" given by the asymptotic properties of a series are mostly exhausted in two transformation steps. The reviewed paper is a solid contribution to the field and confirms this general rule-of-thumb.

Reviewed by *Ulrich D. Jentschura*

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Note: This list reflects references listed in the original paper as accurately as possible with no attempt to correct errors.