22

COMMENTARY, BY WALTER GAUTSCHI

This group of five papers, especially the first and third, has a distinctly "interdisciplinary" character in the sense that classical analysis problems are recast in terms of, and successfully solved by, techniques of linear algebra and, vice versa, problems that have a linear algebra flavor are approached and solved using tools of classical analysis. A similar intriguing mix of analysis and algebra permeates the remaining three papers.

Calculation of Gauss quadrature rules, by Golub and Welsch [53]

The concern here is with the calculation of the n-point Gaussian quadrature rule

$$\int_a^b \omega(t)f(t)\mathrm{d}t = \sum_{\nu=1}^{n} w_\nu f(\tau_\nu) + R_n(f)$$

for the nonnegative weight function $\omega(t)$ on $[a,b]$, i.e., the calculation of the nodes τ_ν and weights w_ν. The connection of this problem with orthogonal polynomials is classical, thanks to work of Gauss [35], Jacobi [61], Christoffel [22], Stieltjes [86], and others: The Gaussian nodes τ_ν are the zeros of π_n, the nth-degree polynomial orthogonal with respect to the weight function ω, and the Gauss weights w_ν are also expressible, in different ways, in terms of these orthogonal polynomials.

An alternative characterization of the Gauss nodes τ_ν can be derived from the classical fact that the ortho*normal* polynomials $\{\tilde{\pi}_k\}$ satisfy a three-term recurrence relation

$$\sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t) = (t-\alpha_k)\tilde{\pi}_k(t) - \sqrt{\beta_k}\tilde{\pi}_{k-1}(t), \quad k = 0,1,2,\ldots,$$
$$\tilde{\pi}_{-1} = 0, \quad \tilde{\pi}_0 = \mu_0^{-1/2},$$

with certain real, resp. positive coefficients α_k, β_k which depend on the weight function ω, and $\mu_0 = \int_a^b \omega(t)\mathrm{d}t$. If $\tilde{\boldsymbol{\pi}}(t) = [\tilde{\pi}_0(t), \tilde{\pi}_1(t), \ldots, \tilde{\pi}_{n-1}(t)]^{\mathrm{T}}$, then indeed,

$$t\tilde{\boldsymbol{\pi}}(t) = \boldsymbol{J}\tilde{\boldsymbol{\pi}}(t) + \sqrt{\beta_n}\tilde{\pi}_n(t)\boldsymbol{e}_n, \quad \boldsymbol{e}_n = [0,0,\ldots,1]^{\mathrm{T}},$$

where $\boldsymbol{J} = \boldsymbol{J}_n$ is the Jacobi matrix of order n for the weight function ω, i.e., the symmetric, tridiagonal matrix having the α_k, $k = 0,1,\ldots,n-1$, on the diagonal,

and the $\sqrt{\beta_k}$, $k = 1, \ldots, n-1$, on the two side diagonals. There follows, for $t = \tau_\nu$, since $\tilde{\pi}_n(\tau_\nu) = 0$,

$$\boldsymbol{J}\tilde{\boldsymbol{\pi}}(\tau_\nu) = \tau_\nu \tilde{\boldsymbol{\pi}}(\tau_\nu), \quad \nu = 1, 2, \ldots, n,$$

so that τ_ν are the eigenvalues of $\boldsymbol{J}$ and $\tilde{\boldsymbol{\pi}}(\tau_\nu)$ corresponding eigenvectors. This is the first important mathematical ingredient of the present paper. The other is an expression for the Gaussian weights,

$$w_\nu = \frac{1}{\tilde{\boldsymbol{\pi}}^{\mathrm{T}}(\tau_\nu)\tilde{\boldsymbol{\pi}}(\tau_\nu)}, \quad \nu = 1, 2, \ldots, n, \tag{22.1}$$

for which the authors refer to Wilf (apparently to [93, Section 2.9, eqn (69) or Ch. 2, Exercise 9]). The formula, however, is older; see Szegö [89, eqn (3.4.8)], where it is attributed to Shohat [85]. The authors re-express this formula in terms of the eigenvectors $\boldsymbol{q}_\nu$ normalized by $\boldsymbol{q}_\nu^{\mathrm{T}}\boldsymbol{q}_\nu = 1$, i.e., in terms of

$$\boldsymbol{q}_\nu = \frac{\tilde{\boldsymbol{\pi}}(\tau_\nu)}{[\tilde{\boldsymbol{\pi}}^{\mathrm{T}}(\tau_\nu)\tilde{\boldsymbol{\pi}}(\tau_\nu)]^{1/2}} = \tilde{\boldsymbol{\pi}}(\tau_\nu) w_\nu^{1/2},$$

by noting that the first component of $\tilde{\boldsymbol{\pi}}(\tau_\nu)$ is $\mu_0^{-1/2}$, hence

$$w_\nu = \mu_0 \boldsymbol{q}_{\nu,1}^2, \quad \nu = 1, 2, \ldots, n,$$

where $\boldsymbol{q}_{\nu,1}$ is the first component of $\boldsymbol{q}_\nu$.

There is a detailed discussion in the paper of how Francis's QR algorithm with appropriate shifts can be adapted to compute the eigenvalues of a symmetric, tridiagonal matrix (the matrix $\boldsymbol{J}$) and the first components of the normalized eigenvectors. Related software in Algol is provided in the microfiche supplement of the paper.

Interestingly, the same eigenvalue/vector characterization of Gauss rules, and even the same numerical method (QR algorithm), have been suggested a year earlier in the physics literature by Gordon [54, eqn (26) and p. 660]. This work has had considerable impact in the physical sciences and engineering, whereas the work of Golub and Welsch has had a wider impact in the areas of computational mathematics and information science. Both works have actually been submitted for publication less than a month apart, the former on October 20, the latter on November 13 of 1967. Rarely have two important and overlapping works, like these, popped up simultaneously in two entirely different venues!

Similar ideas have since been developed for other quadrature rules of Gaussian type. Indeed, Golub himself [45] was the first to derive eigenvalue/vector algorithms for Gauss–Radau and Gauss–Lobatto formulae. Laurie [65] did it for his anti-Gaussian formulae, and Calvetti and Reichel [19] for a symmetric modification thereof. Quadrature rules involving derivative terms of arbitrary orders on the boundary or outside the interval of integration require first the generation of the appropriate Jacobi matrix before the (simple) internal nodes can be calculated from its eigenvalues and the corresponding weights from the

associated eigenvectors; see Golub and Kautsky [47, Section 6] and also Ezzirani and Guessab [32]. This has led to important work on the stable calculation of general interpolatory quadratures (Kautsky and Elhay [63], Elhay and Kautsky [31]). A rather substantial extension is the one to Gauss–Kronrod quadratures due to Laurie [66] (see also the commentary to the last paper). For other types of extended quadrature formulae, see Gout and Guessab [55]. Golub-Welsch type algorithms have been developed also for quadrature rules in the complex plane, for example Gauss-Szegö type formulae on the unit circle (Gragg [57, abstract], [56], Watkins [91, pp. 465–466], Jagels and Reichel [62]), Gauss quadrature on the semicircle (Gautschi and Milovanović [43]), Gauss formulae for the Jacobi weight function with complex parameters (Nuttal and Wherry [78]), or those used to approximate the Bromwich integral in the theory of Laplace transform inversion (Luvison [68], Piessens [79]), and complex Gauss formulae for weighted line integrals in the complex plane (Saylor and Smolarski [84, Section 6]).

There are instances in the area of orthogonal polynomials and quadrature where eigenvalues of more general matrices are of interest, for example banded lower Hessenberg matrices in the case of multiple orthogonal polynomials and related quadrature rules (Coussement and Van Assche [24], Borges [11]), or full-blown upper Hessenberg matrices for zeros of Sobolev orthogonal polynomials (Gautschi and Zhang [44, p. 161]) and also for the Gauss–Szegö quadrature rules mentioned above.

Any advances in improving the QR algorithm for computing eigenvalues and eigenvectors of a symmetric tridiagonal matrix give rise immediately to improved Golub-Welsch algorithms. Some possibilities in this regard are discussed by Laurie [67, Section 2]; for positive definite Jacobi matrices, see also Laurie [67, Section 5] and the references therein.

There still remains, of course, the problem of computing the recurrence coefficients α_k, β_k, if not known explicitly, given the weight function ω. This problem is addressed in Section 4 of the paper, where an algorithm of V.I. Mysovskih is described, which computes these coefficients by a Cholesky decomposition of the Hankel matrix in the moments $\mu_r = \int_a^b t^r \omega(t) \mathrm{d}t$ of the weight function. Any method based on moments, however, is notoriously unstable, owing to severe ill-conditioning (for large n) of the underlying moment map. This was first shown in 1968 by the writer [36]; see also [42, Sections 2.1.4, 2.1.6]. Shortly thereafter, Sack and Donovan, in a technical report [82], introduced the idea of "generalized moments" $m_r = \int_a^b p_r(t)\omega(t)\mathrm{d}t$, where p_r is a polynomial of exact degree r, which, at the suggestion of this writer, they renamed "modified moments" in their formal publication [83]. Under the assumption that the polynomials p_r also satisfy a three-term recurrence relation, but with known coefficients, Sack and Donovan developed an algorithm, later given a more definitive form by Wheeler [92], which computes the desired recurrence coefficients α_k, β_k directly from the modified moments. Wheeler suspected that Chebyshev might already have done something of this nature, which was confirmed by the writer and pinpointed to Chebyshev's 1859 memoir [21], where Wheeler's algorithm indeed appears at the

end of Section 3 in the special case of ordinary moments ($p_r(t) = t^r$) and discrete orthogonal polynomials. The algorithm for ordinary, resp. modified moments was therefore named in [37] the Chebyshev, resp. modified Chebyshev algorithm. The latter is not only more efficient than Mysovskih's algorithm, having complexity $O(n^2)$ instead of $O(n^3)$, but is often also more stable. The condition of the underlying modified moment map has been studied in [37, Section 3.3] and [38]; see also [42, Sections 2.1.5, 2.1.6]. For alternative techniques of computing α_k, β_k, based on discretization, see [42, Section 2.2].

Updating and downdating of orthogonal polynomials with data fitting applications, by Elhay, Golub, and Kautsky [30]

The use, in data fitting applications, of (what today are called) discrete orthogonal polynomials can be traced back to a 1859 memoir of Chebyshev [21]. Forsythe [34], a hundred years later and independently, discussed the same procedure and developed it into a viable computer algorithm. The present paper introduces new ideas of updating and downdating in this context, although similar ideas have previously been applied in connection with the related problem of QR factorization of matrices. Mertens [69] reviews downdating algorithms in statistical applications and in the least squares context attributes the concept of downdating to Legendre and Gauss, the originators of least squares theory.

The problem of data fitting is here understood to be the following weighted least squares problem: Given a set $S_N = \{x_j, y_j, w_j^2\}_{j=1}^N$ of N data points $\{x_j, y_j\}$ and positive weights $\{w_j^2\}$, find the polynomial $\hat{q}_n \in \mathbb{P}_n$ of degree $\leq n$ $(< N)$ such that

$$\sum_{j=1}^{N} w_j^2[y_j - \hat{q}_n(x_j)]^2 \leq \sum_{j=1}^{N} w_j^2[y_j - q(x_j)]^2 \quad \text{for all } q \in \mathbb{P}_n.$$

The inner product and norm naturally associated with this problem are

$$[u, v]_N = \sum_{j=1}^{N} w_j^2 u(x_j) v(x_j), \quad \|u\|_N = \sqrt{[u, u]_N},$$

in terms of which the least squares problem is simply $\|y - \hat{q}\|_N^2 \leq \|y - q\|_N^2$, all $q \in \mathbb{P}_n$. The solution is most conveniently expressed in terms of the polynomials $\{\pi_k\}_{k=0}^{N-1}$ orthonormal with respect to the inner product $[\cdot, \cdot]_N$ (the "discrete orthogonal polynomials"), namely as the nth-degree "Fourier polynomial" of y,

$$\hat{q}_n(x) = \sum_{j=0}^{n} c_j \pi_j(x), \quad c_j = [\pi_j, y]_N.$$

With regard to the least squares problem, updating means the following: Determine the solution $\hat{q}_n$ corresponding to the enlarged set $S_{N+1} = S_N \cup \{x_{N+1}, y_{N+1}, w_{N+1}^2\}$ in terms of the solution $\hat{q}_n$ corresponding to the original

set S_N. Downdating, conversely, means the determination of $\hat{q}_n$ for S_N in terms of $\hat{q}_n$ for S_{N+1}.

There is a similar problem of up- and downdating for the orthogonal polynomials, more precisely for their Jacobi matrices $\boldsymbol{J}_n$ (cf. the commentary to the first paper): Knowing $\boldsymbol{J}_n$ for S_N, find $\boldsymbol{J}_n$ for S_{N+1}, and vice versa. An algorithm of Gragg and Harrod [58, Section 3] using a sequence of Givens similarity transformations, attributed essentially to Rutishauser [81], can be thought of as an updating procedure in this sense, since it introduces one data point and weight at a time.

As one would expect from the authors, both problems of up- and downdating are solved (in several different ways) by reformulating them in terms of matrices and then applying appropriate techniques of numerical linear algebra.

An application of the updating procedure for Jacobi matrices is made in [29] to generate Jacobi matrices for sums of weight functions.

Up- and downdating algorithms have subsequently been developed for least squares problems in the complex plane, for general complex nodes, for example, in [12, Section 4], and for nodes on the unit circle in [80, Section 3], [2]. For an updating procedure in connection with orthogonal rational functions, and function vectors, having prescribed poles, see [90, Section 3] and [27, Section 5].

Matrices, moments and quadrature, by Golub and Meurant [48]

One of the central themes here is the estimation of matrix functionals $\varphi(\boldsymbol{A}) = \boldsymbol{u}^{\mathrm{T}} f(\boldsymbol{A})\boldsymbol{v}$, where $\boldsymbol{A}$ is a symmetric (usually positive definite) matrix, f a smooth function for which $f(\boldsymbol{A})$ is meaningful, and $\boldsymbol{u}$, $\boldsymbol{v}$ are column vectors. A prototype example, and one given the most attention in this work, is estimating the (i,j)-entry of the inverse matrix $\boldsymbol{A}^{-1}$, in which case $f(t) = t^{-1}$ and $\boldsymbol{u} = \boldsymbol{e}_i$, $\boldsymbol{v} = \boldsymbol{e}_j$ are coordinate vectors. The problem has been treated previously by physicists in connection with the estimation of resolvents, where $\boldsymbol{A} = z\boldsymbol{I} - \boldsymbol{H}$, z is an energy, and $\boldsymbol{H}$ a Hamiltonian, thus $\boldsymbol{A}^{-1}$ is the resolvent of $\boldsymbol{H}$. Much related work can also be found in the quantum chemistry literature; see, e.g., [51, Introduction] and the examples and references given therein.

There are three basic steps in solving the problem: (i) The functional is written as an integral, $\varphi(\boldsymbol{A}) = \int_a^b f(\lambda)\mathrm{d}\alpha(\lambda)$, where $\mathrm{d}\alpha$ is a discrete measure supported on the spectrum $\sigma(\boldsymbol{A})$ of $\boldsymbol{A}$ and $[a,b]$ an interval containing $\sigma(\boldsymbol{A})$. This is done by a spectral resolution of $\boldsymbol{A}$, and in the important case $\boldsymbol{u} = \boldsymbol{v}$ yields a positive measure $\mathrm{d}\alpha$. (ii) The integral is estimated by quadrature rules, typically Gauss, Gauss–Radau, or Gauss–Lobatto rules. These, with an increasing number of nodes, are capable of providing increasingly sharper upper and lower bounds for the integral, provided the derivatives of f have constant sign on $[a,b]$ (as is the case, for example, when $f(t) = t^{-1}$, $a > 0$) and the measure $\mathrm{d}\alpha$ is positive. Otherwise, they may still yield estimates of increasing quality. (iii) Generating the quadrature rules requires the discrete orthogonal polynomials for $\mathrm{d}\alpha$, in particular the Jacobi matrix $\boldsymbol{J} = \boldsymbol{J}(\mathrm{d}\alpha)$ of the measure $\mathrm{d}\alpha$ (cf. the commentary

to the first paper), which can be obtained by the Lanczos or the conjugate gradient algorithm. An interesting technical detail is the way the quadrature sums are expressed in terms of the $(1,1)$-element of $f(\boldsymbol{J}^0)$, where $\boldsymbol{J}^0$ is closely related (equal, in the case of Gauss formulae) to the Jacobi matrix $\boldsymbol{J}$ or a leading principal minor matrix thereof.

It is possible to generalize these ideas to the "block" case, where $\boldsymbol{u}$ and $\boldsymbol{v}$ are replaced by an $n \times m$ matrix $\boldsymbol{W}$ (typically with $m = 2$), in which case $d\alpha$ becomes a matrix-valued measure and one has to deal with matrix-valued orthogonal polynomials and quadrature rules, as is done in Sections 3.3 and 4.3 of the present work.

When $f(t) = t^s$ is any power, not necessarily $s = -1$, and $\boldsymbol{u} = \boldsymbol{v}$, the procedure has previously been described by Golub in [46], and in the case $s = -2$, of interest in ℓ_2 error bounds for systems of linear equations, even before by Dahlquist *et al.* in [25] and also in [26, Section 3]. In the latter work, improved approximations are obtained by the conjugate gradient method and the respective errors estimated as described. In a sequel [49] to the present work, and already in [51, Section 4], the case $s = -1$ is further applied to obtain error bounds and stopping criteria in iterative methods for solving linear systems, notably the conjugate gradient method; see also [70], [33], and for the preconditioned conjugate gradient method, [71], [9]. Applications to constructing preconditioners can be found in [10]. Similar ideas have been pursued by M. Arioli and coworkers in a variety of application areas involving partial differential equations and their discretizations ([4], [8] , [6], [7], [3], [5]). A valuable exposition of error estimates in the conjugate gradient method is [88], where some of the recent results are traced back to the original work of Hestenes and Stiefel [59], and the influence of rounding errors is given serious attention. For the latter, see also [51, Section 5], [87, Section 4], and [94]. For a recent comprehensive review of these and related matters, see [72], especially Sections 3.3 and 5.3.

Altogether different applications of the work of Golub and Meurant are to highly ill-conditioned linear algebraic systems, specifically to the determination of the Tikhonov regularization parameter [14], [15], [20], or to the determination of upper and lower bounds for the Lagrange multipliers in constrained least squares and quadratic problems [52]. The blur identification problem in image processing [76, Section 6] contains yet another application.

The work of Golub and Meurant has inspired other researchers to develop variants of their techniques for estimating matrix functionals. We mention, for example, Calvetti *et al.* [17], [18], where next to Gauss and Gauss–Radau quadratures also anti-Gauss formulae are used (see the commentary to the first paper) and Calvetti *et al.* [16], where functionals $\boldsymbol{u}^{\mathrm{T}}[f(\boldsymbol{A})]^{\mathrm{T}} g(\boldsymbol{A})\boldsymbol{u}$ are estimated for matrices $\boldsymbol{A}$ that are no longer necessarily symmetric, and the quadrature and antiquadrature rules are therefore based on the Arnoldi rather than the Lanczos process.

A stable numerical method for inverting shape from moments, by Golub, Milanfar, and Varah [50]

The basic problem here is the determination of an n-sided polygon P in the complex plane, having vertices z_j, $j = 1, 2, \ldots, n$, given its first $2n-2$ "harmonic" moments $c_k = \int\int_P z^k \mathrm{d}x\mathrm{d}y$, $k = 0, 1, \ldots, 2n-3$. If the associated "complex" moments are defined by $\tau_0 = \tau_1 = 0$, $\tau_k = k(k-1)c_{k-2}$, $k = 2, 3, \ldots, 2n-1$, the vertex reconstruction amounts to solving the system of $2n$ nonlinear equations

$$\sum_{j=1}^{n} a_j z_j^k = \tau_k, \quad k = 0, 1, \ldots, 2n-1.$$

These are formally identical with the equations for a Gaussian quadrature formula (with nodes z_j, weights a_j, and moments τ_k of the underlying weight function), except that all these quantities are now complex and, moreover, the first two moments vanish. While the classical Prony's method is still applicable (it determines the coefficients of the monic polynomial of degree n having the z_j as its zeros), it is notoriously unstable. The object of this work is to develop a solution procedure which, though not necessarily perfectly stable, is more stable than Prony's method.

This is done essentially by reformulating the problem, implicit already in [89, eqn (2.2.9)], as a generalized eigenvalue problem involving two Hankel matrices in the moments, or better, in transformed moments obtained by appropriate scaling and shifting.

In practice, the number n of vertices is usually not known a priori and must be estimated from the given sequence of moments, which, to complicate matters, may be corrupted by noise.

There are a number of potential application areas for procedures as here described, one, discussed previously, to tomographic reconstruction, and another, described in the present work, to the problem of geophysical inversion from gravimetric measurements.

The theoretical results of sensitivity analysis are nicely corroborated by numerical examples. There remain, however, a number of issues for further study, for example, a sound statistical analysis of procedures for estimating the number of vertices, especially in the presence of noise, and the incorporation of a priori geometrical constraints. Some of these issues have been taken up in the more recent work [28].

Computation of Gauss–Kronrod quadrature rules, by Calvetti, Golub, Gragg, and Reichel [13]

In order to economically estimate the error $R_n(f)$ of the n-point Gauss quadrature rule (cf. the commentary to the first paper), Kronrod [64] in 1964 constructed (for the weight function $\omega = 1$ on $[-1, 1]$) an extended Gauss formula

$$\int_a^b \omega(t)f(t)\mathrm{d}t = \sum_{\nu=1}^{n} \lambda_\nu^K f(\tau_\nu) + \sum_{\mu=1}^{n+1} \lambda_\mu^{*K} f(\tau_\mu^K) + R_n^K(f),$$

now called the Gauss–Kronrod quadrature formula, by adjoining to the n Gauss nodes τ_ν additional $n+1$ nodes τ_μ^K – the Kronrod nodes – and selecting them, and all weights λ_ν^K, λ_μ^{*K}, such as to achieve maximum degree of exactness $3n+1$ (at least). The same idea, in a germinal form, can be traced back to the late 19th century (cf. [40]). It turns out that the Kronrod nodes must be the zeros of the polynomial π_{n+1}^K of degree $n+1$ orthogonal to all lower-degree polynomials with respect to the (sign-changing) weight function $\omega(t)\pi_n(t;\omega)$ on (a,b), where π_n is the orthogonal polynomial of degree n relative to the weight function ω. While the polynomial π_{n+1}^K (considered for $\omega = 1$ already by Stieltjes in 1894 without reference to quadrature) always exists uniquely, its zeros may or may not all be real and contained in $[a,b]$. An extensive literature thus evolved dealing precisely with this question of reality, and also with the question of positivity of all weights λ_ν^K, λ_μ^{*K}. (For surveys on this and other aspects of Gauss–Kronrod formulae, see Monegato [74], [75], Gautschi [39], and Notaris [77].) In comparison, the question of actually computing the Gauss–Kronrod formula, when it exists, i.e., computing its nodes and weights, has received less attention; see, however, the recent survey by Monegato [73].

Among the most remarkable computational advances in this area is the algorithm of Laurie [66] for computing positive Gauss–Kronrod formulae. Laurie recognizes the equivalence of this problem with an inverse eigenvalue problem for a symmetric tridiagonal matrix with prescribed entries on the side diagonal; see also [23, pp. 15–16]. His algorithm much resembles the Golub-Welsch algorithm (cf. the commentary to the first paper) for ordinary Gauss formulae. In the present work by Calvetti *et al.*, this algorithm is modified and simplified in the sense that the Gauss nodes τ_ν need not be recomputed (as they are in Laurie's algorithm) in cases where they are already known. Indeed, not even the full tridiagonal Jacobi–Kronrod matrix of order $2n+1$ needs to be generated. The resulting new algorithm is then used by the authors to compute also Kronrod extensions of Gauss–Radau and Gauss–Lobatto formulae.

Modifications required to deal with nonpositive Gauss–Kronrod rules are developed in [1].

The work is too recent to have had a major impact, but it can be expected to find many applications, most likely in the area of adaptive quadrature. One such application (to the motion of droplets) is already briefly mentioned in [60, p. 63].

Summary

Golub's work described here is characterized, on the one hand, by the imaginative use of linear algebra techniques in problems originating elsewhere, and on the other hand, by bringing tools outside of linear algebra to bear on problems

involving matrices. Both these features of Golub's work are elaborated in greater detail in the recent essay [41].

Acknowledgment. The writer is grateful for comments by D.P. Laurie, L. Reichel, and Z. Strakoš on an earlier draft of these commentaries.

REFERENCES

1. G. S. Ammar, D. Calvetti, and L. Reichel, Computation of Gauss–Kronrod quadrature rules with non-positive weights. *Electron. Trans. Numer. Anal.*, **9**, 26–38 (1999).
2. G. S. Ammar, W. B. Gragg, and L. Reichel, Downdating of Szegö polynomials and data-fitting applications. *Linear Algebra Appl.*, **172**, 315–336 (1992).
3. M. Arioli, A stopping criterion for the conjugate gradient algorithm in a finite element method framework. *Numer. Math.*, **97**(1), 1–24 (2004).
4. Mario Arioli and Lucia Baldini, A backward error analysis of a null space algorithm in sparse quadratic programming. *SIAM J. Matrix Anal. Appl.*, **23**(2), 425–442 (2001).
5. M. Arioli, D. Loghin, and A. J. Wathen, Stopping criteria for iterations in finite element methods. *Numer. Math.*, **99**(3), 381–410 (2005).
6. Mario Arioli and Gianmarco Manzini, A null space algorithm for mixed finite-element approximations of Darcy's equation. *Comm. Numer. Meth. Engrg.*, **18**(9), 645–657 (2002).
7. Mario Arioli and Gianmarco Manzini, Null space algorithm and spanning trees in solving Darcy's equation. *BIT Numer. Math.*, **43**(Suppl.), 839–848 (2003).
8. M. Arioli, E. Nonlard, and A. Russo, Stopping criteria for iterative methods: applications to PDE's. *Calcolo*, **38**(2), 97–112 (2001).
9. Owe Axelsson and Igor Kaporin, Error norm estimation and stopping criteria in preconditioned conjugate gradient iterations. *Numer. Linear Algebra Appl.*, **8**(4), 265–286 (2001).
10. Michele Benzi and Gene H. Golub, Bounds for the entries of matrix functions with applications to preconditionings. *BIT*, **39**(3), 417–438 (1999).
11. Carlos F. Borges, On a class of Gauss-like quadrature rules. *Numer. Math.*, **67**(3), 271–288 (1994).
12. Adhemar Bultheel and Marc Van Barel, Vector orthogonal polynomials and least squares approximation. *SIAM J. Matrix Anal. Appl.*, **16**(3), 863–885 (1995).
13*. D. Calvetti, G. H. Golub, W. B. Gragg, and L. Reichel, Computation of Gauss–Kronrod quadrature rules. *Math. Comp.*, **69**(231), 1035–1052 (2000).
14. D. Calvetti, G. H. Golub, and L. Reichel, Estimation of the L-curve via Lanczos bidiagonalization. *BIT*, **39**(4), 603–619 (1999).
15. D. Calvetti, P. C. Hansen, and L. Reichel, L-curve curvature bounds via Lanczos bidiagonalization. *Electron. Trans. Numer. Anal.*, **14**, 20–35 (2002).
16. Daniela Calvetti, Sun-Mi Kim, and Lothar Reichel, Quadrature rules based on the Arnoldi process. *SIAM J. Matrix Anal. Appl.*, **26**(3), 765–781 (2005).
17. D. Calvetti, S. Morigi, L. Reichel, and F. Sgallari, Computable error bounds and estimates for the conjugate gradient method. *Numer. Algorithms*, **25**(1–4), 75–88 (2000).
18. D. Calvetti, S. Morigi, L. Reichel, and F. Sgallari, An iteration method with error estimators. *J. Comput. Appl. Math.*, **127**(1–2), 93–119 (2001).
19. Daniela Calvetti and Lothar Reichel, Symmetric Gauss–Lobatto and modified anti-Gauss rules. *BIT*, **43**(3), 541–554 (2003).

20. Daniela Calvetti and Lothar Reichel, Tikhonov regularization of large linear problems. *BIT*, **43**(2), 263–283 (2003).
21. P. L. Chebyshev, Sur l'interpolation par la méthode des moindres carrés. *Mém. Acad. Impér. Sci. St. Petersbourg*, (7) **1**(15), 1–24 (1859). [Also in *Œuvres* I, pp. 473–498.]
22. E. B. Christoffel, Sur une classe particulière de fonctions entières et de fractions continues. *Ann. Mat. Pura Appl.*, (2) **8**, 1–10 (1877). [Also in *Ges. Math. Abhandlungen* I, 65–87.]
23. Moody T. Chu and Gene H. Golub, Structured inverse eigenvalue problems, in *Acta Numerica 2002*, Vol. 11, pp. 1–71, Cambridge University Press, Cambridge (2002).
24. Jonathan Coussement and Walter Van Assche, Gaussian quadrature for multiple orthogonal polynomials. *J. Comput. Appl. Math.*, **178**(1–2), 131–145 (2005).
25. Germund Dahlquist, Stanley C. Eisenstat, and Gene H. Golub, Bounds for the error of linear systems of equations using the theory of moments. *J. Math. Anal. Appl.*, **37**(4), 151–166 (1972).
26. Germund Dahlquist, Gene H. Golub, and Stephen G. Nash, Bounds for the error in linear systems, *Lecture Notes in Control and Information Sci.* 15, pp. 154–172, Springer, Berlin (1979).
27. Steven Delvaux and Marc Van Barel, Orthonormal rational function vectors. *Numer. Math.*, **100**(3), 409–440 (2005).
28. Michael Elad, Peyman Milanfar, and Gene H. Golub, Shape from moments—an estimation theory perspective. *IEEE Trans. Signal Process.*, **52**(7), 1814–1829 (2004).
29. Sylvan Elhay, Gene H. Golub, and Jaroslav Kautsky, Jacobi matrices for sums of weight functions. *BIT*, **32**(1), 143–166 (1992).
30. Sylvan Elhay, Gene H. Golub, and Jaroslav Kautsky, Updating and downdating of orthogonal polynomials with data fitting applications. *SIAM J. Matrix Anal. Appl.*, **12**(2), 327–353 (1991).
31. Sylvan Elhay and Jaroslav Kautsky, Algorithm 655—IQPACK: FORTRAN subroutines for the weights of interpolatory quadratures. *ACM Trans. Math. Software*, **13**(4), 399–415 (1987).
32. Abdelkrim Ezzirani and Allal Guessab, A fast algorithm for Gaussian type quadrature formulae with mixed boundary conditions and some lumped mass spectral approximations. *Math. Comp.*, **68**(225), 217–248 (1999).
33. Bernd Fischer and Gene H. Golub, On the error computation for polynomial based iteration methods, in *Recent advances in iterative methods*, IMA Vol. Math. Appl. 60, Springer, New York, pp. 59–67 (1994).
34. G. E. Forsythe, Generation and use of orthogonal polynomials for data-fitting with a digital computer. *J. Soc. Indust. Appl. Math.*, **5**(2), 74–88 (1957).
35. C. F. Gauss, Methodus nova integralium valores per approximationem inveniendi. *Commentationes Societatis Regiae Scientarium Gottingensis Recentiores*, **3** (1814). [Also in *Werke* III, 163–196.]
36. Walter Gautschi, Construction of Gauss–Christoffel quadrature formulas. *Math. Comp.*, **22**(102), 251–270 (1968).
37. Walter Gautschi, On generating orthogonal polynomials. *SIAM J. Sci. Statist. Comput.*, **3**(3), 289–317 (1982).

38. Walter Gautschi, On the sensitivity of orthogonal polynomials to perturbations in the moments. *Numer. Math.*, **48**(4), 369–382 (1986).
39. Walter Gautschi, Gauss-Kronrod quadrature—a survey, In *Numerical Methods and Approximation Theory III*, G. V. Milovanović (ed.), University of Niš, Niš, pp. 39–66 (1988).
40. Walter Gautschi, A historical note on Gauss–Kronrod quadrature. *Numer. Math.*, **100**(3), 483–484 (2005).
41. Walter Gautschi, The interplay between classical analysis and (numerical) linear algebra — a tribute to Gene H. Golub. *Electron. Trans. Numer. Anal.*, **13**, 119–147 (2002).
42. Walter Gautschi, *Orthogonal polynomials: computation and approximation*, Numerical Mathematics and Scientific Computation, Oxford University Press, Oxford (2004).
43. Walter Gautschi and Gradimir V. Milovanović, Polynomials orthogonal on the semicircle. *J. Approx. Theory*, **46**(3), 230–250 (1986).
44. Walter Gautschi and Minda Zhang, Computing orthogonal polynomials in Sobolev spaces. *Numer. Math.*, **71**(2), 159–183 (1995).
45*. Gene H. Golub, Some modified matrix eigenvalue problems. *SIAM Rev.*, **15**(2), 318–334 (1973).
46. Gene H. Golub, Bounds for matrix moments. *Rocky Mountain J. Math.*, **4**(2), 207–211 (1974).
47. G. H. Golub, and J. Kautsky, Calculation of Gauss quadratures with multiple free and mixed knots. *Numer. Math.*, **41**(2), 147–163 (1983).
48*. Gene H. Golub and Gérard Meurant, Matrices, moments and quadrature, in *Numerical Analysis 1993 (Dundee, 1993)*, Pitman Res. Notes Math. Ser. 303, Longman Sci. Tech., Harlow, pp. 105–156 (1994).
49. G. H. Golub and G. Meurant, Matrices, moments and quadrature II; how to compute the norm of the error in iterative methods. *BIT*, **37**(3), 687–705 (1997).
50. Gene H. Golub, Peyman Milanfar, and James Varah, A stable numerical method for inverting shape from moments. *SIAM J. Sci. Comput.*, **21**(4), 1222–1243 (1999/00) (electronic).
51. Gene H. Golub and Zdeněk Strakoš, Estimates in quadratic formulas. *Numer. Algorithms*, **8**, 241–268 (1994).
52. Gene H. Golub and Urs von Matt, Quadratically constrained least squares and quadratic problems. *Numer. Math.*, **59**(6), 561–580 (1991).
53*. Gene H. Golub and John J. Welsch, Calculation of Gauss quadrature rules. *Math. Comp.*, **23**(106), 221–230 (1969). Microfiche suppl. A1–A10.
54. Roy G. Gordon, Error bounds in equilibrium statistical mechanics. *J. Math. Phys.*, **9**(5), 655–663 (1968).
55. C. Gout and A. Guessab, Extended Lagrange interpolation and nonclassical Gauss quadrature formulae. *Math. Comput. Modelling*, **38**(1–2), 209–228 (2003).
56. William B. Gragg, Positive definite Toeplitz matrices, the Arnoldi process for isometric operators, and Gaussian quadrature on the unit circle. *J. Comput. Appl. Math.*, **46**(1–2), 183–198 (1993).
57. William B. Gragg, The QR algorithm for unitary Hessenberg matrices. *J. Comput. Appl. Math.*, **16**(1), 1–8 (1986).

58. William B. Gragg and William J. Harrod, The numerically stable reconstruction of Jacobi matrices from spectral data. *Numer. Math.*, **44**(3), 317–335 (1984).
59. M. R. Hestenes and E. Stiefel, Methods of conjugate gradients for solving linear syatems. *J. Research Nat. Bur. Standards*, **49**, 409–436 (1952).
60. W. Holländer and S. K. Zaripov, Hydrodynamically interacting droplets at small Reynolds numbers. *Internat. J. Multiphase Flow*, **31**(1), 53–68 (2005).
61. C. G. J. Jacobi, Ueber Gauß neue Methode, die Werthe der Integrale näherungsweise zu finden. *J. Reine Angew. Math.*, **1**, 301–308 (1826).
62. Carl Jagels and Lothar Reichel, Szegö-Lobatto quadrature rules. *Electr. Trans. Numer. Anal.*, (to appear).
63. J. Kautsky and S. Elhay, Calculation of the weights of interpolatory quadratures. *Numer. Math.*, **40**(3), 407–422 (1982).
64. A. S. Kronrod, *Nodes and weights of quadrature formulas. Sixteen-place tables* (Russian), Izdat. Nauka, Moscow (1964). [Authorized translation by Consultants Bureau, New York, 1965.]
65. Dirk P. Laurie, Anti-Gaussian quadrature formulas. *Math. Comp.*, **65**(214), 739–747 (1996).
66. Dirk P. Laurie, Calculation of Gauss–Kronrod quadrature rules. *Math. Comp.*, **66**(219), 1133–1145 (1997).
67. Dirk P. Laurie, Computation of Gauss-type quadrature formulas. *J. Comput. Appl. Math.*, **127**(1–2), 201–217 (2001).
68. Angelo Luvison, On the construction of Gaussian quadrature rules for inverting the Laplace transform. *Proc. IEEE*, **62**, 637–638 (1974).
69. B. J. A. Mertens, Downdating: interdisciplinary research between statistics and computing. *Statistica Neerlandica*, **55**(3), 358–366 (2001).
70. Gérard Meurant, The computation of bounds for the norm of the error in the conjugate gradient algorithm. *Numer. Algorithms*, **16**(1), 77–87 (1997).
71. Gérard Meurant, Numerical experiments in computing bounds for the norm of the error in the preconditioned conjugate gradient algorithm. *Numer. Algorithms*, **23**(3–4), 353–365 (1999).
72. Gérard Meurant and Zdeněk Strakoš, The Lanczos and conjugate gradient algorithms in finite precision arithmetic, in *Acta Numerica 2006*, Vol. 15, (pp. 471–542) Cambridge University Press, Cambridge (2006).
73. Giovanni Monegato, An overview of the computational aspects of Kronrod quadrature rules. *Numer. Algorithms*, **26**(2), 173–196 (2001).
74. Giovanni Monegato, An overview of results and questions related to Kronrod schemes. In *Numerische Integration*, G. Hämmerlin (ed.), Internat. Ser. Numer. Math. 45, Birkhäuser, Basel, pp. 231–240 (1979).
75. Giovanni Monegato, Stieltjes polynomials and related quadrature rules. *SIAM Rev.*, **24**(2), 137–158 (1982).
76. Nhat Nguyen, Peyman Milanfar, and Gene Golub, Efficient generalized cross-validation with applications to parametric image restoration and resolution enhancement. *IEEE Trans. Image Process.*, **10**(9), 1299–1308 (2001).
77. Sotirios E. Notaris, An overview of results on the existence or nonexistence and the error term of Gauss–Kronrod quadrature formulae, in *Approximation and Computation*, R.V.M. Zahar (ed.), Internat. Ser. Numer. Math. 119, Birkhäuser, Boston, pp. 485–496 (1994).

78. J. Nuttall and C. J. Wherry, Gaussian integration for complex weight functions. *J. Inst. Math. Appl.*, **21**(2), 165–170 (1978).
79. Robert Piessens, Comments on: "On the construction of Gaussian quadrature rules for inverting the Laplace transform" by A. Luvison. *Proc. IEEE*, **63**, 817–818 (1975).
80. L. Reichel, G. S. Ammar, and W. B. Gragg, Discrete least squares approximation by trigonometric polynomials. *Math. Comp.*, **57**(195), 273–289 (1991).
81. H. Rutishauser , On Jacobi rotation patterns. In *Experimental Arithmetic, High Speed Computing and Mathematics*, Proc. Sympos. Appl. Math. 15, Amer. Math. Soc., Providence, RI, pp. 219–239 (1963).
82. R. A. Sack and A. F. Donovan, An algorithm for Gaussian quadrature given generalized moments, Technical report, Dept. Math., University of Salford, Salford, UK (1969).
83. R. A. Sack and A. F. Donovan, An algorithm for Gaussian quadrature given modified moments. *Numer. Math.*, **18**(5), 465–478 (1972).
84. Paul E. Saylor and Dennis C. Smolarski, Why Gaussian quadrature in the complex plane?. *Numer. Algorithms*, **26**(3), 251–280 (2001).
85. J. A. Shohat, On a certain formula of mechanical quadratures with non-equidistant ordinates. *Trans. Amer. Math. Soc.*, **31**, 448–463 (1929).
86. T. J. Stieltjes, Quelques recherches sur la théorie des quadratures dites mécaniques. *Ann. Sci. Éc. Norm. Paris*, (3) **1**, 409–426 (1884). [Also in *Œuvres* I, 377–396.]
87. Z. Strakoš and J. Liesen, On numerical stability in large scale linear algebraic computations. *Z. Angew. Math. Mech.*, **85**(5), 307–325 (2005).
88. Zdeněk Strakoš and Petr Tichý, On error estimation in the conjugate gradient method and why it works in finite precision computations. *Electron. Trans. Numer. Anal.*, **13**, 56–80 (2002).
89. Gabor Szegö, *Orthogonal polynomials*, AMS Colloquium Publications 23, Amer. Math. Soc., New York (1939).
90. Marc Van Barel, Dario Fasino, Luca Gemignani, and Nicola Mastronardi, Orthogonal rational functions and structured matrices. *SIAM J. Matrix Anal. Appl.*, **26**(3), 810–829 (2005).
91. David S. Watkins, Some perspectives on the eigenvalue problem. *SIAM Rev.*, **35**(3), 430–471 (1993).
92. John C. Wheeler, Modified moments and Gaussian quadratures. *Rocky Mountain J. Math.*, **4**(2), 287–296 (1974).
93. Herbert S. Wilf, *Mathematics for the physical sciences*, Wiley, New York (1962).
94. Wolfgang Wülling, The stabilization of weights in the Lanczos and conjugate gradient method, *BIT Numer. Math.*, **45**(2), 395–414 (2005).

An asterisk denotes a paper reprinted in this volume.