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ORIGINAL PAPER

A guided tour through my bibliography

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Abstract Since this workshop is dedicated to my "50 years of professional activity", it may not be out of place to give a brief account of what came out of all this activity! Listing the publications is a partial answer, which I am trying to supplement here with some indications of contents. It is impossible, within a reasonable amount of space, to go into any great detail, but just enough information will be given so that anyone who reads this can decide whether to look up an original source for more details. The material is organized into nine sections, each devoted to a particular subject area, and a tenth one with a brief summary of impact. Publications that seem more significant than others are listed immediately following the subsection headings.

Keywords bibliography · Walter Gautschi

1 Special functions

1.1 Gamma function inequalities: [24, 57, 58]

The first paper actually proves (two-sided) inequalities for the incomplete gamma function (for a correction, see Math. Rev. 21 #2067). In a limit case, they improve upon inequalities of E. Hopf for the exponential integral E_1. The related inequalities for the gamma function, $x^{1-s} < \Gamma(x+1)/\Gamma(x+s) < (x+1)^{1-s},\ x > 0,\ 0 < s < 1$, now bearing my name, have received considerably more attention. The other two papers deal with harmonic mean inequalities for the gamma function.

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1.2 Computational algorithm for the complex error function: [46, 49]

Also known in the physics literature as Voigt function, or Faddeeva function, it is a basic function required in spectroscopy, atmospheric transmittance, nuclear reactors, and other areas of physics. In [49] an algorithm is developed to efficiently compute the function in the first quadrant Q of the complex plane. Whereas efficiency is commonly achieved by adopting different methods in different subregions of the domain of interest, here, through a detailed parameter analysis, a single nearly optimal algorithm is developed that provides a prescribed accuracy for all $z \in Q$. When $|z|$ becomes large, it automatically turns into a classical continued fraction approximation. An Algol implementation of the algorithm is provided in [46]. Both papers are widely cited in the physics literature, the former, with 133 citations, in fact being the second most frequently cited paper of mine; cf. Section 10.

1.3 Computation of special functions: [27, 39]

The more important reference here is [39] (with 271 citations the most frequently cited paper). It is basically a work studying "minimal solutions" of three-term recurrence relations and related continued fractions, with applications to the computation of special functions (Bessel, Legendre, Coulomb wave, incomplete beta and gamma functions, and repeated integrals of the error function). The concept of minimality is traced back to the Italian mathematician Pincherle; in fact, an 1894 paper of his, in which minimality is related to convergence of a continued fraction, is resurrected from obscurity. Earlier and subsequent related work can be found in [28, 45, 54, 66], surveys in [7](Section 2), [52, 177], and there are many pieces of published software; cf. Section 9.

The paper [27] analyzes the numerical peformance of first-order (inhomogeneous) recurrence relations, in particular forward vs backward recursion, with applications to "molecular integrals" and exponential integrals [54]. The analysis is supported by many inequalities and monotonicity results for the former integrals, and asymptotic results for both, which may be of independent interest. (The example of the incomplete gamma function is considered, from the same point of view, later in [133].) Another application is made in [36] to the recursive calculation of successive derivatives of $f(z)/z$ at a fixed complex $z \neq 0$, where f is analytic in a disc centered at z and large enough to contain the origin. The first-order recurrence relation satisfied by these derivatives is then stable in forward direction if and only if $f(0) \neq 0$. Computer algorithms are developed in [37] when f is either the exponential or a trigonometric function, the latter being of interest in connection with successive derivatives of the sinc function $(\sin z)/z$. Further improvements in the stability of these algorithms are discussed in [47] and implemented in [48].

1.4 Incomplete gamma function: [74, 75, 178]

The first two papers develop a detailed computational procedure and computer algorithm, also summarized in [76]; the third is a historical profile of this function, written on the occasion of the 100th anniversary of the birth of F.G. Tricomi, who pioneered it.

1.5 Exponential integrals

A uniform (in x) asymptotic approximation of the exponential integral $E_n(x)$ for large n appears in [25], and expansions of E_1 in incomplete gamma functions are given in [146].

1.6 Handbook chapters in "Abramowitz/Stegun": [5, 6]

These are widely cited chapters on the exponential integral and related functions, and on the error function and Fresnel integrals.

1.7 A survey of computational methods: [7]

This surveys a wide range of methods for approximating and computing special functions. Included are methods based on best rational approximation, truncated Chebyshev expansion, Taylor series and asymptotic expansion, Padé approximation and continued fractions, and linear and nonlinear recurrence relations. Software available at the time is also surveyed.

2 Ordinary differential equations

2.1 Numerical integration of oscillatory differential equations: [29]

The methods developed here, based on trigonometric rather than algebraic polynomials, anticipate methods later called "exponentially fitted." They have recently attracted renewed interest and are named after me.

2.2 An early survey of numerical methods for ODEs: [4]

This is the first systematic review of the theory of one-step and multistep methods known at the time. It has largely been overshadowed by Henrici's book on discrete variable methods, which appeared in the same year.

2.3 Global error estimates

An attempt is made in [63] to estimate the global error of one-step methods, at least asymptotically for small steps. In [79], the method is determined, within a class of multistep methods, having minimum coefficient in the asymptotic formula for the global error.

3 Conditioning of matrices and mappings

3.1 Condition of Vandermonde and Vandermonde-like matrices: [30, 60, 86, 105]

Vandermonde-like matrices are Vandermonde matrices in which the consecutive powers are replaced by consecutive polynomials, here orthogonal polynomials, and the nodes are the zeros of the first polynomial not appearing in the matrix.

The four papers listed are the basic papers on norm estimates for inverses of Vandermonde and Vandermonde-like matrices, and hence on condition numbers for these matrices. Confluent Vandermonde matrices, already considered in [30], are revisited in [32]. The results in [30] are applied in [44] to Vandermonde matrices whose nodes are zeros of shifted Jacobi polynomials. Such matrices arise in the numerical inversion of Laplace transforms by a method of Bellman, Kalaba, and Lockett. In [61], further applications are made to real node configurations of optimally conditioned Vandermonde matrices – a problem still unresolved for large-scale matrices – and in [70], with the help of Jensen's formula in the theory of analytic functions, to lower bounds for the condition number of ordinary and confluent Vandermonde matrices with arbitrary complex nodes. The upshot of this work is that Vandermonde matrices with real nodes are always ill-conditioned, exponentially so or worse. For complex nodes, they are usually, but not necessarily, well-conditioned. In the case of Vandermonde-like matrices, the matter depends on the Christoffel numbers or Christoffel function (evaluated at the nodes) of the measure defining the orthogonal polynomials, more precisely, on the ratio of their arithmetic and harmonic means.

A noteworthy case, considered in [110], is the $n \times n$ Vandermonde matrix whose nodes are the first n members of an infinite sequence of complex nodes on the unit circle, specifically a Van der Corput sequence. The (spectral) condition number is then shown to be bounded by $\sqrt{2n}$. It is true that the roots of unity yield optimal condition number 1, but these form a triangular array of nodes as opposed to a linear array, which for practical purposes is more interesting. The survey [170] summarizes much of this work, and in addition contrasts Van der Corput sequences on the unit circle, and also on confocal ellipses, with so-called quasi-cyclic sequences on the same contours.

3.2 The condition of polynomial bases: [72]

The sensitivity of the coefficients of a polynomial of degree $n-1$ in a given basis to small perturbations of the polynomial on a fixed interval $[a, b]$, and vice versa, can be measured by the condition number κ_n of a certain linear map M_n. For the basis of powers, and intervals $[-\omega, \omega]$ symmetric with respect to the origin, κ_n can be expressed explicitly in terms of the coefficients of the Chebyshev polynomials $T_m(x/\omega)$, $m = n-1, n-2$, and shown to grow exponentially fast, at least like $O[(1+\sqrt{2})^n]$. For intervals $[0, \omega]$ the growth is at least $O[(1+\sqrt{2})^{2n}]$. This is in sharp contrast with bases consisting of polynomials orthogonal on a finite interval, considered in [53], in which case the growth of κ_n is typically polynomial when the sensitivity is measured on the interval of orthogonality.

3.3 The condition of algebraic equations: [55]

The roots of an algebraic equation can be quite sensitive to small perturbations in the coefficients of the equation (relative to some given polynomial basis). Here, appropriate condition numbers are defined and analyzed. Best understood is the case of equations expressed in power form, for which the condition of the roots can often be written down explicitly or at least estimated closely. Many examples for this are provided, the most notable one involving the Wilkinson polynomial. In the

case of polynomial equations expressed in a basis of orthogonal polynomials, the condition of the roots can, if not easily expressed or estimated, at least be computed numerically. Examples for this are also provided.

3.4 The condition of moment maps in the theory of orthogonal polynomials and related quadratures

For this, see Sections 5.2 and 5.6.

For the material in Sections 3.2–3.4, see also the survey in [9].

4 Chebyshev-type quadrature

4.1 Chebyshev-type quadrature formulae: [56]

For the integral $\int_{-1}^{1} f(t)\mathrm{d}t$, an n-point Chebyshev quadrature formula is one having equal weights $2/n$, real distinct nodes in $[-1, 1]$, and polynomial degree of exactness n. According to a classical result of Bernstein, such formulae exist only for $1 \leq n \leq 7$ and $n = 9$. This gives rise to the question of how to find substitute formulae, called Chebyshev-type formulae, for the nonexisting Chebyshev formulae. A natural way is to somehow relax the polynomial exactness condition. In [56], this is done for $n = 8, 10, 11, 13$ by replacing polynomial exactness by certain optimality conditions involving the remainder term. It is shown, however, that this comes at the price of having to accept a double node in each case.

4.2 Weighted Chebyshev-type quadrature formulae: [59, 62, 65, 159]

Chebyshev quadrature can be considered also for weighted integrals $\int_{\mathbb{R}} f(t)\mathrm{d}\lambda(t)$. Nonexistence may then be even more prevalent, as e.g. for Laguerre and Hermite measures $\mathrm{d}\lambda(t) = t^{\alpha}e^{-t}\mathrm{d}t$ on $\mathbb{R}_+$ and $\mathrm{d}\lambda(t) = e^{-t^2}\mathrm{d}t$ on $\mathbb{R}$, for which an n-point Chebyshev quadrature formula is known to exist only when $n \leq 2$ (if $\alpha = 0$) and $n \leq 3$, respectively. A similar situation is shown in [59] to exist also for n-point Chebyshev-type quadrature formulae of relaxed degree of exactness $n - s$, $s > 0$, and relaxed conditions on the nodes (to be merely real, not necessarily distinct). A deeper analysis of weighted Chebyshev-type quadrature formulae is given in [62], where formulae are considered that have maximum algebraic degree of exactness and minimum error when applied to the first power not exactly integrated. Called optimal in [62], they always exist. Their construction, however, requires the complete solution of systems of algebraic equations involving generalized power sums. Algebraic tools are developed to solve some special cases, which is then applied to obtain optimal Legendre-weight formulae for $n \leq 17$, Hermite-weight formulae for $n \leq 11$, and Laguerre-weight formulae (with $\alpha = 0$) for $n \leq 7$. In the Legendre case, the optimal formulae of "next-to-highest" algebraic degree are shown in [65] to minimize not only the error term for the first power not exactly integrated, but also the one for all subsequent powers. Hence, they are minimum-norm quadratures in the Hardy space H_2 of functions $f(z)$ analytic in $|z| < r$, $r > 1$, and square-integrable on $|z| = r$.

A short summary of Chebyshev and Chebyshev-type quadrature formulae is given in [69], and a more comprehensive historical review, up to about 1975, in [159].

5 Gauss-type quadrature rules

An extensive historical review, covering the period from Gauss's original 1814 paper to about 1980, and written on the occasion of the 150th anniversary of Christoffel's birth, can be found in [8].

5.1 Geometric properties: [153]

It has been known for some time, either explicitly or implicitly, that for Gauss–Jacobi and other related quadrature formulae on $[-1, 1]$ their weights, suitably normalized, when plotted over the corresponding nodes, come to lie on the upper half of the unit circle, asymptotically for large orders. In [153], this is shown to be true for a large class of weight functions, essentially the Szegö class, not only for the Gauss formulae, but also for Gauss–Radau, Gauss–Lobatto, and, under more restrictive conditions, even for Gauss–Kronrod formulae. There is a close connection with potential theory inasmuch as the unit semicircle is the reciprocal density of the equilibrium measure of the interval $[-1, 1]$. For weight functions with other support, for example a compact set $\Delta \subset [-1, 1]$, the limit curve will be the reciprocal density of the equlilibrium measure of Δ. An illustration of this is given, where Δ is the union of two symmetric, disjoint intervals.

5.2 Generation of Gaussian quadrature formulae: [3, 41, 50, 84, 123]

The problem is to generate Gaussian quadrature formulae for essentially arbitrary (positive) weight functions. The way to do this is classically known: generate the orthogonal polynomials for the given weight function, and obtain the Gauss nodes as the zeros of, and the weights in terms of, these orthogonal polynomials. Also classical, and in fact well into the 20th century, is the implementation of this idea using the moments of the weight function. In [41], the problematic nature of this approach – severe ill-conditioning – is pointed out and analyzed for the first time by estimating (from below) the condition number κ_n of the nonlinear map from the first $2n$ moments to the n-point Gauss quadrature formula. It is found that, typically, $\kappa_n > (1 + \sqrt{2})^{4n}$ for weight functions on $[-1, 1]$. Confluent Vandermonde matrices and the work in [32] are crucial for this analysis. In the same paper, the proposal is made to avoid ill-conditioning by discretizing the inner product and generating the respective discrete instead of the required continuous orthogonal polynomials to approximate the Gauss formulae. The computer algorithm in [42] implements this idea. Further development of this idea had to wait until 1982, when in Section 2.2 of [84] the scope of the method has been expanded and the method itself called "discretized Stieltjes procedure" (in recognition of a brief remark in an 1884 paper of Stieltjes regarding the generation of successive orthogonal polynomials relative to a continuous weight function). The method was further consolidated in [123], where it is implemented in a Fortran routine, and in [3], which contains a Matlab implementation. (The method has recently been referred to as the "Stieltjes–Gautschi method".)

Once (a sufficient number of) the orthogonal polynomials, i.e., their recurrence coefficients collected in a symmetric tridiagonal matrix – the Jacobi matrix – have been generated, the Gauss nodes can be obtaind as the eigenvalues of the Jacobi matrix, and the Gauss weights either from known formulae involving orthogonal polynomials, or in terms of (the first components of) the normalized eigenvectors. The latter seems to be more efficient, judging from a small number of experiments reported on in [160].

Another idea of avoiding ill-conditioning was advanced in 1969 by Sack and Donovan, who proposed the use of modified moments, i.e., weighted integrals of auxiliary orthogonal polynomials p_k rather than powers as in the case of ordinary moments. This is immediately analyzed in [50] with regard to conditioning and found in typical cases (involving the interval $[-1, 1]$) to lead to condition numbers that grow only polynomially rather than exponentially. A more definitive analysis of the underlying condition number is given later in [84] and [97]. In the same paper [50], an algorithm is also developed for generating the Jacobi matrix of order n, given the first $2n + 1$ modified moments. It uses a Cholesky factorization of the $(n + 1 \times n + 1)$ Gram matrix of the polynomials $\{p_k\}$ and therefore has complexity $O(n^3)$. Sack and Donovan, and later in 1974 Wheeler, developed more efficient $O(n^2)$ algorithms. In the case of ordinary moments and discrete orthogonal polynomials, Wheeler's algorithm in fact has already been discovered by Chebyshev in 1859 and is therefore called "modified Chebyshev algorithm" in Section 2.4 of [84].

5.3 Validation of Gaussian quadrature formulae: [87]

Given numerical values of the nodes and weights of a Gauss formula, the question here is to determine their accuracy. In view of the severe ill-conditioning mentioned in the previous subsection, this is a nontrivial problem. Moment-related tests are utterly useless. Two other tests are proposed and shown to be quite effective in the case of a 15-point Gauss formula for the weight function $\exp(-t^3/3)$ on $\mathbb{R}_+$, published in the chemistry literature to 16 decimal digits, but accurate to only 1–2.

5.4 Gauss–Radau and Gauss–Lobatto formulae: [115, 147]

The topics in [115] are generalized Gauss–Radau and generalized Gauss–Lobatto formulae having end point(s) of multiplicity 2. Positivity of the formulae is established for arbitrary weight functions on $[-1, 1]$. General characterizations of the internal nodes and weights are well known, but the weights for the boundary terms require special attention. They are explicitly determined in [115], as rational functions of the order n, for Chebyshev weight functions of all four kinds. For Chebyshev weights of the first kind and Gauss–Radau formulae, more explicit formulae than those generally known are obtained for the internal weights. The superiority of generalized Gauss–Lobatto over ordinary Gauss formulae is illustrated in the case of Fourier coefficients relative to orthogonal Bessel functions.

Generalized Gauss–Radau and Gauss–Lobatto formulae with end point(s) of arbitrary multiplicity $r \geq 1$ are studied in [147]. They are of interest in connection with moment-preserving spline approximation on compact intervals; cf. Section 7.1. Computational procedures are developed to generate these formulae, and numerical

tests seem to indicate that they are positive for all r and for many, if not all, weight functions.

In [139], for Gauss–Radau formulae, the respective Jacobi matrices, as well as all the quadrature weights, are obtained explicitly for general Jacobi weight functions on $[-1, 1]$ and generalized Laguerre weights on $[0, \infty]$. This obviates, for these weight functions, the need to compute eigenvectors of the Jacobi matrix to obtain the quadrature weights, and the explicit formulae are often, especially for the boundary weights, more accurate than the results from eigenvectors. The computation of the Jacobi matrix for high-order Gauss–Lobatto formulae may break down because of underflow, causing division by zero. In the case of Jacobi weight functions on $[-1, 1]$, explicit formulae for the offending elements of the Jacobi matrix, given in [138], eliminates the problem. It is also shown in [138], by numerical experiments, that for Jacobi weight functions, explicit formulae for the weights of both, interior and boundary terms, generally give more accurate results than computation via eigenvectors.

5.5 Gauss–Turán formulae: [132]

These are weighted quadrature rules (with weight function w) of maximum degree of exactness involving not only function values, but also derivatives up to an even order $2s$, all evaluated at the same set of n nodes. The latter must be the zeros of the so-called s-orthogonal polynomial $\pi_{n,s}$ of degree n whose $(2s + 1)$-st power is orthogonal (with respect to w) to all polynomials of degree $< n$. Put differently, $\pi_{n,s}$ is orthogonal to all lower-degree polynomials relative to the positive weight function $\pi_{n,s}^{2s} w$. One has here a case of implicit orthogonality, since the polynomial sought appears also in the weight function. The basic idea of computing the polynomial $\pi_{n,s}$ is to embed it into a sequence of $n + 1$ polynomials $\pi_0, \pi_1, \ldots, \pi_{n-1}, \pi_n$, of which the last one is $\pi_n = \pi_{n,s}$ and all are mutually orthogonal relative to the weight function $\pi_{n,s}^{2s} w$. The problem, therefore, is to compute the Jacobi matrix of order n for $\pi_{n,s}^{2s} w$. A procedure for this is developed in [132], which is stable, but owing to the implicit nature of the problem requires the solution of a set of $2n$ nonlinear equations. This is accomplished by the Newton–Kantorovich method and basically requires only knowledge of the Jacobi matrix of order $(s + 1)n$ for the weight function w and the respective Gauss formula of order $(s + 1)n$. For the $2s + 1$ weights of the Gauss–Turán formula associated with each node, an upper triangular system of linear equations is derived, the solution of which again requires only the $(s + 1)n$-point Gauss formula for w. Special attention is paid to the Chebyshev weight function $w(t) = (1 - t^2)^{-1/2}$, for which the orthogonal (Chebyshev) polynomials are s-orthogonal for all s.

5.6 Gauss–Kronrod formulae: [104, 106, 108, 164]

Given an n-point Gauss quadrature formula relative to some weight function w, it may be extended to a $(2n + 1)$-point formula by inserting $n + 1$ additional nodes and choosing them, and all the weights, in such a way as to maximize the degree of exactness. This is the idea behind Gauss–Kronrod quadrature. It is known that the $n + 1$ nodes to be inserted must be the zeros of the polynomial π_{n+1}^S of degree $n + 1$, called Stieltjes polynomial, which is "orthogonal" to all lower-degree polynomials with respect to the sign-variable "weight function" $\pi_n w$, where π_n is the nth-degree

orthogonal polynomial relative to the weight function w. The reality of the zeros of π_{n+1}^S – the Kronrod nodes – is by no means guaranteed, nor is the fact that they are all mutually distinct and contained in the interval of orthogonality, or even interlacing with the given Gauss nodes. There is an extensive and still growing literature dealing with these questions, and also with the question of positivity. The state of knowledge, as of 1988, is summarized in [164]. In [104], these questions are examined in detail for the Gegenbauer weight function $w(t) = (1 - t^2)^{\lambda - 1/2}$, first explicitly for $1 \leq n \leq 4$, and then, in part numerically and in part algebraically, for values of n up to 40. For each fixed n, a dynamic approach is taken: starting from a λ-interval in which the property p of interest is known to hold, the parameter λ is moved away from this interval until the property breaks down, which is signaled by an algebraic condition (for example, the vanishing of the resultant of two polynomials). In this way the exact interval $\lambda_n^p < \lambda < \Lambda_n^p$ can be determined in which property p holds. It is conjectured that there are such exact intervals also for any $n > 40$. A similar analysis is undertaken for general Jacobi weight functions $w(t) = (1 - t)^\alpha (1 + t)^\beta$, the task then being to obtain the region D_n^p in the (α, β)-plane in which property p holds for a given n. This is carried out numerically/algebraically for n up to 10.

All the desired properties are shown in [106] to hold for Gauss–Kronrod formulae involving a one-parameter family of weight functions considered already in 1930 by Geronimus. Not only are all these properties satisfied, but the formulae can be written down fairly explicitly and, moreover, they have exceptionally high degree of exactness. The same is shown in [108] to be (almost always) true for weight functions of Bernstein–Szegö type, i.e., a Chebyshev weight of any of the four kinds divided by a quadratic polynomial which remains positive on $[-1, 1]$. (The Geronimus weight is the special case where the quadratic polynomial is even.) The theory, as a limit case, extends to linear divisor polynomials as well. There is yet another situation, considered in [128], which gives rise to equally favorable Gauss–Kronrod formulae, at least for n sufficiently large, namely the case in which the orthogonal polynomials for the underlying weight function satisfy a three-term recurrence relation which ultimately has constant coefficients.

The problem of computing an n-point Gauss–Kronrod formula is addressed in [98], where a system of $3n + 2$ nonlinear equations involving modified moments is derived for all the unknown quantities (the $n + 1$ Kronrod nodes and $2n + 1$ weights). The system is solved by a careful implementation of the Newton–Kantorovich method. A detailed analysis of the condition of the underlying moment map is also provided. For repeated Kronrod extensions à la Patterson, it is found in [165] that Newton's method quickly deteriorates with increasing n and eventually fails to converge for reasons of severe ill-conditioning. The method preferred in [3] is a more recent method due to Laurie using eigenvalues and eigenvectors.

5.7 Error bounds for analytic functions: [88]

When n-point Gaussian quadrature relative to a weight function w on $[-1, 1]$ is applied to an analytic function f, the error is expressible as a contour integral $(2\pi \mathrm{i})^{-1} \int_\Gamma K_n(z) f(z) \mathrm{d}z$, where Γ is a contour in the domain of analyticity of f encircling the interval $[-1, 1]$. The kernel K_n depends solely on the weight function w. In order to bound the error, it is useful to have a sharp bound of $|K_n(z)|$ for $z \in \Gamma$. The task in [88] is to find a point z_n on Γ such that $|K_n(z_n)| = \max_{z \in \Gamma} |K_n(z)|$.

Once found, the kernel $K_n(z_n)$ can be computed by a continued fraction algorithm for minimal solutions of three-term recurrence relations; cf. Section 1.3. (The same algorithm is useful also for evaluating certain correction terms that arise when poles are present in the integrand.) In the case of a circular contour with center at the origin and radius $r > 1$, our task is resolved for a large class of weight functions with the help of a monotonicity result in [89] for Gauss quadrature approximations of the moments of w. In fact, z_n is either r or $-r$, depending on whether $w(t)/w(-t)$ is nondecreasing or nonincreasing on $(-1, 1)$. Technically more challenging is the case of elliptic contours, where precise results are obtained only for the four Chebyshev weight functions. The maximum is then again attained on the real axis, except for Chebyshev weights of the second kind and n odd, when it is attained on the imaginary axis. (A detailed discussion of the case n even is given in [109].) For more general Jacobi weight functions, the problem is explored numerically. This work is continued in [112], where error bounds for Gauss–Radau and Gauss–Lobatto formulae are derived in the same spirit, and in [111], where the same is done for generalized Gauss–Radau and generalized Gauss–Lobatto formulae having end point(s) of multiplicity 2.

Contour integration techniques for error estimation are surveyed in [172], partly in a historical perspective.

5.8 Rational/polynomial Gauss quadrature: [134]

When integrating functions that have poles outside, possibly near, the interval of integration, it seems natural to utilize quadrature rules that are exact for a mixture of polynomials and elementary rational functions having the same poles, or at least the most important ones, as the function to be integrated. Such formulae of Gaussian type, exactly integrating as many polynomials and rational functions as possible, are developed in [174] and, in a more definitive manner, in [134]. This calls for the construction of Gauss quadrature formulae for weight functions modified by a rational function; cf. Section 6.1. The idea is extended in [137] to Gauss–Kronrod and Gauss–Turán type formulae as well as to rational Gauss formulae for Cauchy principal value integrals. Interpolatory quadrature rules, for example Fejér rules (see Section 5 of [142]), can also be "rationalized." The use of rational Gauss formulae for integrals of interest in solid state physics is proposed in [122].

5.9 Applications

Gauss quadrature has been applied in various contexts: in [92] to integrals – Einstein and Fermi functions – of interest in solid state physics and also in the summation of slowly convergent series [113], in [103] to Cauchy principal value integrals involving a coth-kernel, in [117] to integrals over the positive real line with prescribed algebraic behavior of the integrand at zero and at infinity, in [136] to certain integrals of interest in wavelet analysis, and in [143, 144, 152, 154] to the evaluation of special functions (hypergeometric, confluent hypergeometric, Bessel, Macdonald, Airy functions, and Kontorovich-Lebedev integral transforms).

6 Orthogonal polynomials

6.1 Generation of orthogonal polynomials: [3, 84]

The generation of orthogonal polynomials, meaning the generation of their Jacobi matrix, goes hand in hand with the generation of Gauss-type quadrature rules, and the principal methods – discretization and moment-based methods – have already been mentioned in Section 5.2. The major reference here is [84] (with 100 citations the third most frequently cited paper). In addition, there are modification algorithms which generate new orthogonal polynomials from old ones by multiplying the weight function of the latter by a rational function. The major reference for this, until recently, was [161], but today, the techniques presented in Section 2.4 of [3] are simpler and more effective. A related type of modification – multiplying the weight function of the old polynomials by the square of the nth degree (old) orthogonal polynomial π_n – is studied in [120], where for each n the sequence of new polynomials is called induced (by the orthogonal polynomial π_n); see Section 7.3 for an application. Another important problem is the computation of Cauchy integrals of orthogonal polynomials, in particular the Cauchy transform of a positive measure, where the theory of minimal solutions of three-term recurrence relations and related algorithms find an application; see [80].

Constructive methods and software for, and applications of, orthogonal polynomials have been reviewed at various stages of their development in expository articles, [11, 13, 93, 148, 163, 166, 167, 169, 171, 173, 176, 179], of which the first two and [169] are the more extensive ones. The article [13] is actually a concise summary of the book [3], but also contains exercises.

6.2 Special (nonclassical) orthogonal polynomials: [91, 152]

The recurrence coefficients of orthogonal polynomials with weight function supported on $[-1, -\xi] \cup [\xi, 1]$, $0 < \xi < 1$, and having algebraic singularities with indices p and q at $\pm\xi$ resp. ± 1, are shown in [91] to be computable directly by simple nonlinear recursions and, in the case $p = q = \pm 1/2$, to be explicitly known. Interestingly, in the case $p = q = -1/2$, the corresponding n-point Gaussian quadrature formula has equal weights whenever n is even. Orthogonal polynomials with unusual weight functions w are generated and applied in [83], where w is the reciprocal gamma function on $\mathbb{R}_+$, in [150], where w is densely oscillating, or exponentially decaying, near the origin, and in [152], where $w(t) = \exp(-e^t)$ on $\mathbb{R}_+$ is decaying "super-exponentially" at infinity.

6.3 Orthogonal polynomials on the semicircle: [102]

In [94, 96] a new type of complex orthogonal polynomials is introduced for which the inner product (u, v) – the integral of the product uv over the upper unit semicircle – is non-Hermitian. It is, however, quasi-definite, as is shown by examining moment determinants, implying that the (monic) complex orthogonal polynomials exist uniquely. They satisfy a three-term recurrence relation with one set of coefficients purely imaginary and the other positive. All zeros of each of these polynomials are simple, contained in the interior D_+ of the upper half of the unit disc, and

distributed symmetrically with respect to the imaginary axis. Each polynomial also satisfies a linear second-order complex differential equation. The zeros determine a Gaussian quadrature rule over the semicircle, whose nodes and weights can be computed in terms of the eigenvalues and eigenvectors of a real tridiagonal matrix which, however, is no longer symmetric, as in the classical case. The Gauss formula can also be used for integration over the full circle if the latter is broken up into two halves and the lower half transformed into the upper by a change of variables. In this way, Cauchy's theorem, e.g., can be implemented numerically [168].

The theory is generalized in [102] to weighted inner products over the semicircle and simplified considerably, using orthogonality and the associated polynomials of the second kind as principal tools and thereby avoiding moment determinants altogether. Special attention is paid to Jacobi and Gegenbauer weight functions (on D_+) and to the zeros of the respective (complex) orthogonal polynomials. It is proved, in part with the help of the gamma function inequality of Section 1.1, that in the case of Gegenbauer weights the zeros are all simple and contained in D_+, and numerical exploration suggests the same for Jacobi weights. For arbitrary symmetric weight functions it is shown that all zeros are in D_+ with the possible exception of a single (simple) zero on the imaginary axis on or above the point i. That the exception can indeed occur is proved in [107]. A linear second-order differential equation again holds, at least in the case of Gegenbauer weights.

6.4 Sobolev orthogonal polynomials: [126, 131]

These are polynomials orthogonal in Sobolev spaces, the inner product thus involving derivative terms up to some order $s \geq 1$, each being endowed with its own (positive) measure, often discrete for derivatives of order ≥ 1. The recurrence relation satisfied by Sobolev polynomials is now of increasing order; computing its coefficients is again a major task, which is considered in [126]. Two methods are developed: The first is based on modified moments of the constitutive measures and generalizes the modified Chebyshev algorithm for ordinary orthogonal polynomials ($s = 0$). Because of intrinsic complexities, this is done only in the special, but important, case $s = 1$. The second method, applicable for arbitrary $s \geq 1$, generalizes the discretized Stieltjes procedure. The study of the zeros of Sobolev orthogonal polynomials is an important problem, which is here explored computationally, making use of the fact that they are the eigenvalues of an upper Hessenberg matrix formed with the recurrence coefficients. For Sobolev polynomials with $s = 1$ and inner products involving Jacobi and generalized Laguerre measures, a number of conjectures are formulated with regard to reality, location, and interlacing of the zeros. For a class of Sobolev orthogonal polynomials with $s = 1$ and compactly supported measures, the asymptotic distribution of zeros not only of Sobolev polynomials, but also of their first derivative, is analyzed in [131] by potential-theoretic methods and illustrated numerically.

A rather special type of Sobolev orthogonality is considered in [129], where the "ground measure" is absolutely continuous and there occurs only one derivative, of order $r \geq 1$, with the associated measure being atomic, i.e., concentrated at a single point $c \in \mathbb{R}$. In this case, the Sobolev orthogonal polynomial $q_k(x)$ of degree k, multiplied by $(x - c)^{r+1}$, is expressible as a linear combination of either $q_j(x)$, $|j - k| \leq r + 1$, or $p_j(x)$, $|j - k| \leq r + 1$, the polynomials orthogonal with respect to

the ground measure. Stable methods are developed for computing the respective coefficients, and the numerical behavior – not always unproblematic – of these new (finite-order) recurrences is analyzed along with the location of the zeros, of which some may be complex.

7 Approximation

7.1 Moment-preserving spline approximation: [99, 100]

Work on this problem began with [90], where a function f on $\mathbb{R}_+$ was to be approximated by a step function s in such a way that f and s have as many moments in common as possible. Both, the location and height of the jumps of s, are assumed to be freely variable. The problem has arisen in connection with the moment-preserving approximation of the Maxwell distribution and has been "solved" in the physics literature by methods known to be highly unstable. Here it is observed that the problem is equivalent to constructing a Gaussian quadrature formula relative to a weight function which depends on f and which is positive if f is monotonically decreasing on $\mathbb{R}_+$. The problem is thus brought into the realm of stable methods for constructing orthogonal polynomials. Numerical data is presented not only for the Maxwell distribution, but also for the Bose–Einstein and Fermi–Dirac distributions. In [99] the problem is generalized to moment-preserving approximation on $\mathbb{R}_+$ by spline functions of fixed degree and variable knots. Under appropriate assumptions on f, the problem is shown to have a unique solution if and only if a Gauss quadrature formula exists, with distinct positive nodes, for a certain weight function, not necessarily positive on $\mathbb{R}_+$, depending on f. Unique existence is assured, e.g., if f is completely monotonic on $\mathbb{R}_+$. Analogous problems on a compact interval, considered in [100], are considerably more intricate as they require generalized Gauss–Radau and generalized Gauss–Lobatto quadrature formulae for their solution; cf. Section 5.4. A summary of this work is given in [118].

7.2 Fourier analysis: [51]

The object here is to approximate the nth (complex) Fourier coefficient $c_n(f)$ of a 2π-periodic function f, given the values of f at N equally spaced points in $[0, 2\pi)$. The most common solution is the discrete Fourier transform $\hat{c}_n(f)$, which is reasonable if no information about f is known other than the N function values. The approximation, indeed, is optimal in the discrete L_2-norm (relative to the N equidistant points), and moreover is accessible to the fast Fourier transform for speedy evaluation. On the other hand, $\hat{c}_n(f)$, because of its N-periodicity $\hat{c}_{n+N}(f) = \hat{c}_n(f)$, may fall short in reflecting important properties of $c_n(f)$, as for example its decay properties as $n \to \infty$. An alternative approach, therefore, is to first use the data to find an approximation φ of f and then approximate $c_n(f)$ by $c_n(\varphi)$. In many cases it is found that $c_n(\varphi) = \tau_n \hat{c}_n(f)$, where τ_n – called attenuation factor – is independent of f and depends only on the approximation process $P : f \to \varphi$. This approximation, still amenable to fast Fourier transform evaluation, by virtue of the attenuation factors may faithfully reproduce the asymptotic behavior of $c_n(f)$ as $n \to \infty$. The paper [51] develops a general theory of attenuation factors. The basic

result is that for the existence of attenuation factors it is necessary and sufficient that the process P be linear and translation invariant. The theorem extends to approximation processes P that use also derivative values of f at the data points, in which case there is an attenuation factor associated with the Fourier transform of each derivative. Multiple attenuation factors occur also for approximation processes P that are r-translation invariant, $r > 1$, i.e., translation invariant over r, but not fewer, consecutive subintervals. The theory is illustrated by many examples, in which φ are polynomial and nonpolynomial spline interpolants, including deficient splines, as well as other piecewise polynomial interpolants.

7.3 Extended Lagrange interpolation: [119, 127]

Both, [119] and [127], analyze the extension of Lagrange interpolation at the n zeros of an nth-degree orthogonal (relative to a weight function w) polynomial π_n to Lagrange interpolation at $2n + 1$ points by introducing $n + 1$ additional abscissae of interpolation. Following an idea of A. Bellen, the additional abscissae, similarly as in Kronrod extension of Gaussian quadrature, are taken to be the zeros of the polynomial of degree $n + 1$ orthogonal with respect to the weight function $\pi_n^2 w$ (not $\pi_n w$, as in Kronrod extension!), an "induced" orthogonal polynomial in the terminology of [120].

The first paper considers mean convergence (in $L_w^2[-1, 1]$) as $n \to \infty$, for arbitrary continuous functions $f \in C[-1, 1]$. By a well-known result of Erdős and Turán, this indeed holds for n-point interpolation of f at the zeros of π_n, and the question is whether the same remains true for the extended $(2n + 1)$-point interpolation. The principal result in [119] relates to Chebyshev weight functions w and is basically a negative one: mean convergence for all $f \in C[-1, 1]$ fails to hold for Chebyshev weight functions of the first, third, and fourth kind, but holds trivially, i.e., as a consequence of the Erdős–Turán result, for the Chebyshev weight function of the second kind. Extensive numerical exploration, based on a sufficient condition for mean convergence due to Bellen, however, suggests its validity for Jacobi weight functions with parameters α, β suitably restricted.

The second paper [127] looks at what Erdős and Turán called "quadrature convergence," i.e., convergence to zero of the weighted integral of the interpolation error (not its square!). This trivially holds for n-point interpolation as above, and also for the extended $(2n + 1)$-point interpolation, if the interpolatory $(2n + 1)$-point quadrature rule based on the $2n + 1$ abscissae of interpolation is positive. The latter is shown to be indeed the case for all four Chebyshev weight functions by determining the quadrature weights explicitly. Moreover, it is shown that positivity of the $(2n + 1)$-point quadrature rule always holds if the inserted $n + 1$ abscissae interlace with the n original ones and the n Gaussian weights for w satisfy certain inequalities. These have been checked numerically for Jacobi weight functions with parameters α, β and found valid for all $|\alpha| \leq 1/2$, $|\beta| \leq 1/2$.

7.4 Continued fraction approximation: [68, 85]

In [68], attention is drawn to a curious anomaly in the convergence of certain continued fractions: if the continued fraction is interpreted as an infinite series, the terms

of the series initially decrease rapidly in absolute value, causing the partial sums to have essentially (i.e., to many decimal digits) the same value over a long range of the summation index. Eventually, however, the terms begin to increase again and peak at a relatively large value before decreasing again and finally converging to zero. The series thus seems initially to converge to some number, but in fact converges to the correct limit only during the "final descent" of the terms. The phenomenon, termed "apparent convergence to the wrong limit," has been encountered in connection with ratios of Kummer functions and their evaluation by means of a continued fraction of Perron. It is concretely illustrated in the special cases of Bessel function and incomplete gamma function ratios.

The convergence behavior of continued fractions (with real elements) and appropriate stopping rules are studied via infinite series also in [85], where for a realistic assessment of convergence the importance of transient, as opposed to asymptotic, convergence rates is emphasized, and in [71], where two continued fractions, one of Gauss, the other of Perron, are compared for evaluating modified Bessel function ratios.

The convergents of a continued fraction representation of the modified Bessel function of order 1, given in the applied mathematics literature, are shown in [116] to be Gauss–Chebyshev quadrature approximations to an integral representation of the function in question, in fact, approximations from below. Alternative Gauss–Radau quadratures of the same integral yield approximations from above. The same sort of two-sided approximations can be established for modified Bessel functions of any order $\nu > -1/2$.

7.5 Padé approximation: [89]

In [89], three (only looseley connected) aspects are discussed regarding Padé approximants associated with Hamburger series: (a) Necessary and sufficient conditions for normality of the Padé table, classically expressed in terms of moment determinants, are formulated in terms of orthogonal and related polynomials. (b) In the case of a weight function w (defining the moments) supported on a symmetric interval I, different monotonicity properties are derived for the higher-order coefficients (those beyond the moments) in the power series expansion of the Padé approximants, depending on whether $w(t)/w(-t)$ is strictly increasing, constant equal to 1, or strictly decreasing on I. They have found application in the development of error bounds for Gaussian quadrature of analytic functions; cf. Section 5.7. (c) The Padé approximants themselves are computed using stable methods for constructing Gaussian quadrature formulae and orthogonal polynomials (those in Sections 5.2 and 6.1).

7.6 Summation of slowly convergent series: [113, 114]

As observed already in Section 4 of [92], slowly convergent series whose terms are a Laplace transform of some known function f, or the derivative of a Laplace transform, evaluated at integer values, can be summed in the form of a weighted integral of f over $\mathbb{R}_+$, the weight functions involved being Einstein and Fermi functions. The sequence of the respective Gaussian quadrature approximations to these integrals then often converges quite rapidly and thus provides an effective

summation procedure. This is implemented in [113] for series whose general term is a rational function, possibly multiplied by a fractional power. Among the examples given is one that arose in the study of an interesting spiral devised by P.J. Davis (see [10]). Series that occur in plate contact problems are treated similarly in [114], but eventually are reduced to the problem of evaluating a Cauchy transform of a certain measure on [0, 1]; cf. Section 6.1. Another application is made in [149] to the computation of the Hardy–Littlewood function. Brief summaries appear in [167] and [175].

8 Miscellaneous

There are a number of isolated articles on a variety of topics. Some, like [1, 17–23, 26, 31, 64, 82, 140, 151, 157, 158, 162, 185, 186, 193, 194, 196, 197, 199, 201], are of marginal interest, others are more substantial.

In [12], the problem is considered of producing contour plots of analytic functions using Matlab and Maple facilities in combination with the solution of ordinary differential equations. Applications are made to the partial sums of the exponential series. (The same technique has been applied already in [49] to obtain an altitude map for the error of the Gauss–Hermite quadrature approximation to the complex error function.)

Fejér quadrature rules are considered in [40]. They are interpolatory on $[-1, 1]$, having as nodes the zeros of the Chebyshev polynomials of the first and second kind. Since, by a result of Fejér, both are positive, a well-known theorem of Pólya implies that they converge for all functions continuous on $[-1, 1]$. It is shown in [40] that they also converge for functions that have monotone singularities at one or both end points of $[-1, 1]$ and are integrable there. This is of interest in connection with discretization methods for computing Gaussian quadrature rules and orthogonal polynomials (Sections 5.2 and 6.1), where the first Fejér rule is an important vehicle of discretization.

In [73], modified moments of the weight function $t^\alpha \ln(1/t), \alpha > -1$, on $[0, 1]$, using shifted Legendre polynomials, are evaluated explicitly.

While test matrices for the assessment of computer routines for solving linear algebraic systems and eigenvalue problems have been available for some time, the same could not be said for test algebraic equations to assess rootfinding routines. In [77], two families of such test equations are developed, the first having predominantly complex roots, the other exclusively real roots. Both have integer coefficients and involve parameters which can be used to control the condition of the roots from well-conditioned to arbitrarily ill-conditioned ones. The exact roots, of course, must be computable directly, without recourse to a rootfinding algorithm.

In [78], lower bounds are established for the largest zero of an orthogonal polynomial and applied to Jacobi, Gegenbauer, generalized Laguerre, and Hermite polynomials. Other inequalities for the largest zero of Jacobi polynomials, and also for the polynomials themselves, are conjectured in [156].

In [81], the interest centers on the errors, measured in the energy norm, of optimal relaxation methods in dependence on the initial residual vector, particularly the behavior of its high-order components in the coordinate system of principal axes. The analysis rests heavily on the theory of orthogonal polynomials.

The paper [95] solves a statistical problem of interest in principal component analysis, namely to find a single orthogonal matrix which transforms several symmetric positive definite matrices simultaneously to nearly diagonal form as best as possible. The algorithm developed has become known in the statistics literature as the FG-algorithm, a name given it in the paper.

Two papers, [101] and [141], deal with the Hilbert transform of Jacobi resp. generalized Laguerre and Hermite measures, which is expressible explicitly in terms of a hypergeometric function in the first case, and Tricomi's incomplete gamma function resp. Dawson's integral in the others. The numerical evaluation of these expressions, especially the first, is not easy.

In [121], in connection with the three-term recurrence relation for discrete orthogonal polynomials, attention is drawn to a phenomenon of "pseudostability", already encountered in Section 4 of [101]. It helps to explain a type of instability that has been observed in the discretized Stieltjes procedure.

The role played by moments in numerical quadrature problems is discussed in [130]. The paper also contains new conjectures regarding the positivity of certain Newton–Cotes formulae with Jacobi and other weight functions.

The paper [135] is devoted to adaptive quadrature and has been motivated by serious deficiencies in the routines `quad` and `quad8` of earlier Matlab releases. Two new Matlab routines are developed and extensively tested, one an adaptive Simpson rule, the other based on a 4-point Gauss–Lobatto formula and two successive Kronrod extensions. A modified version of the latter has since replaced the old `quad` and `quad8` routines.

A very recent paper, [155], comments on a letter of Euler to Daniel Bernoulli, in which Euler mentions his (failed) attempt to interpolate the common logarithm at the successive powers of 10. (A shorter commentary is to appear in a forthcoming volume in Series IVA of Euler's *Opera omnia*, [202].) The trouble is that the procedure converges too fast, causing the limiting function to be an entire function. Interestingly, though, this entire function is related to a q-extension of the logarithm, where $q = 1/10$, and in the case of the logarithm to base ω, considered by Euler almost 20 years later, $q = 1/\omega$.

There are a number of papers dealing with historical and contemporary figures in mathematics: an assessment of the impact (or lack thereof) of Christoffel's work on quadrature during and after his lifetime [187], tributes to, or commentaries on, the work of Philip Rabinowitz [124], Luigi Gatteschi [125], and Gene H. Golub [145, 200], several appreciations of the life and work of A. Ostrowski [188, 189, 192, 198], an obituary of Y. L. Luke [190], and some reflections and recollections on my own career [195] (on the occasion of my 65th birthday).

The story of my involvement in de Branges's proof of the Bieberbach conjecture is told in [191].

9 Software

Many individual pieces of software have been written, especially in the area of special functions: [33–35, 38, 43, 67]. Among major software packages (in Fortran) are [123] and its quadruple-precision version `ORTHPOLq` on the Web at `http://www.cs.purdue.edu/archives/2001/wxg/codes`. The same Web

Site, with "2001" replaced by "2002", contains the package OPQ of Matlab routines, a companion piece to the book [3].

10 Impact (citations)

According to the *ISI Web of Science*, the ten most frequently cited papers, as of July 2006, are as follows (with the number of citations given in parentheses):

[39] (271); [49] (133); [84] (100); [46] (74); [41] (73); [50] (67); [123] (53); [88] (43); [93] (36); [105] (31)

In closing, let me say that a good part of my "professional activities" consisted of teaching, lecturing, and editorial and translation work, all of which has left some marks: the textbook [2] in the first instance, practically all of the conference proceeding papers in the second, and the edited volumes [14–16], and the translations [180–183], in the third instance. All work that has been enjoyable and rewarding.

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