Algorithm xxx — ORTHPOL: A package of routines for generating orthogonal polynomials and Gauss-type quadrature rules*

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ABSTRACT. A collection of subroutines and examples of their uses, as well as the underlying numerical methods, are described for generating orthogonal polynomials relative to arbitrary weight functions. The object of these routines is to produce the coefficients in the three-term recurrence relation satisfied by the orthogonal polynomials. Once these are known, additional data can be generated, such as zeros of orthogonal polynomials and Gauss-type quadrature rules, for which routines are also provided.

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1. INTRODUCTION

Classical orthogonal polynomials, such as those of Legendre, Chebyshev, Laguerre and Hermite, have been used for purposes of approximation in widely different disciplines and over a long period of time. Their popularity is due in part to the ease with which they can be employed, and in part to the wealth of analytic results known for them. Widespread use of non-classical orthogonal polynomials, in contrast, has been impeded by a lack of effective and generally applicable constructive methods. The present set of computer routines has been developed over the past ten years in the hope of remedying this impediment and of encouraging the use of nonstandard orthogonal polynomials. A number of applications indeed have already been made, for example to numerical quadrature (Cauchy principal value integrals with coth-kernel [38], Hilbert transform of Jacobi weight functions [37], integration over half-infinite intervals [28], rational Gauss-type quadrature [30, *Work supported, in part, by National Research Foundation grants, most recently by grant DMS-9023403.

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to moment-preserving spline approximation [21,35,11], to the summation of slowly convergent series [26,27], and, perhaps most notably, to the proof of the Bieberbach conjecture [24].

In most applications, orthogonality is with respect to a positive weight function, \( w \), on a given interval or union of intervals, or with respect to positive weights, \( w_i \), concentrated on a discrete set of points, \( \{x_i\} \), or a combination of both. For convenience of notation, we subsume all these cases under the notion of a positive measure, \( d\lambda \), on the real line \( \mathbb{R} \). That is, the respective inner product is written as a Riemann-Stieltjes integral,

\[
(u, v) = \int_{\mathbb{R}} u(t)v(t)d\lambda(t),
\]

where the function \( \lambda(t) \) is the indefinite integral of \( w \) for the continuous part, and a step function with jumps \( w_i \) at \( x_i \) for the discrete part. We assume that (1.1) is meaningful whenever \( u, v \) are polynomials. There is then defined a unique set of (monic) orthogonal polynomials,

\[
\pi_k(t) = t^k + \text{lower-degree terms}, \quad k = 0, 1, 2, \ldots,
\]

(1.2)

\[
(\pi_k, \pi_\ell) = 0 \quad \text{if} \quad k \neq \ell.
\]

We speak of “continuous” orthogonal polynomials if the support of \( d\lambda \) is an interval, or a union of intervals, of “discrete” orthogonal polynomials if the support of \( d\lambda \) consists of a discrete set of points, and of orthogonal polynomials of “mixed type” if the support of \( d\lambda \) has both a continuous and discrete part. In the first and last case, there are infinitely many orthogonal polynomials — one for each degree —, whereas in the second case there are exactly \( N \) orthogonal polynomials, \( \pi_0, \pi_1, \ldots, \pi_{N-1} \), where \( N \) is the number of support points. In all cases, we denote the polynomials by \( \pi_k(\cdot) = \pi_k(\cdot; d\lambda) \), or \( \pi_k(\cdot; w) \), if we want to indicate their dependence on the measure \( d\lambda \) or weight function \( w \), and use similar notations for other quantities depending on \( d\lambda \) or \( w \).

It is a distinctive feature of orthogonal polynomials, compared to other orthogonal systems, that they satisfy a three-term recurrence relation,

\[
\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \quad k = 0, 1, 2, \ldots,
\]

(1.3)

\[
\pi_0(t) = 1, \quad \pi_{-1}(t) = 0.
\]
with coefficients $\alpha_k = \alpha_k(d\lambda) \in \mathbb{R}$, $\beta_k = \beta_k(d\lambda) > 0$ that are uniquely determined by the measure $d\lambda$. By convention, the coefficient $\beta_0$, which multiplies $\pi_{-1} = 0$ in (1.3), is defined by

$$\beta_0 = \beta_0(d\lambda) = \int_{\mathbb{R}} d\lambda(t).$$

(1.4)

The knowledge of these coefficients is absolutely indispensable for any sound computational use and application of orthogonal polynomials [19,25]. One of the principal objectives of the present package is precisely to provide routines for generating these coefficients. Routines for related quantities are also provided, such as Gauss-type quadrature weights and nodes, hence also zeros of orthogonal polynomials.

Occasionally (e.g., in [21,35,11,30,31]), one needs to deal with indefinite (i.e., sign-changing) measures $d\lambda$. The positivity of the $\beta_k$ is then no longer guaranteed, indeed not even the existence of all orthogonal polynomials. Nevertheless, our methods can still be formally applied, albeit at the risk of possible breakdowns or instabilities.

There are basically four methods used here to generate recursion coefficients: (i) *Methods based on explicit formulae*. These relate to classical orthogonal polynomials, and are implemented in the routine `recur` of §2. (ii) *Methods based on moment information*. These are dealt with in §3, and are represented by a single routine, `cheb`. Its origin can be traced back to work of Chebyshev on discrete least squares approximation. (iii) *Bootstrap methods based on inner product formulae for the coefficients, and orthogonal reduction methods*. We have attributed the idea for the former method to Stieltjes and referred to it in [19] as the Stieltjes procedure. The prototype is the routine `sti` in §4, applicable for discrete orthogonal polynomials. An alternative routine is `lancz`, which accomplishes the same purpose, but uses the method of Lanczos. Either of these routines can be used in `mcdis`, which applies to continuous as well as mixed-type orthogonal polynomials. In contrast to all previous routines, `mcdis` uses a discretization process, and thus furnishes only approximate answers whose accuracies can be controlled by the user. The routine, however, is by far the most sophisticated and flexible routine in this package, one that requires, or can greatly benefit from, ingenuity of the user. The same kind of discretization is also applicable to moment-related methods, yielding the routine `mccheb`. (iv) *Modification algorithms*. These are routines generating recursion coefficients for measures modified by a rational factor, utilizing the recursion coefficients of the original measure, which are assumed to be known. They can be thought of as
algorithmic implementations of the Christoffel, or generalized Christoffel, theorem and are incorporated in the routines chri and gchri of §5. An important application of all these routines is made in §6, where routines are provided that generate the weights and nodes of quadrature rules of Gauss, Gauss-Radau, and Gauss-Lobatto type.

Each routine has a single-precision and double-precision version with similar names, except for the prefix “d” in double-precision procedures. The latter are generally a straightforward translation of the former. An exception is the routine dlga used in drecur for computing the logarithm of the gamma function, which employs a different method than the single-precision companion routine alga.

All routines of the package have been checked for ANSI conformance, and have been tested on two computers: the Cyber 205 and a Sun 4/670 MP workstation. The former has machine precisions $\epsilon^s \approx 7.11 \times 10^{-15}$, $\epsilon^d \approx 5.05 \times 10^{-29}$ in single and double precision, respectively, while the latter has $\epsilon^s \approx 5.96 \times 10^{-8}$, $\epsilon^d \approx 1.11 \times 10^{-16}$. The Cyber 205 has a large floating-point exponent range, extending from approximately $-8617$ to $+8645$ in single as well as double precision, whereas the Sun 4/670 has the rather limited exponent range $[-38, 38]$ in single precision, but a larger range, $[-308, 308]$, in double precision. All output cited relates to work on the Cyber 205.

The package is organized as follows: Section 0 contains (slightly amended) netlib routines, namely r1mach and d1mach, providing basic machine constants for a variety of computers. Section 1 contains all the driver routines — named test1, test2, etc. — which are used (and described in the body of this paper) to test the subroutines of the package. The complete output of each test is listed immediately after the driver. Sections 2–6 constitute the core of the package: the single- and double-precision subroutines described in the equally-numbered sections of this paper. All single-precision routines are provided with comments and instructions for their use. These, of course, apply to the double-precision routines as well.

2. CLASSICAL WEIGHT FUNCTIONS

Among the most frequently used orthogonal polynomials are the Jacobi polynomials, generalized Laguerre polynomials, and Hermite polynomials, supported respectively on a finite interval, half-infinite interval, and the
whole real line. The respective weight functions are
\[ w(t) = w^{(\alpha, \beta)}(t) = (1 - t)^\alpha (1 + t)^\beta \text{ on } (-1, 1), \quad \alpha > -1, \quad \beta > -1: \quad \text{Jacobi}, \]
\[ w(t) = w^{(\alpha)}(t) = t^\alpha e^{-t} \text{ on } (0, \infty), \quad \alpha > -1: \quad \text{generalized Laguerre}, \]
\[ w(t) = e^{-t^2} \text{ on } (-\infty, \infty): \quad \text{Hermite}. \]

Special cases of the Jacobi polynomials are the Legendre polynomials \((\alpha = \beta = 0)\), the Chebyshev polynomials of the first \((\alpha = \beta = -\frac{1}{2})\), second \((\alpha = \beta = \frac{1}{2})\), third \((\alpha = -\beta = -\frac{1}{2})\) and fourth \((\alpha = -\beta = \frac{1}{2})\) kind, and the Gegenbauer polynomials \((\alpha = \beta = \lambda - \frac{1}{2})\). The Laguerre polynomials are the special case \(\alpha = 0\) of the generalized Laguerre polynomials.

For each of these polynomials, the corresponding recursion coefficients \(\alpha_k = \alpha_k(w), \beta_k = \beta_k(w)\) are explicitly known (see, e.g., [5, pp. 217–221]), and are generated in single precision by the routine **recur**. Its calling sequence is

\[ \text{recur}(n, \text{ipoly}, \text{al}, \text{be}, a, b, ierr). \]

On entry,

- **n** is the number of recursion coefficients desired;
  type integer

- **ipoly** is an integer identifying the polynomial as follows:
  1 = Legendre polynomial on \((-1,1)\)
  2 = Legendre polynomial on \((0,1)\)
  3 = Chebyshev polynomial of the first kind
  4 = Chebyshev polynomial of the second kind
  5 = Chebyshev polynomial of the third kind
  6 = Jacobi polynomial with parameters \(\text{al}, \text{be}\)
  7 = generalized Laguerre polynomial with parameter \(\text{al}\)
  8 = Hermite polynomial

- **al, be** are the input parameters \(\alpha, \beta\) for Jacobi and generalized Laguerre polynomials; type real;
  they are only used if \(\text{ipoly} = 6\) or 7, and in the latter case only \(\text{al}\) is used.
On return, 

\[ a, b \] are real arrays of dimension \( n \) with \( a(k), b(k) \) containing the coefficients \( \alpha_{k-1}, \beta_{k-1} \), respectively, \( k = 1, 2, \ldots, n \)

\( ierr \) is an error flag, where
\[
\begin{align*}
\text{ ierr } &= 0 \text{ on normal return,} \\
\text{ ierr } &= 1 \text{ if either } a \text{ or } b \text{ are out of range} \\
&\quad \text{ when } ipoly = 6 \text{ or } ipoly=7, \\
\text{ ierr } &= 2 \text{ if there is potential overflow in the} \\
&\quad \text{ evaluation of } \beta_0 \text{ when } ipoly = 6 \text{ or} \\
&\quad \text{ ipoly = 7; in this case } \beta_0 \text{ is set equal} \\
&\quad \text{ to the largest machine-representable} \\
&\quad \text{ number,} \\
\text{ ierr } &= 3 \text{ if } n \text{ is out of range,} \\
\text{ ierr } &= 4 \text{ if } ipoly \text{ is not one of the} \\
&\quad \text{ admissible integers.}
\end{align*}
\]

No provision has been made for Chebyshev polynomials of the fourth kind, since their recursion coefficients are obtained from those for the third-kind Chebyshev polynomials simply by changing the sign of the \( \alpha \)'s (and leaving the \( \beta \)'s unchanged).

The corresponding double-precision routine is \texttt{drecur}; it has the same calling sequence, except for real data types now being double-precision.

In the cases of Jacobi polynomials (\( ipoly = 6 \)) and generalized Laguerre polynomials (\( ipoly = 7 \)), the recursion coefficient \( \beta_0 \) (and only this one) involves the gamma function \( \Gamma \). Accordingly, a function routine, \texttt{alga}, is provided that computes the logarithm \( \ln \Gamma \) of the gamma function, and a separate routine, \texttt{gamma}, computing the gamma function by exponentiating its logarithm. Their calling sequences are

\[
\begin{align*}
\text{ function alga(x) } \\
\text{ function gamma(x,ierr),}
\end{align*}
\]

where \( ierr \) is an output variable set equal to 2 or 0 depending on whether the gamma function does, or does not, overflow, respectively. The corresponding double-precision routines have the names \texttt{dlga} and \texttt{dgamma}. All these routines require machine-dependent constants for reasons explained below.
The routine \texttt{alga} is based on a rational approximation valid on the interval $\left[\frac{1}{2}, \frac{3}{2}\right]$. Outside this interval, the argument $x$ is written as

$$x = x_e + m,$$

where

$$x_e = \begin{cases} 
  x - \lfloor x \rfloor + 1 & \text{if } x - \lfloor x \rfloor \leq \frac{1}{2}, \\
  x - \lfloor x \rfloor & \text{otherwise}
\end{cases}$$

is in the interval $\left(\frac{1}{2}, \frac{3}{2}\right]$ and $m \geq -1$ is an integer. If $m = -1$ (i.e., $0 < x \leq \frac{1}{2}$), then $\ln \Gamma(x) = \ln \Gamma(x_e) - \ln x$, while for $m > 0$, one computes $\ln \Gamma(x) = \ln \Gamma(x_e) + \ln p$, where $p = x_e(x_e + 1) \cdots (x_e + m - 1)$. If $m$ is so large, say $m \geq m_0$, that the product $p$ would overflow, then $\ln p$ is computed (at a price!) as $\ln p = \ln x_e + \ln (x_e + 1) + \cdots + \ln (x_e + m - 1)$. It is here, where a machine-dependent integer is required, namely $m_0 = \text{smallest integer } m$ such that $1 \cdot 3 \cdot 5 \cdots (2m+1)/2^m$ is greater than or equal to the largest machine-representable number, $R$. By Stirling’s formula, the integer $m_0$ is seen to be the smallest integer $m$ satisfying $\left((m+1)/e\right) \ln((m+1)/e) \geq (\ln R - \frac{1}{2} \ln 8)/e$, hence equal to $\lfloor e \cdot t((\ln R - \frac{1}{2} \ln 8)/e) \rfloor$, where $t(y)$ is the inverse function of $y = t \ln t$. For our purposes, the low-accuracy approximation of $t(y)$, given in [16, pp. 51–52], and implemented in the routine $t$, is adequate.

The rational approximation chosen on $\left[\frac{1}{2}, \frac{3}{2}\right]$ is one due to W.J. Cody and K.E. Hillstrom, namely the one labeled $n = 7$ in Table II of [9]. It is designed to yield about 16 correct decimal digits (cf. [9, Table I]), but because of numerical cancellation furnishes only about 13-14 correct decimal digits.

Since rational approximations for $\ln \Gamma$ having sufficient accuracies for double-precision computation do not seem to be available in the literature, we used a different approach for the routine \texttt{dlga}, namely the asymptotic approximation (cf. [1, Eq. 6.1.42], where the constants $B_{2m}$ are Bernoulli numbers)

$$\ln \Gamma(y) = \left(y - \frac{1}{2}\right) \ln y - y + \frac{1}{2} \ln(2\pi) + \sum_{m=1}^{n} \frac{B_{2m}}{2m(2m-1)} y^{-(2m-1)} + R_n(y)$$

(2.4)
for values of \( y > 0 \) large enough to have

\[
|R_n(y)| \leq \frac{1}{2} 10^{-d},
\]

(2.5)

where \( d \) is the number of decimal digits carried in double-precision arithmetic, another machine-dependent real number. If (2.5) holds for \( y \geq y_0 \), and if \( x \geq y_0 \), we compute \( \ln \Gamma(x) \) from the asymptotic expression (2.4) (where \( y = x \) and the remainder term is neglected). Otherwise, we let \( k_0 \) be the smallest positive integer \( k \) such that \( x + k \geq y_0 \), and use

\[
\ln \Gamma(x) = \ln \Gamma(x + k_0) - \ln (x(x + 1) \cdots (x + k_0 - 1)),
\]

(2.6)

where the first term on the right is computed from (2.4) (with \( y = x + k_0 \)).

Since for \( y > 0 \),

\[
|R_n(y)| \leq \frac{|B_{2n+2}|}{(2n+2)(2n+1)} y^{-(2n+1)}
\]

(cf. [1, Eq. 6.1.42]), the inequality (2.5) is satisfied if

\[
y \geq \exp \left\{ \frac{1}{2n+1} \left[ d \ln 10 + \ln \frac{2|B_{2n+2}|}{(2n+2)(2n+1)} \right] \right\}.
\]

(2.7)

In our routine \texttt{dlga}, we have selected \( n = 9 \). For double-precision accuracy on the Cyber 205, we have \( d \approx 28.3 \), for which (2.7) then gives \( y \geq \exp\{.121188\ldots + .053905\ldots\} \approx 32.6 \).

For single-precision calculation we selected the method of rational approximation, rather than the asymptotic formula (2.4) and (2.6), since we found that the former is generally more accurate, by a factor, on the average, of about 20 and as large as 300. Neither method yields full machine accuracy. The former, as already mentioned, loses accuracy in the evaluation of the approximation. The latter suffers loss of accuracy because of cancellation occurring in (2.6), which typically amounts to a loss of 2–5 significant decimal digits in the gamma function itself.

Since these errors affect only the coefficient \( \beta_0 \) (and only if \texttt{ipoly} = 6 or 7), they are of no consequence unless the output of the routine \texttt{recur} serves as input to another routine, such as \texttt{gauss} (cf. §6), which makes essential use of \( \beta_0 \). In this case, for maximum single-precision accuracy, it is recommended that \( \beta_0 \) be first obtained in double precision by means of \texttt{drecur} with \( n = 1 \), and then converted to single precision.
3. MOMENT-RELATED METHODS

It is a well-known fact that the first \( n \) recursion coefficients \( \alpha_k(d\lambda) \), \( \beta_k(d\lambda) \), \( k = 0, 1, \ldots, n - 1 \) (cf. (1.3)), are uniquely determined by the first \( 2n \) moments \( \mu_k \) of the measure \( d\lambda \),

\[
\mu_k = \mu_k(d\lambda) = \int_{\mathbb{R}} t^k d\lambda(t), \quad k = 0, 1, 2, \ldots, 2n - 1. \tag{3.1}
\]

Formulae are known, for example, which express the \( \alpha \)'s and \( \beta \)'s in terms of Hankel determinants in these moments. The trouble is that these formulae become increasingly sensitive to small errors as \( n \) becomes large. There is an inherent reason for this: the underlying (nonlinear) map \( K_n: \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n} \) has a condition number, \( \text{cond } K_n \), which grows exponentially with \( n \) (cf. [19, §3.2]). Any method that attempts to compute the desired coefficients from the moments in (3.1), therefore, is doomed to fail, unless \( n \) is quite small, or extended precision is being employed. That goes in particular for an otherwise elegant method due to Chebyshev (who developed it for the case of discrete measures \( d\lambda \)) that generates the \( \alpha \)'s and \( \beta \)'s directly from the moments (3.1), bypassing determinants altogether (cf. [4], [19, §2.3]).

Variants of Chebyshev’s algorithm with more satisfactory stability properties have been developed by Sack and Donovan [46] and Wheeler [50] (independently of Chebyshev’s work). The idea is to forego the moments (3.1) as input data, and instead depart from so-called modified moments. These are defined by replacing the power \( t^k \) in (3.1) by an appropriate polynomial \( p_k(t) \) of degree \( k \),

\[
\nu_k = \nu_k(d\lambda) = \int_{\mathbb{R}} p_k(t) d\lambda(t), \quad k = 0, 1, 2, \ldots, 2n - 1. \tag{3.2}
\]

For example, \( p_k \) could be one of the classical orthogonal polynomials. More generally, we shall assume that \( \{p_k\} \) are monic polynomials satisfying a three-term recurrence relation similar to the one in (1.3),

\[
p_{k+1}(t) = (t - a_k)p_k(t) - b_kp_{k-1}(t), \quad k = 0, 1, 2, \ldots, \tag{3.3}
\]

\[
p_0(t) = 1, \quad p_{-1}(t) = 0,
\]

with coefficients \( a_k \in \mathbb{R}, b_k \geq 0 \) that are known. (In the special case \( a_k = 0, b_k = 0 \), we are led back to powers and ordinary moments.) There now
exists an algorithm, called modified Chebyshev algorithm in [19, §2.4], which takes the $2n$ modified moments in (3.2) and the $2n - 1$ coefficients $\{a_k\}_{k=0}^{2n-2}$, $\{b_k\}_{k=0}^{2n-2}$ in (3.3), and from them generates the $n$ desired coefficients $\alpha_k(d\lambda)$, $\beta_k(d\lambda)$, $k = 0, 1, \ldots, n - 1$. It generalizes Chebyshev’s algorithm, which can be recovered (if need be) by putting $a_k = b_k = 0$. The modified Chebyshev algorithm is embodied in the subroutine cheb, which has the calling sequence

\begin{verbatim}
cheb(n,a,b,fnu,alpha,beta,s,ierr,s0,s1,s2)
dimension a(*),b(*),fnu(*),alpha(n),beta(n),s(n),
s0(*),s1(*),s2(*)
\end{verbatim}

On entry,

- $n$ is the number of recursion coefficients desired; type integer
- $a, b$ are arrays of dimension $2 \times n - 1$ holding the coefficients $a(k) = a_{k-1}$, $b(k) = b_{k-1}$, $k = 1, 2, \ldots, 2n - 1$
- $fnu$ is an array of dimension $2 \times n$ holding the modified moments $fnu(k) = \nu_{k-1}$, $k = 1, 2, \ldots, 2n$

On return,

- $alpha, beta$ are arrays of dimension $n$ containing the desired recursion coefficients $alpha(k) = \alpha_{k-1}$, $beta(k) = \beta_{k-1}$, $k = 1, 2, \ldots, n$
- $s$ is an array of dimension $n$ containing the numbers $s(k) = \int_{\mathbb{R}} x_k^2 d\lambda$, $k = 1, 2, \ldots, n$
- $ierr$ is an error flag, equal to 0 on normal return, equal to 1 if $|\nu_0|$ is less than the machine zero, equal to 2 if $n$ is out of range, equal to $-(k-1)$ if $s(k)$, $k = 1, 2, \ldots, n$, is about to underflow, and equal to $+(k-1)$, if it is about to overflow.
The arrays $s_0, s_1, s_2$ of dimension $2 \times n$ are needed for working space.

There is again a map $K_n: \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ underlying the modified Chebyshev algorithm, namely the map taking the $2n$ modified moments into the $n$ pairs of recursion coefficients. The condition of the map $K_n$ (actually of a somewhat different, but closely related map) has been studied in [19, §3.3] and [23] in the important case where the polynomials $p_k$ defining the modified moments are themselves orthogonal polynomials, $p_k(\cdot) = p_k(\cdot; d\mu)$, with respect to a measure $d\mu$ (for example, one of the classical ones) for which the recursion coefficients $a_k, b_k$ are known. The upshot of the analysis then is that the condition of $K_n$ is characterized by a certain positive polynomial $g_n(\cdot; d\lambda)$ of degree $4n - 2$, depending only on the target measure $d\lambda$, in the sense that

$$\text{cond } K_n = \int_{\mathbb{R}} g_n(t; d\lambda) d\mu(t). \quad (3.4)$$

Thus, the numerical stability of the modified Chebyshev algorithm is determined by the magnitude of $g_n$ on the support of $d\mu$.

The occurrence of underflow [overflow] in the computation of the $\alpha$’s and $\beta$’s, especially on computers with limited exponent range, can often be avoided by multiplying all modified moments by a sufficiently large [small] scaling factor before entering the routine. On exit, the coefficient $\beta_0$ (and only this one!) then has to be divided by the same scaling factor. (There may occur harmless underflow of auxiliary quantities in the routine \texttt{cheb}, which is difficult to avoid since some of these quantities actually are expected to be zero.)

Example 3.1. $d\lambda_\omega(t) = \left[(1 - \omega^2 t^2)(1 - t^2)\right]^{-1/2} dt$ on $(-1,1)$, $0 \leq \omega < 1$.

This example is of some historical interest, in that it has already been considered by Christoffel [8, Example 6]; see also [44]. Computationally, the example is of interest as there are empirical reasons to believe that for the choice $d\mu(t) = (1 - t^2)^{-1/2} dt$ on $(-1,1)$ — which appears rather natural — the modified Chebyshev algorithm is exceptionally stable, uniformly in $n$, in the sense that in (3.4) one has $g_n \leq 1$ on supp $d\mu$ for all $n$ (cf. [22, Example 5.2]). With the above choice of $d\mu$, the polynomials $p_k$ are clearly the Chebyshev polynomials of the first kind, $p_0 = T_0, p_k = 2^{-k} T_k, k \geq 1,$ and the modified moments are given by

$$\nu_0 = \int_{-1}^{1} d\lambda_\omega(t), \quad \nu_k = \frac{1}{2^{k-1}} \int_{-1}^{1} T_k(t)d\lambda_\omega(t), \quad k = 1, 2, 3, \ldots \quad (3.5)$$
They are expressible in terms of the Fourier coefficients $C_r(\omega^2)$ in

\[(1 - \omega^2 \sin^2 \theta)^{-1/2} = C_0(\omega^2) + 2 \sum_{r=1}^{\infty} C_r(\omega^2) \cos 2r\theta \quad (3.6)\]

by means of (cf. [19, Example 3.3])

\[
\begin{align*}
\nu_0 &= \pi C_0(\omega^2), \\
\nu_{2m} &= \frac{(-1)^m \pi}{2^{m-1}} C_m(\omega^2) \quad m = 1, 2, 3, \ldots \\
\nu_{2m-1} &= 0
\end{align*}
\]

The Fourier coefficients $\{C_r(\omega^2)\}$ in turn can be accurately computed as minimal solution of a certain three-term recurrence relation (see [19, pp. 310–311]).

The ordinary moments

\[
\begin{align*}
\mu_0 &= \nu_0, \\
\mu_k &= \int_{-1}^{1} t^k d\lambda_\omega(t), \quad k = 1, 2, 3, \ldots 
\end{align*}
\]

likewise can be expressed in terms of the Fourier coefficients $C_r(\omega^2)$ by writing $t^{2m}$ as a linear combination of Chebyshev polynomials $T_0, T_2, \ldots, T_{2m}$ (cf. Eq. (22) on p. 454 of [43]). The result is

\[
\begin{align*}
\mu_{2m} &= \frac{(-1)^m \pi}{2^{2m-1}} \sum_{r=0}^{m} (-1)^r \gamma_r(m) C_{m-r}(\omega^2), \\
\mu_{2m-1} &= 0,
\end{align*}
\]

where

\[
\begin{align*}
\gamma_0^{(m)} &= 1, \\
\gamma_r^{(m)} &= \frac{2m + 1 - r}{r} \gamma_{r-1}^{(m)}, \quad r = 1, 2, \ldots, m - 1, \\
\gamma_m^{(m)} &= \frac{m + 1}{2m} \gamma_{m-1}^{(m)}.
\end{align*}
\]

The driver routine test1 (in §1 of the package) generates for $\omega^2 = .1(.2).9, .99, .999$ the first $n$ recurrence coefficients $\beta_k(d\lambda_\omega)$ (all $\alpha_k = 0$), both
in single and double precision, using modified moments if \texttt{modmom}=.true.,
and ordinary moments otherwise. In the former case, \( n = 80 \), in the latter, \( n = 20 \). It prints the double-precision values of \( \beta_k \) together with the relative errors of the single-precision values (computed as the difference of the double-precision and single-precision values divided by the double-precision value). In \texttt{test1}, as well as in all subsequent drivers, not all error flags are interrogated for possible malfunction. The user is urged, however, to do so as a matter of principle.

\[
\begin{array}{cccc}
\omega^2 & k & \beta_k^{\text{double}} & \text{err } \beta_k^{\text{single}} \\
.1 & 0 & 3.224882697440438796459832725 & 1.433(-14) \\
 & 1 & .5065840806382684475158495727 & 1.187(-14) \\
 & 5 & .2499999953890031901881028267 & 1.109(-14) \\
 & 11 & .24999999999999999996365048540 & 1.454(-18) \\
 & 18 & .250000000000000000000 & 0.000 \\
.5 & 0 & 3.708149354602743836867700694 & 9.005(-15) \\
 & 1 & .5430534189555363746250333773 & 2.431(-14) \\
 & 8 & .249999984631723296083779480 & 4.109(-15) \\
 & 20 & .2499999999999999978894635584 & 8.442(-18) \\
 & 35 & .250000000000000000000 & 0.000 \\
.9 & 0 & 5.156184226696346376405141543 & 6.950(-15) \\
 & 1 & .6349731661452458711622492613 & 7.920(-15) \\
 & 19 & .249999995692595094629502830 & 1.820(-14) \\
 & 43 & .249999999999999998282104100896 & 6.872(-16) \\
 & 79 & .24999999999999999999999999962 & 1.525(-26) \\
.999 & 0 & 9.682265121100594060678208257 & 1.194(-13) \\
 & 1 & .7937821421385176965531719571 & 6.311(-14) \\
 & 19 & .249906389439820920047452537 & 1.026(-14) \\
 & 43 & .2499955822633680825859750068 & 8.282(-15) \\
 & 79 & .2499998417688157876153069211 & 1.548(-15) \\
\end{array}
\]

\textbf{TABLE 3.1.} Selected output from \texttt{test1} in the case of modified moments

The routine
The routine \texttt{fmm} as well as its double-precision version \texttt{dmm} are listed immediately after the routine \texttt{test1}.

In Table 3.1, we show selected results from the output of \texttt{test1}, when \texttt{modmom=.true.}. (Complete results are given in the package immediately after \texttt{test1}.) The values for \( k = 0 \) are expressible in terms of the complete elliptic integral, \( \beta_0 = 2K(\omega^2) \), and were checked, where possible, against the 16S-values in Table 17.1 of [1]. In all cases, there was agreement to all 16 digits. The largest relative error observed was \( 2.43 \times 10^{-13} \) for \( \omega^2 = 0.999 \) and \( k = 2 \). When \( \omega^2 \leq 0.99 \), the error was always less than \( 2.64 \times 10^{-14} \), which confirms the extreme stability of the modified Chebyshev algorithm in this example. It can be seen (as was to be expected) that for \( \omega^2 \) not too close to 1, the coefficients converge rapidly to \( \frac{1}{4} \).

In contrast, Table 3.2 shows selected results (for complete results, see the package) in the case of ordinary moments (\texttt{modmom=.false.}) and demonstrates the severe instability of the Chebyshev algorithm. We remark that the moments themselves are all accurate to essentially machine precision, as has been verified by additional computations.

| \( \omega^2 \) | \( k \) | \( \text{err} \beta_k \) | \( \omega^2 \) | \( k \) | \( \text{err} \beta_k \) |
|---------------|-------|----------------|---------------|-------|----------------|
| .1            | 1     | 1.187(–14)     | .9            | 1     | 3.270(–15)     |
|               | 7     | 2.603(–10)     |               | 7     | 4.819(–10)     |
|               | 13    | 9.663(–6)      |               | 13    | 1.841(–5)      |
|               | 19    | 4.251(–1)      |               | 19    | 6.272(–1)      |
| .5            | 1     | 2.431(–14)     | .999          | 1     | 6.311(–14)     |
|               | 7     | 5.571(–10)     |               | 7     | 1.745(–9)      |
|               | 13    | 9.307(–6)      |               | 13    | 8.589(–5)      |
|               | 19    | 5.798(–1)      |               | 19    | 4.808(0)       |

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TABLE 3.2. Selected output from test1 in the case of ordinary moments

The next example deals with another weight function for which the modified Chebyshev algorithm performs rather well.

Example 3.2. \( d\lambda_\sigma(t) = t^\sigma \ln(1/t) dt \) on \((0,1], \sigma > -1\).

What is nice about this example is that both modified and ordinary moments of \( d\lambda_\sigma \) are known in closed form. The latter are obviously given by

\[
\mu_k(d\lambda_\sigma) = \frac{1}{\sigma + 1 + k}, \quad k = 0, 1, 2, \ldots, \tag{3.11}
\]

whereas the former, relative to shifted monic Legendre polynomials (ipoly=2 in recur), are (cf. [17])

\[
\left(\frac{2k!}{k!^2}\right) \nu_k(d\lambda_\sigma) = \begin{cases} 
(-1)^{k-\sigma} \frac{\sigma!(k - \sigma - 1)!}{(k + \sigma + 1)!}, & 0 \leq \sigma < k, \, \sigma \text{ an integer,} \\
\frac{1}{\sigma + 1} \left\{ \frac{1}{\sigma + 1} + \sum_{r=1}^{\sigma} \left( \frac{1}{\sigma + 1 + r} - \frac{1}{\sigma + 1 - r} \right) \right\} \prod_{r=1}^{k} \frac{\sigma + 1 - r}{\sigma + 1 + r}, & \text{otherwise.}
\end{cases} \tag{3.12}
\]

The routines \texttt{fmm} and \texttt{dmm} appended to test2 in §1 of the package, similarly as the corresponding routines in Example 3.1, generate the first \( 2 \times n \) modified moments \( \nu_0, \nu_1, \ldots, \nu_{2n-1} \), if \texttt{modmom=.true.}, and the first \( 2 \times n \) ordinary moments, otherwise. The calling sequence of \texttt{fmm} is

\[
\texttt{fmm(n,modmom,intexp,sigma,fnu}).
\]

The logical variable \texttt{intexp} is to be set \texttt{.true.}, if \( \sigma \) is an integer, and \texttt{.false.} otherwise. In either case, the input variable \texttt{sigma} is assumed of type \texttt{real}.

The routine \texttt{test2} generates the first \( n \) recursion coefficients \( \alpha_k(d\lambda_\sigma), \beta_k(d\lambda_\sigma) \) in single and double precision for \( \sigma = -\frac{1}{2}, 0, \frac{1}{2} \), where \( n = 100 \) for the modified Chebyshev algorithm (\texttt{modmom=.true.}), and \( n = 12 \) for the classical Chebyshev algorithm (\texttt{modmom=.false.}). Selected double-precision results to 25 significant digits, when modified moments are used, are shown in Table 3.3. (The complete results are given in the package after test2.)
| $\sigma$ | $k$ | $\alpha_k$ | $\beta_k$ |
|---|---|---|---|
| -.5 | 0  | 0.11111111111111111111111111111111 | 4.000000000000000000000000000000 |
| 12 | .4994971916094638566242202 | 0.06231277082877488477563886 |
| 24 | .4998662912324218943801592 | 0.06245372557342242600457226 |
| 48 | .499652635485445800661969 | 0.062488557177486847423618 |
| 99 | .4999916184024356271670789 | 0.06249733823051821636937156 |
| 0 | 0  | 0.250000000000000000000000000000000000 | 1.000000000000000000000000000000000000 |
| 12 | .4992831802157361310272625 | 0.06238356835953571123560330 |
| 24 | .499806283948614639850153 | 0.0624710064469111001639128 |
| 48 | .499944083797023879356424 | 0.0624928126811096742373889 |
| 99 | .4999877992015903283047919 | 0.0624983267061692596204896 |
| .5 | 0  | 0.360000000000000000000000000000000000 | 1.4444444444444444444444444444 |
| 12 | .4993755732917555644203267 | 0.06237082738280752611960887 |
| 24 | .4998324497706394888722725 | 0.06246581011945496883543089 |
| 48 | .4999567275223771727791521 | 0.062491153327102716695932 |
| 99 | .4999896931841789781887674 | 0.06249787251281682973825635 |

**TABLE 3.3.** Selected output from test2 in the case of modified moments

The largest relative errors observed, over all $k = 0, 1, \ldots, 99$, were respectively $6.211 \times 10^{-11}$, $2.237 \times 10^{-12}$, $1.370 \times 10^{-12}$ for the $\alpha$’s, and $1.235 \times 10^{-10}$, $4.446 \times 10^{-12}$, $2.724 \times 10^{-12}$ for the $\beta$’s, attained consistently at $k = 99$. The accuracy achieved is slightly less than in Example 3.1, for reasons explained in [22, Example 5.3].

The complete results for $\sigma = -\frac{1}{2}$ are also available in [27, Appendix, Table 1]. (They differ occasionally by 1 unit in the last decimal place from those produced here, probably because of a slightly different computation of the modified moments.) The results for $\sigma = 0$ can be checked up to $k = 15$ against the 30S-values given in [47, p. 92], and for $16 \leq k \leq 19$ against 12S-values in [10, Table 3]. There is complete agreement to all 25 digits in the former case, and agreement to 12 digits in the latter, although there are occasional end figure discrepancies of 1 unit. These are believed to be due to rounding errors committed in [10], since similar discrepancies occur also in the range $k \leq 15$. We do not know of any tables for $\sigma = \frac{1}{2}$, but a test will be given in §5, Example 5.1.
The use of ordinary moments (\texttt{modmom=.false.}) produces predictably worse results, the relative errors of which are shown in Table 3.4.

| $k$ | $\sigma$ | err $\alpha_k$ | err $\beta_k$ | $\sigma$ | err $\alpha_k$ | err $\beta_k$ | $\sigma$ | err $\alpha_k$ | err $\beta_k$ |
|-----|----------|----------------|---------------|----------|----------------|---------------|----------|----------------|---------------|
| 2   | .5       | 1.8(–13)      | 7.7(–14)     | 0        | 4.2(–13)      | 7.6(–13)     | .5       | 1.6(–12)      | 2.6(–13)     |
| 5   | 2.2(–9)  | 1.2(–9)       | 4.2(–9)      | 1.2(–10) | 1.3(–8)       | 6.6(–9)      |
| 8   | 1.1(–5)  | 5.5(–6)       | 4.3(–6)      | 3.8(–6)  | 6.0(–5)       | 5.2(–6)      |
| 11  | 2.5(–1)  | 1.7(–1)       | 1.3(0)       | 3.2(–1)  | 2.2(0)        | 4.7(–1)      |

\textbf{TABLE 3.4.} Selected output from \texttt{test2} in the case of ordinary moments

4. STIELTJES, ORTHOGONAL REDUCTION, AND DISCRETIZATION PROCEDURES

4.1. \textit{The Stieltjes procedure.} It is well known that the coefficients $\alpha_k(d\lambda)$, $\beta_k(d\lambda)$ in the basic recurrence relation (1.3) can be expressed in terms of the orthogonal polynomials (1.2) and the inner product (1.1) as follows:

\[
\alpha_k(d\lambda) = \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)}, \quad k \geq 0; \\
\beta_0(d\lambda) = (\pi_0, \pi_0), \quad \beta_k(d\lambda) = \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})}, \quad k \geq 1.
\] (4.1)

Provided the inner product can be readily calculated, (4.1) suggests the following “bootstrap” procedure: Compute $\alpha_0$ and $\beta_0$ by the first relations in (4.1) for $k = 0$. Then use the recurrence relation (1.3) for $k = 0$ to obtain $\pi_1$. With $\pi_0$ and $\pi_1$ known, apply (4.1) for $k = 1$ to get $\alpha_1$, $\beta_1$, then again (1.3) to obtain $\pi_2$, and so on. In this way, alternating between (4.1) and (1.3), we can bootstrap ourselves up to as many of the coefficients $\alpha_k$, $\beta_k$ as are desired. We attributed this procedure to Stieltjes, and called it Stieltjes’s procedure in [19].

In the case of discrete orthogonal polynomials, i.e., for inner products of the form

\[
(u, v) = \sum_{k=1}^{N} w_k u(x_k) v(x_k), \quad w_k > 0,
\] (4.2)
Stieltjes's procedure is easily implemented; the resulting routine is called \texttt{sti}, and has the calling sequence

\begin{verbatim}
sti(n,ncap,x,w,alpha,beta,ierr,p0,p1,p2).
\end{verbatim}

On entry,

- \texttt{n} is the number of recursion coefficients desired; type integer
- \texttt{ncap} is the number of terms, \( N \), in the discrete inner product; type integer
- \texttt{x,w} are arrays of dimension \texttt{ncap} holding the abscissae \( x(k) = x_k \) and weights \( w(k) = w_k, k = 1,2,\ldots,\texttt{ncap} \), of the discrete inner product.

On return,

- \texttt{alpha,beta} are arrays of dimension \texttt{n} containing the desired recursion coefficients \( \alpha(k) = \alpha_{k-1}, \beta(k) = \beta_{k-1}, k = 1,2,\ldots,\texttt{n} \)
- \texttt{ierr} is an error flag having the value 0 on normal return, and the value 1 if \texttt{n} is not in the proper range \( 1 \leq n \leq N \); if during the computation of a recursion coefficient with index \( k \) there is impending underflow or overflow, \texttt{ierr} will have the value \(-k\) in case of underflow, and the value \(+k\) in case of overflow. (No error flag is set in case of harmless underflow.)

The arrays \texttt{p0, p1, p2} are working arrays of dimension \texttt{ncap}. The double-precision routine has the name \texttt{dsti}.

Occurrence of underflow [overflow] can be forestalled by multiplying all weights \( w_k \) by a sufficiently large [small] scaling factor prior to entering the routine. Upon return, the coefficient \( \beta_0 \) will then have to be readjusted by dividing it by the same scaling factor.
4.2. Orthogonal reduction method. Another approach to producing the recursion coefficients $\alpha_k, \beta_k$ from the quantities $x_k, w_k$ defining the inner product (4.2) is based on the observation (cf. [2], [29, §7]) that the symmetric tridiagonal matrix of order $N + 1$,

$$J(d\lambda_N) = \begin{bmatrix}
1 & \sqrt{\beta_0} & 0 \\
\sqrt{\beta_0} & \alpha_0 & \sqrt{\beta_1} \\
& \sqrt{\beta_1} & \alpha_1 & \ddots \\
& & \ddots & \ddots & \sqrt{\beta_{N-1}} \\
0 & & & \sqrt{\beta_{N-1}} & \alpha_{N-1}
\end{bmatrix} \quad (4.3)
$$

(the “extended Jacobi matrix” for the discrete measure $d\lambda_N$ implied in (4.2)), is orthogonally similar to the matrix

$$\begin{bmatrix}
1 \\
\sqrt{w^T} \\
\sqrt{w} & D_x
\end{bmatrix}, \quad \sqrt{w} = \begin{bmatrix}
\sqrt{w_1} \\
\vdots \\
\sqrt{w_N}
\end{bmatrix}, \quad D_x = \begin{bmatrix}
x_1 & 0 \\
& \ddots \\
0 & x_N
\end{bmatrix}. \quad (4.4)
$$

Hence, the desired matrix $J(d\lambda_N)$ can be obtained by applying Lanczos’s algorithm to the matrix (4.4). This is implemented in the routine

$$\text{lancz}(n, ncap, x, w, \alpha, \beta, ierr, p0, p1),$$

which uses a judiciously constructed sequence of Givens transformations to accomplish the orthogonal similarity transformation (cf. [45,3,41,2]; the routine lancz is adapted from the routine RKPW in [41, p. 328]). The input and output parameters of the routine lancz have the same meaning as in the routine sti, except that ierr can only have the value 0 or 1, while p0, p1 are again working arrays of dimension ncap. The double-precision version of the routine is named dlancz.

The routine lancz is generally superior to the routine sti: The procedure used in sti may develop numerical instability from some point on, and therefore give inaccurate results for larger values of n. It furthermore is subject to underflow and overflow conditions. None of these shortcomings is shared by the routine lancz. On the other hand, there are cases where sti does better than lancz (cf. Example 4.5).

We illustrate the phenomenon of instability (which is explained in [32]) in the case of the “discrete Chebyshev” polynomials.
Example 4.1. The inner product (4.2) with $x_k = -1 + 2 \frac{k-1}{N-1}$, $w_k = \frac{2}{N}$, $k = 1, 2, \ldots, N$.

This generates discrete analogues of the Legendre polynomials, which they indeed approach as $N \to \infty$. The recursion coefficients are explicitly known:

$$\alpha_k = 0, \quad k = 0, 1, \ldots, N-1;$$
$$\beta_0 = 2, \quad \beta_k = \left(1 + \frac{1}{N-1}\right)^2 \left(1 - \left(\frac{k}{N}\right)^2\right) \left(4 - \frac{1}{k^2}\right)^{-1} \quad (4.5)$$
$$k = 1, 2, \ldots, N-1.$$

To find out how well the routines sti and lancz generate them (in single precision), when $N = 40, 80, 160, 320$, we wrote the driver test3, which computes the respective absolute errors for the $\alpha$’s and relative errors for the $\beta$’s.

Selected results for Stieltjes’s algorithm are shown in Table 4.1. The gradual deterioration, after some point (depending on $N$), is clearly visible. Lanczos’s method, in contrast, preserves essentially full accuracy; the largest error in the $\alpha$’s is $1.42(-13)$, $2.27(-13)$, $4.83(-13)$, $8.74(-13)$ for $N = 40, 80, 160, 320$, respectively, and $3.38(-13)$, $6.63(-13)$, $2.17(-12)$, $5.76(-12)$ for the $\beta$’s.

| $N$ | $n$ | $\text{err } \alpha$ | $\text{err } \beta$ | $N$ | $n$ | $\text{err } \alpha$ | $\text{err } \beta$ |
|-----|-----|---------------------|---------------------|-----|-----|---------------------|---------------------|
| 40  | $\leq 35$ | $1.91(-13)$ | $7.78(-13)$ | 160 | $\leq 76$ | $2.98(-13)$ | $7.61(-13)$ |
| 36  | 3.01(-12) | 1.48(-11) | 85 | 1.61(-9) | 1.57(-8) |
| 37  | 6.93(-11) | 3.55(-10) | 94 | 1.25(-4) | 1.17(-3) |
| 38  | 2.57(-9) | 1.30(-8) | 103 | 2.64(-3) | 1.51(-1) |
| 39  | 1.93(-7) | 9.58(-7) | 112 | 2.35(-3) | 1.16(-1) |
| 80  | $\leq 53$ | $2.04(-13)$ | $6.92(-13)$ | 320 | $\leq 106$ | $8.65(-13)$ | $7.39(-13)$ |
| 57  | 2.04(-10) | 5.13(-10) | 117 | 3.96(-10) | 7.73(-10) |
| 61  | 3.84(-7) | 9.35(-7) | 128 | 2.46(-6) | 4.67(-6) |
| 65  | 1.94(-3) | 4.61(-3) | 139 | 2.94(-2) | 6.27(-2) |
| 69  | 1.87(-1) | 6.14(0) | 150 | 1.15(-3) | 2.18(-2) |

TABLE 4.1. Errors in the recursion coefficients $\alpha_k, \beta_k$ of (4.5) computed by Stieltjes’s procedure
4.3. Multiple-component discretization procedure. We assume now a measure $d\lambda$ of the form

$$d\lambda(t) = w(t)dt + \sum_{j=1}^{p} y_j \delta(t - x_j)dt, \quad p \geq 0,$$

consisting of a continuous part, $w(t)dt$, and (if $p > 0$) a discrete part written in terms of the Dirac $\delta$-function. The support of the continuous part is assumed to be an interval or a finite union of disjoint intervals, some of which may extend to infinity. In the discrete part, the abscissae $x_j$ are assumed pairwise distinct, and the weights positive, $y_j > 0$. The inner product (1.1), therefore, has the form

$$(u,v) = \int_{\mathbb{R}} u(t)v(t)w(t)dt + \sum_{j=1}^{p} y_j u(x_j)v(x_j).$$

The basic idea of the discretization procedure is rather simple: One approximates the continuous part of the inner product, i.e., the integral in (4.7), by a sum, using a suitable quadrature scheme. If the latter involves $N$ terms, this replaces the inner product (4.7) by a discrete inner product $(\cdot,\cdot)_{N+p}$ consisting of $N + p$ terms, the $N$ “quadrature terms” and the $p$ original terms. In effect, the measure $d\lambda$ in (4.6) is approximated by a discrete $(N+p)$-point measure $d\lambda_{N+p}$. We then compute the desired recursion coefficients from the formula (4.1), in which the inner product $(\cdot,\cdot)$ is replaced, throughout, by $(\cdot,\cdot)_{N+p}$. Thus, in effect, we approximate

$$\alpha_k(d\lambda) \approx \alpha_k(d\lambda_{N+p}), \quad \beta_k(d\lambda) \approx \beta_k(d\lambda_{N+p}).$$

The quantities on the right can be computed by the methods of §4.1 or §4.2, i.e., employing the routines sti or lancz.

The difficult part of this approach is to find a discretization that results in rapid convergence, as $N \to \infty$, of the approximations on the right of (4.8) to the exact values on the left, even in cases where the weight function $w$ in (4.6) exhibits singular behavior. (The speed of convergence, of course, is unaffected by the discrete part of the inner product (4.7).) To be successful in this endeavor often requires considerable inventiveness on the part of the user. Our routines, mcdis and dmcdis, that implement this idea in single resp. double precision, however, are designed to be flexible enough to promote the use of effective discretization procedures.
Indeed, if the support of the weight function $w$ in (4.7) is contained in the (finite or infinite) interval $(a, b)$, it will often be useful to first decompose that interval into a finite number of subintervals,

$$\text{supp } w \subset [a, b] = \bigcup_{i=1}^{m} [a_i, b_i], \quad m \geq 1,$$

and to approximate the inner product separately on each subinterval $[a_i, b_i]$, using an appropriate weighted quadrature rule. Thus, we write the integral in (4.7) as

$$\int_{\mathbb{R}} u(t)v(t)w(t)dt = \sum_{i=1}^{m} \int_{a_i}^{b_i} u(t)v(t)w_i(t)dt,$$

where $w_i$ is an appropriate weight function on $[a_i, b_i]$. The intervals $[a_i, b_i]$ are not necessarily disjoint. For example, the weight function $w$ may be the sum $w = w_1 + w_2$ of two weight functions on $[a, b]$, which we may want to treat individually (cf. Example 4.2 below). In that case, one would take $[a_1, b_1] = [a_2, b_2] = [a, b]$ and $w_1$ on the first interval, $w_2$ on the other. Alternatively, we may simply want to use a composite quadrature rule to approximate the integral, in which case (4.9) is a partition of $[a, b]$ and $w_i(t) = w(t)$ for each $i$. Still another example is a weight function $w$ which is already supported on a union of disjoint intervals; in this case, (4.9) would be the same union, or possibly a refined union where some of the subintervals are further partitioned.

In whichever way (4.9) and (4.10) are constructed, each integral on the right of (4.10) is now approximated by an appropriate quadrature rule,

$$\int_{a_i}^{b_i} u(t)v(t)w_i(t)dt \approx Q_i(uv),$$

where

$$Q_i f = \sum_{r=1}^{N_i} w_{r,i} f(x_{r,i}).$$

This gives rise to the approximate inner product

$$(u, v)_{N+p} = \sum_{i=1}^{m} \sum_{r=1}^{N_i} w_{r,i}u(x_{r,i})v(x_{r,i}) + \sum_{j=1}^{p} y_j u(x_j)v(x_j),$$

where $N = \sum_{i=1}^{m} N_i$. 22
In our routine \texttt{mcdis}, we have chosen, for simplicity, all \( N_i \) to be the same integer \( N_0 \),

\[ N_i = N_0, \quad i = 1, 2, \ldots, m, \quad (4.14) \]

so that \( N = mN_0 \). Furthermore, if \( n \) is the number of \( \alpha_k \) and the number of \( \beta_k \) desired, we have used the following iterative procedure to determine the coefficients \( \alpha_k, \beta_k \) to a prescribed (relative) accuracy \( \varepsilon \): We let \( N_0 \) increase through a sequence \( \{N_0[^{[s]}]\}_{s=0,1,2,...} \) of integers, for each \( s \) use Stieltjes’s (or Lanczos’s) algorithm to compute \( \alpha_k[^{[s]}] = \alpha_k(d\lambda_{mN_0[^{[s]}]+p}), \beta_k[^{[s]}] = \beta_k(d\lambda_{mN_0[^{[s]}]+p}), k = 0, 1, \ldots, n - 1 \), and stop the iteration for the first \( s \geq 1 \) for which all inequalities

\[ |\beta_k[^{[s]}] - \beta_k[^{[s-1]}]| \leq \varepsilon \beta_k[^{[s]}], \quad k = 0, 1, \ldots, n - 1, \quad (4.15) \]

are satisfied. An error flag is provided if within a preset range \( N_0[^{[s]}] \leq N_0^{\text{max}} \) the stopping criterion \( (4.15) \) cannot be satisfied. Note that the latter is based solely on the \( \beta \)-coefficients. This is because, unlike the \( \alpha \)'s, they are known to be always positive, so that it makes sense to insist on relative accuracy. (In our routine we actually replaced \( \beta_k[^{[s]}] \) on the right of \( (4.15) \) by its absolute value to insure proper termination in cases of sign-changing measures \( d\lambda \).)

In view of the formulae \( (4.1) \), it is reasonable to expect, and indeed has been observed in practice, that satisfaction of \( (4.15) \) entails sufficient absolute accuracy for the \( \alpha \)'s if they are zero or small, and relative accuracy otherwise.

Through a bit of experimentation, we have settled on the following sequence of integers \( N_0[^{[s]}] \):

\[ N_0[^{[0]}] = 2n, \quad N_0[^{[s]}] = N_0[^{[s-1]}] + \Delta_s, \quad s = 1, 2, \ldots, \]

\[ \Delta_1 = 1, \quad \Delta_s = 2^{[s/5]} \cdot n, \quad s = 2, 3, \ldots. \quad (4.16) \]

It should be noted that if the quadrature formula \( (4.11) \) is exact for each \( i \), whenever \( u \cdot v \) is a polynomial of degree \( \leq 2n - 1 \) (which is the maximum degree occurring in the inner products of \( (4.1) \), when \( k \leq n - 1 \)), then our procedure converges after the very first iteration step! Therefore, if each quadrature rule \( Q_i \) has (algebraic) degree of exactness \( \geq d(N_0) \), and
\[ d(N_0)/N_0 = \delta + O(N_0^{-1}) \] as \( N_0 \to \infty \), then we let \( N_0^{[0]} = 1 + \lfloor (2n - 1)/\delta \rfloor \) in an attempt to get exact answers after one iteration. Normally, \( \delta = 1 \) (for interpolatory rules) or \( \delta = 2 \) (for Gauss-type rules).

The calling sequence of the multiple-component discretization routine is

\[ \text{mcdis}(n, ncapm, mc, mp, xp, yp, quad, eps, iq, idelta, irout, finl, finr, endl, endr, xfer, wfer, alpha, beta, ncap, kount, ierr, ie, be, x, w, xm, wm, p0, p1, p2) \]

\[ \text{dimension} \ xp(*), yp(*), endl(mc), endr(mc), xfer(ncapm), wfer(ncapm), alpha(n), beta(n), be(n), x(ncapm), w(ncapm), xm(*), wm(*), p0(*), p1(*), p2(*), \]

\[ \text{logical} \ finl, finr \]

On entry,

- \( n \) is the number of recursion coefficients desired; type integer
- \( ncapm \) is the integer \( N_0^{\text{max}} \) above, i.e., the maximum integer \( N_0 \) allowed (\( ncapm = 500 \) will usually be satisfactory)
- \( mc \) is the number of component intervals in the continuous part of the spectrum; type integer
- \( mp \) is the number of points in the discrete part of the spectrum; type integer; if the measure has no discrete part, set \( mp = 0 \)
- \( xp, yp \) are arrays of dimension \( mp \) containing the abscissae and the jumps of the point spectrum
- \( quad \) is a subroutine determining the discretization of the inner product on each component interval, or a dummy routine if \( iq \neq 1 \) (see below); specifically, \( \text{quad}(n, x, w, i, ierr) \) produces the abscissae \( x(r) = x_{r,i} \) and weights
\( w(r) = w_{r,i}, \ r = 1, 2, \ldots, n, \) of the \( n \)-point discretization of the inner product on the interval \([a_i, b_i]\) (cf. (4.13)); an error flag \( \text{ierr} \) is provided to signal the occurrence of an error condition in the quadrature process.

\text{eps} is the desired relative accuracy of the nonzero recursion coefficients; type real.

\text{iq} is an integer selecting a user-supplied quadrature routine \text{quad} if \( \text{iq} = 1 \) or the ORTHPOL routine \text{qgp} (see below) otherwise.

\text{idelta} is a nonzero integer, typically 1 or 2, inducing fast convergence in the case of special quadrature routines; the default value is \( \text{idelta} = 1 \).

\text{irout} is an integer selecting the routine for generating the recursion coefficients from the discrete inner product; specifically, \( \text{irout} = 1 \) selects the routine \text{sti}, and \( \text{irout} \neq 1 \) the routine \text{lancz}.

The logical variables \text{finl}, \text{finr} and the arrays \text{endl}, \text{endr}, \text{xfer}, \text{wfer} are input variables to the subroutine \text{qgp} and are used (and hence need to be properly dimensioned) only if \( \text{iq} \neq 1 \).

On return,

\text{alpha}, \text{beta} are arrays of dimension \( n \) holding the desired recursion coefficients \( \text{alpha} (k) = \alpha_{k-1}, \beta_{k-1}, \ k = 1, 2, \ldots, n \).

\text{ncap} is the integer \( N_0 \) yielding convergence.

\text{kount} is the number of iterations required to achieve convergence.
**ierr** is an error flag, equal to 0 on normal return, equal to –1 if \( n \) is not in the proper range, equal to \( i \) if there is an error condition in the discretization on the \( i \)th interval, and equal to \( \text{n capm} \) if the discretized Stieltjes procedure does not converge within the discretization resolution specified by \( \text{n capm} \).

**ie** is an error flag inherited from the routine \text{sti} or \text{lancz} (whichever is used).

The arrays \( \text{be, x, w, xm, wm, p0, p1, p2} \) are used for working space, the last five having dimension \( \text{mc} \times \text{n capm} + \text{mp} \).

A general-purpose quadrature routine, \text{qgp}, is provided for cases in which it may be difficult to develop special discretizations that take advantage of the structural properties of the weight function \( w \) at hand. The routine assumes the same setup (4.9)–(4.14) used in \text{mcdis}, with disjoint intervals \([a_i, b_i]\), and provides for \( Q_i \) in (4.12) the Fejér quadrature rule, suitably transformed to the interval \([a_i, b_i]\), with the same number \( N_i = N_0 \) of points for each \( i \). Recall that the \( N \)-point Fejér rule on the standard interval \([-1,1]\) is the interpolatory quadrature formula

\[
Q_N^F f = \sum_{r=1}^N w_r^F f(x_r^F),
\]

(4.17)

where \( x_r^F = \cos((2r-1)\pi/2N) \) are the Chebyshev points. The weights are all positive and can be computed explicitly in terms of trigonometric functions (cf., e.g., [15]). The rule (4.17) is now applied to the integral in (4.11) by transforming the interval \([-1,1]\) to \([a_i, b_i]\) via some monotone function \( \phi_i \) (a linear function if \([a_i, b_i]\) is finite) and letting \( f = uvw_i \):

\[
\int_{a_i}^{b_i} u(t)v(t)w_i(t)dt = \int_{-1}^{1} u(\phi_i(\tau))v(\phi_i(\tau))w_i(\phi_i(\tau))\phi_i'(\tau)d\tau
\approx \sum_{r=1}^N w_r^F w_i(\phi_i(x_r^F))\phi_i'(x_r^F) \cdot u(\phi_i(x_r^F))v(\phi_i(x_r^F)).
\]

Thus, in effect, we take in (4.13)

\[
x_{r,i} = \phi_i(x_r^F), \quad w_{r,i} = w_r^F w_i(\phi_i(x_r^F))\phi_i'(x_r^F), \quad i = 1, 2, \ldots, m.
\]

(4.18)
If the interval \([a_i, b_i]\) is half-infinite, say of the form \([0, \infty]\), we use \(\phi_i(t) = (1 + t)/(1 - t)\), and similarly for intervals of the form \([-\infty, b]\) and \([a, \infty]\). If \([a_i, b_i] = [-\infty, \infty]\), we use \(\phi_i(t) = t/(1 - t^2)\).

The routine \texttt{qgp} has the following calling sequence:

```fortran
subroutine qgp(n,x,w,i(ierr,mc,finl,finr,endl,endr,xfer,wfer)
dimension x(n),w(n),endl(mc),endr(mc),xfer(*),wfer(*)
logical finl,finr
```

On entry,

- \(n\) is the number of terms in the Fejér quadrature rule
- \(i\) indexes the interval \([a_i, b_i]\) for which the quadrature rule is desired; an interval that extends to \(-\infty\) has to be indexed by 1, one that extends to \(+\infty\) by \(mc\)
- \(mc\) is the number of component intervals; type integer
- \(finl\) is a logical variable to be set .true. if the extreme left interval is finite, and .false. otherwise
- \(finr\) is a logical variable to be set .true. if the extreme right interval is finite, and .false. otherwise
- \(endl\) is an array of dimension \(mc\) containing the left endpoints of the component intervals; if the first of these extends to \(-\infty\), \(endl(1)\) is not being used by the routine
- \(endr\) is an array of dimension \(mc\) containing the right endpoints of the component intervals; if the last of these extends to \(+\infty\), \(endr(mc)\) is not being used by the routine
xfer, wfer are working arrays holding the standard Fejér nodes and weights, respectively; they are dimensioned in the routine mcdis.

On return,

x, w are arrays of dimension n holding the abscissae and weights (4.18) of the discretized inner product for the ith component interval

ierr has the integer value 0.

The routine calls on the subroutines fejer, symtr and tr, which are appended to the routine qgp in §4 of the package. The first generates the Fejér quadrature rule, the others perform variable transformations. The user has to provide his own function routine wf(x, i) to calculate the weight function w_i(x) on the ith component interval.

Example 4.2. Chebyshev weight plus a constant: \( w_c(t) = (1 - t^2)^{-1/2} + c, c > 0, -1 < t < 1. \)

It would be difficult, here, to find a single quadrature rule for discretizing the inner product and obtain fast convergence. However, using in (4.9) \( m = 2, [a_1, b_1] = [a_2, b_2] = [-1, 1], \) and \( w_1(t) = (1 - t^2)^{-1/2}, w_2(t) = c \) in (4.11), and taking for Q1 the Gauss-Chebyshev, and for Q2 the Gauss-Legendre n-point rule (the latter multiplied by c), yields convergence to \( \alpha_k(w_c), \beta_k(w_c), k = 0, 1, \ldots, n - 1, \) in one iteration (provided \( \delta \) is set equal to 2)! Actually, we need \( N_0 = n + 1, \) in order to test for convergence; cf. (4.15). The driver test4 implements this technique and calculates the first \( n = 80 \) beta-coefficients to a relative accuracy of \( 5000 \times \varepsilon^8 \) for \( c = 1, 10, 100. \) (All \( \alpha_k \) are zero.) Attached to the driver is the quadrature routine qchle used in this example. It, in turn, calls for the Gauss quadrature routine gauss, to be described later in §6. Anticipating convergence after one iteration, we put \( ncapm = 81. \)

The weight function of Example 4.2 provides a continuous link between the Chebyshev polynomials \( (c = 0) \) and the Legendre polynomials \( (c = \infty); \) the recursion coefficients \( \beta_k(w_c) \) indeed converge (except for \( k = 0 \)) to those of the Legendre polynomials, as \( c \to \infty. \)

Selected results of test4 (where irout in mcdis can be arbitrary) are shown in Table 4.2. The output variable kount is 1 in each case, confirming convergence after one iteration. The coefficients \( \beta_0(w_c) \) are easily seen to be

\[ \begin{align*}
\text{Example 4.2. Chebyshev weight plus a constant: } w_c(t) &= (1 - t^2)^{-1/2} + c, \quad c > 0, -1 < t < 1. \\
\text{It would be difficult, here, to find a single quadrature rule for discretizing} \\
\text{the inner product and obtain fast convergence. However, using in (4.9) } \nonumber \\
m = 2, [a_1, b_1] = [a_2, b_2] = [-1, 1], \quad \text{and } w_1(t) = (1 - t^2)^{-1/2}, \; w_2(t) = c \nonumber \\
\text{in (4.11), and taking for Q1 the Gauss-Chebyshev, and for Q2 the Gauss-Legendre n-point rule (the latter multiplied by c), yields convergence to } \nonumber \\
\alpha_k(w_c), \beta_k(w_c), \; k = 0, 1, \ldots, n - 1, \; \text{in one iteration (provided } \delta \text{ is set equal to 2)! Actually, we need } \nonumber \\
N_0 = n + 1, \; \text{in order to test for convergence; cf. (4.15). The driver test4 implements this technique and calculates the first } \nonumber \\
n = 80 \beta\text{-coefficients to a relative accuracy of } 5000 \times \varepsilon^8 \; \text{for } c = 1, 10, 100. \; (\text{All } \alpha_k \text{ are zero.}) \text{ Attached to the driver is the quadrature routine qchle used in this example. It, in turn, calls for the Gauss quadrature routine gauss, to be described later in §6. Anticipating convergence after one iteration, we put } ncapm = 81. \nonumber \\
The weight function of Example 4.2 provides a continuous link between the Chebyshev polynomials \( (c = 0) \) and the Legendre polynomials \( (c = \infty); \) the recursion coefficients \( \beta_k(w_c) \) indeed converge (except for \( k = 0 \)) to those of the Legendre polynomials, as \( c \to \infty. \)

Selected results of test4 (where irout in mcdis can be arbitrary) are shown in Table 4.2. The output variable kount is 1 in each case, confirming convergence after one iteration. The coefficients \( \beta_0(w_c) \) are easily seen to be} \nonumber 
\end{align*} \]
\[ \pi + 2c. \]

| \( k \) | \( \beta_k(w^1) \) | \( \beta_k(w^{10}) \) | \( \beta_k(w^{100}) \) |
|-------|----------------|----------------|----------------|
| 0     | 5.141592654   | 23.14159265    | 203.1415927    |
| 1     | .4351692451   | .3559108398    | .3359108398    |
| 5     | .2510395775   | .2504824840    | .2505324193    |
| 12    | .2500610870   | .2500682357    | .2501336338    |
| 25    | .2500060034   | .2500082010    | .2500326887    |
| 51    | .2500001724   | .2500021136    | .2500127264    |
| 79    | .2500001724   | .2500021136    | .2500127264    |

**TABLE 4.2.** Selected recursion coefficients \( \beta_k(w^c) \) for \( c = 1, 10, 100 \)

**Example 4.3.** Jacobi weight with one mass point at the left endpoint:
\[ w^{(\alpha,\beta)}(x ; y) = [\mu_0^{(\alpha,\beta)}]^{-1}(1-x)^{\alpha}(1+x)^{\beta} + y \delta(x+1) \text{ on } (-1,1), \mu_0^{(\alpha,\beta)} = 2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)/\Gamma(\alpha+\beta+2), \alpha > -1, \beta > -1, y > 0. \]

The recursion coefficients \( \alpha_k, \beta_k \) are known explicitly (see [6, Eqs. (6.23), (3.5)]) and can be expressed, with some effort, in terms of the recursion coefficients \( \alpha_J^k, \beta_J^k \) for the Jacobi weight \( w^{(\alpha,\beta)}(\cdot) = w^{(\alpha,\beta)}(\cdot ; 0) \). The formulae are:

\[
\alpha_0 = \frac{\alpha_J^0 - y}{1 + y}, \quad \beta_0 = \beta_J^0 + y, \\
\alpha_k = \alpha_J^k + \frac{2k(\alpha+k)}{(\alpha+\beta+2k)(\alpha+\beta+2k+1)}(c_k - 1) + \frac{2(\beta+k+1)(\alpha+\beta+k+1)}{(\alpha+\beta+2k+1)(\alpha+\beta+2k+2)} \left( \frac{1}{c_k} - 1 \right), \\
\beta_k = \frac{c_k}{c_k - 1} \beta_J^k, \quad k = 1, 2, 3, \ldots, \tag{4.19}
\]

where

\[
c_0 = 1 + y, \quad c_k = \frac{1 + \frac{(\beta+k+1)(\alpha+\beta+k+1)}{k(\alpha+k)}yd_k}{1 + yd_k}, \quad k = 1, 2, \ldots, \tag{4.20}
\]

\(^1\) In [6], the interval is taken to be [0,2], rather than [-1,1]. There is a typographical error in the first formula of (6.23), which should have the numerator \( 2\beta + 2 \) instead of \( 2\beta + 1 \).
and

\[ d_1 = 1, \]
\[ d_k = \frac{(\beta + k)(\alpha + \beta + k)}{(\alpha + k - 1)(k - 1)} d_{k-1}, \quad k = 2, 3, \ldots. \quad (4.21) \]

Again, it is straightforward with \texttt{mcdis} to get exact results (modulo rounding) after one iteration, by using the Gauss-Jacobi quadrature rule (see \texttt{gauss} in §6) to discretize the continuous part of the measure. The driver \texttt{test5} generates in this manner the first \( n = 40 \) recursion coefficients \( \alpha_k, \beta_k, k = 0, 1, \ldots, n-1 \), to a relative accuracy of \( 5000 \times \varepsilon^8 \), for \( y = \frac{1}{2}, 1, 2, 4, 8 \). For each \( \alpha = -0.8(0.2)1 \) and \( \beta = -0.8(0.2)1 \), it computes the maximum relative errors (absolute error, if \( \alpha_k \approx 0 \)) of the \( \alpha_k, \beta_k \) by comparing them with the exact coefficients. These have been computed in double precision by a straightforward implementation of the formulae (4.19)–(4.21).

As expected, the output of \texttt{test5} reveals convergence after one iteration, the variable \texttt{kount} having consistently the value 1. The maximum relative error in the \( \alpha_k \) is found to generally lie between \( 2 \times 10^{-8} \) and \( 3 \times 10^{-12} \), the one in the \( \beta_k \) between \( 7.5 \times 10^{-12} \) and \( 8 \times 10^{-12} \); they are attained for \( k \) at or near 39. The discrepancy between the errors in the \( \alpha_k \) and those in the \( \beta_k \) is due to the \( \alpha_k \) being considerably smaller than the \( \beta_k \), by 3–4 orders of magnitude. Replacing the routine \texttt{sti} in \texttt{mcdis} by \texttt{lancz} yields very much the same error picture.

It is interesting to note that the addition of a second mass point at the other endpoint makes an analytic determination of the recursion coefficients intractable (cf. [6, p. 713]). Numerically, however, it makes no difference whether there are two or more mass points, and whether they are located inside, or outside, or on the boundary of the support interval. It was observed, however, that if at least one mass point is located outside the interval \([-1,1]\), the procedure \texttt{sti} used in \texttt{mcdis} becomes severely unstable\footnote{This has also been observed in the similar Example 4.8 of [19], but was incorrectly attributed to a phenomenon of ill-conditioning. Indeed, the statement made at the end of Example 4.8 can now be retracted: stable methods do exist, namely the method embodied by the routine \texttt{mcdis} in combination with \texttt{lancz}.} and must be replaced by \texttt{lancz}.

\textbf{Example 4.4.} Logistic density function: \( w(x) = e^{-x}/(1 + e^{-x})^2 \) on \( (-\infty, \infty) \).
In this example we illustrate a slight variation of the discretization procedure (4.9)–(4.13), which ends up with a discrete inner product of the same type as in (4.13) (and thus implementable by the routine mcdis) but derived in a somewhat different manner. The idea is to integrate functions with respect to the density \( w \) by splitting the integral into two parts, one from \(-\infty\) to 0, the other from 0 to \( \infty \), changing variables in the first part, and thus obtaining

\[
\int_{-\infty}^{\infty} f(t)w(t)dt = \int_{0}^{\infty} f(-t) \frac{e^{-t}}{(1 + e^{-t})^2} dt + \int_{0}^{\infty} f(t) \frac{e^{-t}}{(1 + e^{-t})^2} dt. \tag{4.22}
\]

Since \((1 + e^{-t})^{-2}\) quickly tends to 1 as \( t \to \infty \), a natural discretization of both integrals is provided by the Gauss-Laguerre quadrature rule applied to the product \( f(\pm t) \cdot (1 + e^{-t})^{-2} \). This amounts to taking, in (4.13), \( m = 2 \) and

\[
x_{r,1} = -x^L_r, \; x_{r,2} = x^L_r, \quad w_{r,1} = w_{r,2} = \frac{w^L_r}{(1 + e^{-x^L_r})^2}, \quad r = 1, 2, \ldots, N,
\]

where \( x^L_r, w^L_r \) are the Gauss-Laguerre \( N \)-point quadrature nodes and weights.

The driver test6 incorporates this discretization into the routines mcdis and dmcdis, runs them for \( n = 40 \) with error tolerances \( 5000 \times \varepsilon^a \) and \( 1000 \times \varepsilon^d \), respectively, and prints the absolute errors in the \( \alpha \)'s (\( \alpha_k = 0 \), in theory) and the relative errors in the \( \beta \)'s. (We used the default value \( \delta = 1 \).) Also printed are the number of iterations \#it (= kount) in (4.15) and the corresponding final value \( N^f_0 \) (= ncap). In single precision, we found \#it = 1, \( N^f_0 = 81 \), and in double precision, \#it = 5, \( N^f_0 = 281 \). Both routines returned with the error flags equal to 0, indicating a normal course

| \( k \) | \( \beta_k \) | \( \text{err } \alpha_k \) | \( \text{err } \beta_k \) |
|-------|-------------|-----------------|-----------------|
| 0     | 1.000000000000000000000000000000000 | 4.572(-13) | 1.918(-13) |
| 1     | 3.28968133696452872944830 | 1.682(-13) | 5.641(-13) |
| 6     | 89.44760352315950188817832 | 2.187(-12) | 2.190(-12) |
| 15    | 555.7827839879296775066697 | 1.732(-13) | 2.915(-12) |
| 26    | 1668.58022268668421827788 | 3.772(-12) | 4.112(-12) |
| 39    | 3753.5340251948983877223544 | 2.482(-11) | 4.533(-12) |

TABLE 4.3. Selected output from test6
of events. A few selected double-precision values of the coefficients $\beta_k$ along with absolute errors in the $\alpha$’s and relative errors in the $\beta$’s are shown in Table 4.3. The results are essentially the same no matter whether sti or lancz is used in mcdis. The maximum errors observed are $2.482 \times 10^{-11}$ for the $\alpha$’s, and $4.939 \times 10^{-12}$ for the $\beta$’s, which are well within the single-precision tolerance $\varepsilon = 5000 \times \varepsilon^s$.

On computers with limited exponent range, convergence difficulties may arise, both with sti and lancz, owing to underflow in many of the Laguerre quadrature weights. This seems to perturb the problem significantly enough to prevent the discretization procedure from converging.

Example 4.5. Half-range Hermite measure: $w(x) = e^{-x^2}$ on $(0, \infty)$.

This is an example of a measure for which there do not seem to exist natural discretizations other than those based on composite quadrature rules. Therefore, we applied our general-purpose routine qgp (and its double-precision companion dqgp), using, after some experimentation, the partition $[0, \infty] = [0, 3] \cup [3, 6] \cup [6, 9] \cup [9, \infty]$. The driver test7 implements this, with $n = 40$ and an error tolerance $50 \times \varepsilon^s$ in single precision, and $1000 \times \varepsilon^d$ in double precision.

The single-precision routine mcdis (using the default value $\delta = 1$) converged after one iteration, returning $\text{ncap} = 81$, whereas the double-precision

| $k$ | $\alpha_k$ | $\text{err } \alpha_k$ | $\beta_k$ | $\text{err } \beta_k$ |
|-----|------------|-------------------------|-----------|-------------------------|
| 0   | 0.5641895835477562869480795 | \text{1.096(–13)} | 0.8862269254527580136490837 | \text{3.180(–13)} |
| 1   | \text{0.9884253928468002854870634} | \text{1.514(–13)} | 0.1816901138162093284622325 | \text{7.741(–14)} |
| 6   | \text{2.080620336400833224817622} | \text{1.328(–13)} | \text{1.00234785101101042224538} | \text{5.801(–14)} |
| 15  | \text{3.214270636071128227448914} | \text{2.402(–14)} | \text{2.500927917133702669954321} | \text{8.186(–14)} |
| 26  | \text{4.203048578872001952660277} | \text{1.415(–13)} | \text{4.333867901229950443604430} | \text{7.878(–14)} |
| 39  | \text{5.13153286894296519319692} | \text{6.712(–13)} | \text{6.500356237707132938035155} | \text{1.820(–14)} |

TABLE 4.4. Selected output from test7
routine `dmcdis` took four iterations to converge, and returned `ncapd = 201`. Selected results (where `err α_k` and `err β_k` both denote relative errors) are shown in Table 4.4. The maximum error `err α_k` occurred at `k = 10`, and had the value $1.038 \times 10^{-12}$, whereas `max_k err β_k = 3.180 \times 10^{-13}` is attained at `k = 0`. The latter is within the error tolerance $\varepsilon$, the former only slightly larger. Comparison of the double-precision results with Table I on the microfiche supplement to [12] revealed agreement to all 20 decimal digits given there, for all `k` in the range $0 \leq k \leq 19$. Interestingly, the routine `sti` in `mcdis` did consistently better than `lancz` on the `β`’s, by a factor as large as 235 (for `k = 33`), and is comparable with `lancz` (sometimes better, sometimes worse) on the `α`’s.

Without composition, i.e., using `mc=1` in `mcdis`, it takes 8 iterations ($N_0^f = 521$) in single precision, and 10 iterations ($N_0^f = 761$) in double precision, to satisfy the much weaker error tolerances $\varepsilon = \frac{1}{2} \times 10^{-6}$ and $\varepsilon^d = \frac{1}{2} \times 10^{-12}$, respectively. All single-precision results, however, turn out to be accurate to about 12 decimal places. (This is because of the relatively large final increment $\Delta_8 = 2n = 80$ in $N_0$ (cf. (4.16)) that forces convergence.)

4.4. Discretized modified Chebyshev algorithm. The whole apparatus of discretization (cf. (4.9)–(4.14)) can also be employed in connection with the modified Chebyshev algorithm (cf. §3), if one discretizes modified moments rather than inner products. Thus, one approximates (cf. (4.14), (4.16))

$$\nu_k(d\lambda) \approx \nu_k(d\lambda_{mN_0^{[s]}+p}) \quad (4.23)$$

and iterates the modified Chebyshev algorithm with `s = 0, 1, 2, ...` until the convergence criterion (4.15) is satisfied. (It would be unwise to test convergence on the modified moments, for reasons explained in [19, §2.5].) This is implemented in the routine `mccheb`, whose calling sequence is

```
mcheb(n,ncapm,mc,mp,xp,yp,quad,eps,iq,idelta,finl,finr,endl,endl,xfer,wxfer,a,b,fnu,alp,a,bncap,s,be,x,w,xm,wm,ss0,s1,s2)
```

Its input and output parameters have the same meaning as in the routine `mcdis`. In addition, the arrays `a, b` of dimension $2 \times n-1$ are to be supplied with the recursion coefficients $a(k) = a_{k-1}, b(k) = b_{k-1}, k = 1, 2, ..., 2 \times n-1$, defining the modified moments. The arrays `be,x,w,xm,wm,ss0,s1,s2`
are used for working space. The double-precision version of the routine has the name \texttt{dmcheb}.

The discretized modified Chebyshev algorithm must be expected to behave similarly as its close relative, the modified Chebyshev algorithm. In particular, if the latter suffers from ill-conditioning, so does the former.

Example 4.6. Example 3.1, revisited.

We recompute the $n = 40$ first recursion coefficients $\alpha_k, \beta_k$ of Example 3.1 to an accuracy of $100 \times \epsilon^s$ in single precision, using the routine \texttt{mccheb} instead of the routine \texttt{cheb}. For the discretization of the modified moments we employed the Gauss-Chebyshev quadrature rule:

$$\int_{-1}^{1} f(t)(1 - \omega^2 t^2)^{-1/2}(1 - t^2)^{-1/2} dt \approx \frac{\pi}{N} \sum_{r=1}^{N} f(x_r)(1 - \omega^2 x_r^2)^{-1/2}, \quad (4.24)$$

where $x_r = \cos((2r - 1)\pi/2N)$ are the Chebyshev points. This is accomplished by the driver \texttt{test8}. The results of this test (shown in the package) agree to all 10 decimal places with those of \texttt{test1}. The routine \texttt{mccheb} converged in one iteration, with \texttt{ncap} = 81, for $\omega^2 = .1, .3, .5, .7, .9$, in 4 iterations, with \texttt{ncap} = 201, for $\omega^2 = .99$, and in 8 iterations, with \texttt{ncap} = 521, for $\omega^2 = .999$. A double-precision version of \texttt{test8} was also run with $\epsilon = 1.2 \times 10^{-20}$ (not shown in the package) and produced correct results to 20 decimals in one iteration (\texttt{ncap} = 81) for $\omega^2 = .1, .3, .5, .7$, in 3 iterations (\texttt{ncap} = 161) for $\omega^2 = .9$, in 6 iterations (\texttt{ncap} = 361) for $\omega^2 = .99$, and in 11 iterations (\texttt{ncap} = 921) for $\omega^2 = .999$.

5. MODIFICATION ALGORITHMS

Given a positive measure $d\lambda(t)$ supported on the real line, and two polynomials $u(t) = \pm \Pi_{\rho=1}^{r}(t - u_{\rho}), v(t) = \Pi_{\sigma=1}^{s}(t - v_{\sigma})$ whose ratio is finite on the support of $d\lambda$, we may ask for the recursion coefficients $\hat{\alpha}_k = \alpha_k(d\hat{\lambda}), \hat{\beta}_k = \beta_k(d\hat{\lambda})$ of the modified measure

$$d\hat{\lambda}(t) = \frac{u(t)}{v(t)} d\lambda(t), \quad t \in \text{supp}(d\lambda), \quad (5.1)$$

assuming known the recursion coefficients $\alpha_k = \alpha_k(d\lambda), \beta_k = \beta_k(d\lambda)$ of the given measure. Methods that accomplish the passage from the $\alpha$’s and $\beta$’s to the $\hat{\alpha}$’s and $\hat{\beta}$’s will be called modification algorithms. The simplest case
\( s = 0 \) (i.e., \( v(t) \equiv 1 \)) and \( u \) positive on \( \text{supp}(d\lambda) \) has already been considered by Christoffel [7], who represented the polynomial \( u(\cdot)\pi_k(\cdot) = u(\cdot)\pi_k (\cdot ; d\lambda) \) in determinantal form in terms of the polynomials \( \pi_j(\cdot) = \pi_j(\cdot ; d\lambda), j = k, k+1, \ldots, k+r \). This is now known as Christoffel’s theorem. Christoffel, however, did not address the problem of how to generate the new coefficients \( \hat{\alpha}_k, \hat{\beta}_k \) in terms of the old ones. For the more general modification (5.1), Christoffel’s theorem has been generalized by Uvarov [48,49]. The coefficient problem stated above, in this general case, has been treated in [20], and previously by Galant [13] in the special case \( v(t) \equiv 1 \).

The passage from \( d\lambda \) to \( d\hat{\lambda} \) can be carried out in a sequence of elementary steps involving real linear factors \( t - x \), or real quadratic factors \( (t - x)^2 + y^2 \), either in \( u(t) \) or in \( v(t) \). The corresponding elementary steps in the passage from the \( \alpha \)'s and \( \beta \)'s to the \( \hat{\alpha} \)'s and \( \hat{\beta} \)'s can all be performed by means of certain nonlinear recurrences. Some of these, however, when divisions of the measure \( d\lambda \) are involved, are liable to instabilities. An alternative method can then be used, which appeals to the modified Chebyshev algorithm supplied with appropriate modified moments. These latter are of independent interest and find application, e.g., in evaluating the kernel in the contour integral representation of the Gauss quadrature remainder term.

5.1 Nonlinear recurrence algorithms. The routine that carries out the elementary modification steps is called \texttt{chri} and has the calling sequence

\[
\texttt{chri(n,i,opt,a,b,x,y,hr,hi,alpha,beta,ierr)}.
\]

On entry,

\begin{itemize}
  \item \texttt{n} is the number of recursion coefficients desired; type integer
\end{itemize}
iopt is an integer identifying the type of modification as follows:

1: \(d\hat{\lambda}(t) = (t - x)d\lambda(t)\)
2: \(d\hat{\lambda}(t) = ((t - x)^2 + y^2)d\lambda(t), \ y > 0\)
3: \(d\hat{\lambda} = (t^2 + y^2)d\lambda(t)\) with \(d\lambda(t)\) and \(\text{supp}(d\lambda)\) assumed symmetric with respect to the origin and \(y > 0\)
4: \(d\hat{\lambda}(t) = d\lambda(t)/(t - x)\)
5: \(d\hat{\lambda}(t) = d\lambda(t)/((t - x)^2 + y^2), \ y > 0\)
6: \(d\hat{\lambda}(t) = d\lambda(t)/(t^2 + y^2)\) with \(d\lambda(t)\) and \(\text{supp}(d\lambda)\) assumed symmetric with respect to the origin and \(y > 0\)
7: \(d\hat{\lambda}(t) = (t - x)^2d\lambda(t)\)

a, b are arrays of dimension n+1 holding the recursion coefficients \(a(k) = \alpha_k(d\lambda), \ b(k) = \beta_k(d\lambda), \ k = 1, 2, \ldots, n+1\)

x, y are real parameters defining the linear and quadratic factors (or divisors) of \(d\lambda\)

hr, hi are the real and imaginary part, respectively, of \(\int_{\mathbb{R}} d\lambda(t)/(z - t)\), where \(z = x + iy\); the parameter hr is used only if \(\text{iopt} = 4\) or 5, the parameter hi only if \(\text{iopt} = 5\) or 6.

On return,

alpha, beta are arrays of dimension n containing the desired recursion coefficients \(\alpha_k(d\hat{\lambda}), \ \beta_k(d\hat{\lambda}), \ k = 1, 2, \ldots, n\)

ierr is an error flag, equal to 0 on normal return, equal to 1 if \(n \leq 1\) (the routine assumes that \(n\) is larger than or equal to 2), and equal to 2 if the integer \(\text{iopt}\) is inadmissible.

It should be noted that in the cases \(\text{iopt} = 1\) and \(\text{iopt} = 4\), the modified measure \(d\hat{\lambda}\) is positive [negative] definite if \(x\) is to the left [right] of the support of \(d\lambda\), but indefinite otherwise. Nevertheless, it is permissible to
have $x$ inside the support of $d\lambda$ (or inside its convex hull), provided the resulting measure $d\hat{\lambda}$ is still quasi-definite (cf. [20]).

For $i_{\text{opt}} = 1, 2, \ldots, 6$, the methods used in $\text{chri}$ are straightforward implementations of the nonlinear recurrence algorithms respectively in Eq. (3.7), (4.7), (4.8), (5.1), (5.8) and (5.9) of [20]. The only minor modification required concerns $\hat{\beta}_0 = \beta_0(d\lambda)$. In [20], this constant was taken to be 0, whereas here it is defined to be $\hat{\beta}_0 = \int_{\mathbb{R}} d\hat{\lambda}(t)$. Thus, for example, if $i_{\text{opt}} = 2$,

$$
\hat{\beta}_0 = \int_{\mathbb{R}} ((t - x)^2 + y^2)d\lambda(t) = \int_{\mathbb{R}} ((t - \alpha_0 + \alpha_0 - x)^2 + y^2)d\lambda(t)
$$

$$
= \int_{\mathbb{R}} ((t - \alpha_0)^2 + (\alpha_0 - x)^2 + y^2)d\lambda(t),
$$

since $\int_{\mathbb{R}} (t - \alpha_0)d\lambda(t) = \int_{\mathbb{R}} \pi_1(t)d\lambda(t) = 0$. Furthermore (cf. (4.1)),

$$
\int_{\mathbb{R}} (t - \alpha_0)^2d\lambda(t) = \beta_0\beta_1,
$$

so that the formula to be used for $\hat{\beta}_0$ is

$$
\hat{\beta}_0 = \beta_0(\beta_1 + (\alpha_0 - x)^2 + y^2) \quad (i_{\text{opt}} = 2).
$$

Similar calculations need to be made in the other cases.

The case $i_{\text{opt}} = 7$ incorporates a $QR$ step with shift $x$, following Kautsky and Golub [42], and uses an adaptation of the algorithm in [51, Eq. (67.11), p. 567] to carry out the $QR$ step. The most significant modification made is the replacement of the test $c \neq 0$ by $|c| > \varepsilon$, where $\varepsilon = 5 \times \varepsilon^s$ is a quantity close to, but slightly larger than, the machine precision. (Without this modification, the algorithm could fail.)

The methods used in $\text{chri}$ are believed to be quite stable when the measure $d\lambda$ is modified multiplicatively ($i_{\text{opt}} = 1, 2, 3$ and 7). When divisions are involved ($i_{\text{opt}} = 4, 5$ and 6), however, the algorithms rapidly become unstable as the point $z = x + iy \in \mathbb{C}$ moves away from the support interval of $d\lambda$. (The reason for this instability is not well understood at present; see, however, Galant [14].) For such cases there is an alternative routine, $\text{gchri}$ (see §5.2), that can be used.
Example 5.1. Checking the results (for $\sigma = \frac{1}{2}$) of test2.

We apply chri (and the corresponding double precision routine dchri) with iopt = 1, $x = 0$, to $d\lambda_\sigma(t) = t^\sigma \ln (1/t)$ on (0,1) with $\sigma = -\frac{1}{2}$, to recompute the results of test2 for $\sigma = \frac{1}{2}$. This can be done by a minor modification, named test9, of test2. Selected results from it, showing the relative discrepancies between the single-precision values $\alpha_k$, $\beta_k$, resp. double-precision values $\alpha_k^d$, $\beta_k^d$, computed by the modified Chebyshev algorithm and the modification algorithm, are shown in Table 5.1 (cf. Table 3.3). The maximum errors occur consistently for the last value of $k$ ($= 98$).

| $\sigma$ | $k$ | err $\alpha_k$ | err $\beta_k$ | err $\alpha_k^d$ | err $\beta_k^d$ |
|----------|-----|----------------|----------------|-----------------|----------------|
| .5       | 0   | 7.895(-14)     | 4.796(-14)     | 2.805(-28)      | 7.952(-28)     |
|          | 12  | 3.280(-12)     | 6.195(-12)     | 8.958(-26)      | 1.731(-25)     |
|          | 24  | 7.648(-12)     | 1.478(-11)     | 2.065(-25)      | 3.985(-25)     |
|          | 48  | 2.076(-11)     | 4.088(-11)     | 5.683(-25)      | 1.121(-24)     |
|          | 98  | 6.042(-11)     | 1.201(-10)     | 1.504(-24)      | 2.987(-24)     |

Table 5.1. Comparison between modified Chebyshev algorithm and modification algorithm in Example 5.1 (cf. Example 3.2)

Example 5.2. Induced orthogonal polynomials.

Given an orthogonal polynomial $\pi_m(\cdot; d\lambda)$ of fixed degree $m \geq 1$, the sequence of orthogonal polynomials $\tilde{\pi}_{k,m}(\cdot) = \pi_k(\cdot; \pi_m^2 d\lambda)$, $k = 0, 1, 2, \ldots$, has been termed induced orthogonal polynomials in [33]. Since their measure $d\tilde{\lambda}_m$ modifies the measure $d\lambda$ by a product of quadratic factors,

$$d\tilde{\lambda}_m(t) = \prod_{\mu=1}^{m} (t-x_\mu)^2 \cdot d\lambda(t),$$

(5.2)

where $x_\mu$ are the zeros of $\pi_m$, we can apply the routine chri (with iopt=7) $m$ times to compute the $n$ recursion coefficients $\tilde{\alpha}_{k,m} = \alpha(k d\tilde{\lambda}_m)$, $\tilde{\beta}_{k,m} = \beta_k(d\tilde{\lambda}_m)$, $k = 0, 1, \ldots, n-1$, from the $n + m$ coefficients $\alpha_k = \alpha_k(d\lambda)$, $\beta_k = \beta_k(d\lambda)$, $k = 0, 1, \ldots, n-1+m$. The subroutines indp and dindp in the driver test10 implement this procedure in single resp. double precision. The driver itself uses them to compute the first $n = 20$ recursion coefficients of the
induced Legendre polynomials with \( m = 0, 1, \ldots, 11 \). It also computes the maximum absolute errors in the \( \hat{\alpha}'s (\hat{\alpha}_{k,m} = 0 \) for all \( m \) ) and the maximum relative errors in the \( \hat{\beta}'s \) by comparing single-precision with double-precision results.

An excerpt of the output of test10 is shown in Table 5.2. It already suggests a high degree of stability of the procedure employed by \texttt{indp}. This is reinforced by an additional test (not shown in the package) generating \( n = 320 \) recursion coefficients \( \hat{\alpha}_{k,m}, \hat{\beta}_{k,m}, 0 \leq k \leq 319 \), for \( m = 40, 80, 160, 320 \) and \( d\lambda \) being the Legendre, the 1st-kind Chebyshev, the Laguerre, and the Hermite measure. Table 5.3 shows the maximum absolute error in the \( \hat{\alpha}_{k,m}, 0 \leq k \leq 319 \) (relative error in the Laguerre case), and the maximum relative error in the \( \hat{\beta}_{k,m}, 0 \leq k \leq 319 \).

| \( k \) | \( m = 0, \hat{\beta}_{k,m} \) | \( m = 2, \hat{\beta}_{k,m} \) | \( m = 6, \hat{\beta}_{k,m} \) | \( m = 11, \hat{\beta}_{k,m} \) |
|-------|-----------------|-----------------|-----------------|-----------------|
| 0     | 2.0000000000    | 0.1777777777    | 0.0007380787    | 0.0000007329    |
| 1     | 0.3333333333    | 0.5238095238    | 0.5030303030    | 0.5009523810    |
| 6     | 0.2517482517    | 0.1650550769    | 0.2947959861    | 0.2509913424    |
| 12    | 0.2504347826    | 0.2467060415    | 0.2521022519    | 0.1111727541    |
| 19    | 0.2501732502    | 0.2214990335    | 0.2274818789    | 0.2509466619    |

| \( \text{err} \hat{\alpha} \) | \( 0.000(0) \) | \( 1.350(-13) \) | \( 9.450(-13) \) | \( 1.357(-12) \) |
| \( \text{err} \hat{\beta} \) | \( 1.737(-14) \) | \( 2.032(-13) \) | \( 2.055(-12) \) | \( 3.748(-12) \) |

**TABLE 5.2.** Induced Legendre polynomials

| \( m \) | \( \text{Legendre} \) | \( \text{Chebyshev} \) | \( \text{Laguerre} \) | \( \text{Hermite} \) |
|-----|-----------------|-----------------|-----------------|-----------------|
| 40  | 3.4(-11) 1.5(-10) 1.9(-9) 7.9(-9) 3.0(-10) 6.0(-10) 1.8(-9) 2.7(-10) |
| 80  | 1.4(-10) 5.4(-10) 2.1(-9) 2.2(-9) 5.8(-10) 9.2(-10) 7.9(-9) 9.2(-10) |
| 160 | 1.5(-9)  5.1(-9)  9.5(-9) 1.1(-8)  7.8(-10)  1.4(-9)  1.1(-8)  6.8(-10) |
| 320 | 3.3(-9)  2.1(-8)  9.6(-9)  2.1(-8)  3.9(-9)  7.2(-9)  2.5(-8)  1.1(-9) |

**TABLE 5.3.** Accuracy of the recursion coefficients for some classical induced polynomials
5.2. Methods based on the modified Chebyshev algorithm. As was noted earlier, the procedure chri becomes unstable for modified measures involving division of $d\lambda(t)$ by $t - x$ or $(t - x)^2 + y^2$ as $z = x + iy \in \mathbb{C}$ moves away from the “support interval” of $d\lambda$, i.e., from the smallest interval containing the support of $d\lambda$. We now develop a procedure that works better the further away $z$ is from that interval.

The idea is to use modified moments of $d\hat{\lambda}$ relative to the polynomials $\pi_k(\cdot; d\lambda)$ to generate the desired recursion coefficients $\hat{\alpha}_k, \hat{\beta}_k$ via the modified Chebyshev algorithm (cf. §3). The modified moments in question are

$$\nu_k = \nu_k(x; d\lambda) = \int_{\mathbb{R}} \frac{\pi_k(t; d\lambda)}{t - x} d\lambda(t), \quad k = 0, 1, 2, \ldots, \quad (5.3)$$

for linear divisors, and

$$\nu_k = \nu_k(x, y; d\lambda) = \int_{\mathbb{R}} \frac{\pi_k(t; d\lambda)}{(t - x)^2 + y^2} d\lambda(t), \quad k = 0, 1, 2, \ldots, \quad (5.4)$$

for quadratic divisors. Both can be expressed in terms of the integrals

$$\rho_k = \rho_k(z; d\lambda) = \int_{\mathbb{R}} \frac{\pi_k(t; d\lambda)}{z - t} d\lambda(t), \quad z \in \mathbb{C}\setminus\text{supp}(d\lambda), \quad k = 0, 1, 2, \ldots, \quad (5.5)$$

the first by means of

$$\nu_k(x; d\lambda) = -\rho_k(z; d\lambda), \quad z = x, \quad (5.6)$$

the others by means of

$$\nu_k(x, y; d\lambda) = -\frac{\text{Im} \rho_k(z; d\lambda)}{\text{Im} z}, \quad z = x + iy. \quad (5.7)$$

The point to observe is that $\{\rho_k(z; d\lambda)\}$ is a minimal solution of the basic recurrence relation (1.3) for the orthogonal polynomials $\{\pi_k(\cdot; d\lambda)\}$ (cf. [18]). The quantities $\rho_k(z; d\lambda), k = 0, 1, \ldots, n$, therefore can be computed accurately by a backward recurrence algorithm ([18, §5]) which, for $\nu > n$, produces approximations $\rho_k^{[\nu]}(z; d\lambda)$ converging to $\rho_k(z; d\lambda)$ when $\nu \to \infty$, for any fixed $k$,

$$\rho_k^{[\nu]}(z; d\lambda) \to \rho_k(z; d\lambda), \quad \nu \to \infty. \quad (5.8)$$

The procedure is implemented in the routine

\begin{verbatim}
  knum(n,nu0,numax,z,eps,a,b,rho,nu,ierr,rold),
\end{verbatim}
which computes $\rho_k(z; d\lambda)$ for $k = 0, 1, \ldots, n$ to a relative precision $\text{eps}$. The results are stored as $\text{rho}(k) = \rho_{k-1}(z; d\lambda)$, $k = 1, 2, \ldots, n+1$, in the complex array $\text{rho}$ of dimension $n+1$. The user has to provide a starting index $\nu_0 = \nu_0 > n$ for the backward recursion, which the routine then increments by units of 5 until convergence to within $\text{eps}$ is achieved. If the requested accuracy $\text{eps}$ cannot be realized for some $\nu \leq \text{numax}$, the routine exits with $\text{ierr} = \text{numax}$. Likewise, if $\nu_0 > \text{numax}$, the routine exits immediately, with the error flag $\text{ierr}$ set equal to $\nu_0$. Otherwise, the value of $\nu$ for which convergence is obtained is returned as output variable $\nu$. The arrays $a$, $b$ of dimension $\text{numax}$ are to hold the recursion coefficients $a(k) = \alpha_{k-1}(d\lambda)$, $b(k) = \beta_{k-1}(d\lambda)$, $k = 1, 2, \ldots, \text{numax}$, for the given measure $d\lambda$. The complex array $\text{rold}$ of dimension $n+1$ is used for working space. In the interest of rapid convergence, the routine should be provided with a realistic estimate of $\nu_0$. For classical measures, such estimates are known (cf. [18, §5]) and are implemented here by the function routines

$$
\text{nu0jac}(n, z, \text{eps}), \text{nu0lag}(n, z, \alpha, \text{eps}), \text{nu0her}(n, z, \text{eps}).
$$

The first is for Jacobi measures, the second for generalized Laguerre measures with parameter $\alpha_1 = \alpha > -1$, and the last for the Hermite measure. Note that $\nu_0$ for Jacobi measures does not depend on the weight parameters $\alpha$, $\beta$, in contrast to $\nu_0$ for the generalized Laguerre measure.

The name $\text{knum}$ comes from the fact that $\rho_n(z; d\lambda)$ in (5.5) is the numerator in the kernel

$$
K_n(z; d\lambda) = \frac{\rho_n(z; d\lambda)}{\pi_n(z; d\lambda)} (5.9)
$$

of the remainder term of the $n$-point Gaussian quadrature rule for analytic functions (cf., e.g., [36]). For the sequence of kernels $K_0$, $K_1$, $\ldots$, $K_n$ we have the following routine:

```
subroutine kern(n,nu0,numax,z,eps,a,b,ker,nu,ierr,rold)
complex z,ker,rold,p0,p,pml
dimension a(numax),b(numax),ker(*),rold(*)
call knum(n,nu0,numax,z,eps,a,b,ker,nu,ierr,rold)
if(ierr.ne.0) return
p0=(0.,0.)
p=(1.,0.)
do 10 k=1,n
```

41
pm1=p0
p0=p
p=(z-a(k))*p0-b(k)*pm1
ker(k+1)=ker(k+1)/p
10 continue
return
end

The meaning of the input and output parameters is the same as in knum. The double precision version of the routine is named dkern.

All the ingredients are now in place to describe the workings of gchri, the alternative routine to chri when the latter is unstable. First, the routine knum is used to produce the first $2n$ modified moments $\nu_k(x;d\lambda)$ resp. $\nu_k(x,y;d\lambda)$, $k = 0,1,\ldots,2n-1$. These are then supplied to the routine cheb along with the recursion coefficients $\alpha_k(d\lambda)$, $\beta_k(d\lambda)$ (needed anyhow for the computation of the $\nu_k$), which produces the desired coefficients $\alpha_k(d\hat{\lambda})$, $\beta_k(d\hat{\lambda})$, $k = 0,1,\ldots,n-1$. The routine has the calling sequence

\[
gchri(n,iopt,nu0,numax,eps,a,b,x,y,alpha,beta,\nu,ierr,ierrc,fnu,rho,rold,s,s0,s1,s2).
\]

On entry,

- $n$ is the number of recursion coefficients desired; type integer
- $iopt$ is an integer identifying the type of modification as follows:
  1: $d\hat{\lambda}(t) = d\lambda(t)/(t-x)$, where $x$ is assumed outside the smallest interval containing supp$(d\lambda)$
  2: $d\lambda(t) = d\lambda(t)/((t-x)^2 + y^2)$, $y > 0$
- $nu0$ is an integer $\nu_0 \geq 2n$ estimating the starting index for the backward recursion to compute the modified moments; if no other choices are available, take $nu0 = 3 \times n$
numax is an integer used to terminate backward recursion in case of nonconvergence; a conservative choice is \texttt{numax}=500

eps is a relative error tolerance; type real

\texttt{a,b} are arrays of dimension \texttt{numax} to be supplied with the recursion coefficients \texttt{a}(k) = \alpha_{k-1}(d\lambda), \texttt{b}(k) = \beta_{k-1}(d\lambda), \ k = 1,2,\ldots, \texttt{numax}

\texttt{x,y} are real parameters defining the linear and quadratic divisors of \(d\lambda\).

On return,

\texttt{alpha,beta} are arrays of dimension \texttt{n} containing the desired recursion coefficients \texttt{alpha}(k) = \hat{\alpha}_{k-1}
\texttt{beta}(k) = \hat{\beta}_{k-1}, \ k = 1,2,\ldots, \texttt{n}

\texttt{nu} is the index \(\nu\) for which the error tolerance \texttt{eps} is satisfied for the first time; if it is never satisfied, \texttt{nu} will have the value \texttt{numax}

\texttt{ierr} is an error flag, where
\begin{itemize}
  \item \texttt{ierr} = 0 on normal return
  \item \texttt{ierr} = 1 if iopt is inadmissible
  \item \texttt{ierr} = \texttt{nu0} if \texttt{nu0} > \texttt{numax}
  \item \texttt{ierr} = \texttt{numax} if the backward recurrence algorithm does not converge.
  \item \texttt{ierr} = -1 if \texttt{n} is not in range
\end{itemize}

\texttt{ierrc} is an error flag inherited from the routine \texttt{cheb}.

The real arrays \texttt{fnu,s,s0,s1,s2} are working space, all of dimension \(2 \times \texttt{n}\) except \texttt{s}, which has dimension \texttt{n}. The complex arrays \texttt{rho, rold} are also working space, both of dimension \(2n\). The routine calls on the subroutines \texttt{knum} and \texttt{cheb}. The double-precision version of \texttt{gchri} has the name \texttt{dgchri}.
Since the routine *gchri* is based on the modified Chebyshev algorithm, it shares with the latter its proneness to ill-conditioning, particularly in cases of measures supported on an infinite interval. On finitely supported measures, however, it can be quite effective, as will be seen in the next example.

Example 5.3. The performance of *chri* and *gchri*.

To illustrate the severe limitations of the routine *chri* in situations where divisions of the measure $d\lambda$ are involved, and at the same time to document the effectiveness of *gchri*, we ran both routines with $n = 40$ for Jacobi measures $d\lambda(\alpha,\beta)$ with parameters $\alpha, \beta = -0.8(.4)8$, $\beta \geq \alpha$. This is done in *test11*.

The routine *test11* first tests division by $t - x$, where $x = -1.001, -1.01, -1.04, -1.07, -1.1$. Both routines *chri* and *gchri* are run in single and double precision, the latter with $\varepsilon = 10 \times 10^6$ and $\varepsilon = 100 \times 10^4$, respectively. The double-precision results are used to determine the absolute errors in the $\hat{\alpha}$'s and the relative errors in the $\hat{\beta}$'s for each routine. The required coefficients $\alpha_k, \beta_k, 0 \leq k \leq \nu_{\text{max}} - 1$ ($\nu_{\text{max}} = 500$ for single precision, and 800 for double precision) are supplied by *recur* and *drecur* with $\text{ipoly} = 6$. The routine *nu0jac* is used to provide the starting recurrence index $\nu_0$ resp. $\nu_0^d$. In Tables 5.4 and 5.5, relating respectively to linear and quadratic divisors, we give only the results for the Legendre measure ($\alpha = \beta = 0$). The first line in each 3-line block of Table 5.4 shows $x, \nu_0, \nu_0^d$ and the maximum (over $k, 0 \leq k \leq 39$) errors in the $\hat{\alpha}_k$ and $\hat{\beta}_k$ for *gchri*, followed by the analogous information (excepting the $\nu_0$'s) for *chri*. The recurrence index $\nu$ yielding convergence was found (not shown in *test11*) to be $\nu = \nu_0 + 5$ and $\nu^d = \nu_0^d + 5$, without exception.
TABLE 5.4. Performance of \( gchri \) and \( chri \) for elementary divisors \( t - x \) of the Legendre measure \( d\lambda(t) \)

It can be seen from the leading lines in Table 5.4 that \( chri \) rapidly loses accuracy as \( x \) moves away from the interval \([-1,1]\), all single-precision accuracy being gone by the time \( x \) reaches \(-1.1\). Similar, if not more rapid, erosion of accuracy is observed for the other parameter values of \( \alpha, \beta \). The next two lines in each 3-line block show “reconstruction errors”, i.e., the maximum errors in the \( \alpha \)'s and \( \beta \)'s if the \( \hat{\alpha} \)'s and \( \hat{\beta} \)'s produced by \( gchri \), \( chri \) and \( dgchri \), \( dchri \) are fed back to the routines \( chri \) and \( dchri \) with \( iopt = 1 \) to recover the original recursion coefficients in single and double precision. The first of these two lines shows the errors in reconstructing these coefficients from the output of \( gchri \) (resp. \( dgchri \)), the second from the output of \( chri \) (resp. \( dchri \)). Rather remarkably, the coefficients are recovered to essentially full accuracy, even when the input coefficients (produced
by \texttt{chri} and \texttt{dchri}) are very inaccurate! This is certainly a phenomenon that deserves further study. It can also be seen from Table 5.4 (and the more complete results in §1 of the package) that \texttt{gchri} consistently produces accurate results, some slight deterioration occurring only very close to \(x = -1\), where the routine has to work harder.

The second half of \texttt{test11} tests division by \((t - x)^2 + y^2\), where \(z = x + iy\) is taken along the upper half of the ellipse

\[
\mathcal{E}_\rho = \{z \in \mathbb{C} : z = \frac{1}{2} \left( \rho e^{i\vartheta} + \frac{1}{\rho} e^{-i\vartheta} \right), 0 \leq \vartheta \leq 2\pi \}, \rho > 1, \quad (5.10)
\]

which has foci \(\pm 1\) and sum of the semiaxes equal to \(\rho\). (These ellipses are contours of constant \(\nu_0\) for Jacobi measures.) We generated information analogous to the one in Table 5.4, for \(\rho = 1.05, 1.1625, 1.275, 1.3875, 1.5\), except that all quantities are averaged over 19 equally spaced points on \(\mathcal{E}_\rho\) corresponding to \(\vartheta = j\pi/20, j = 1, 2, \ldots, 19\). Selected results (bars indicate averaging), again for the Legendre case, are shown in Table 5.5. They reveal a behavior very similar to the one in Table 5.4 for linear divisors.

| \(\rho\) | \(\hat{\nu}_0\) | \(\hat{\nu}_0^d\) | \(\bar{\alpha}\) | \(\bar{\beta}\) | \(\bar{\alpha}\) | \(\bar{\beta}\) |
|---|---|---|---|---|---|---|
| 1.05 | 390 | 700 | 7.879(-13) | 1.440(-12) | 7.685(-14) | 1.556(-13) |
| | | | 2.024(-14) | 8.442(-14) | 3.016(-28) | 1.742(-27) |
| reconstruction | | | 7.814(-13) | 1.433(-12) | 1.768(-26) | 3.042(-26) |
| | | | 6.554(-14) | 1.279(-13) | 1.541(-27) | 3.061(-27) |
| errors | | | 2.295(-14) | 8.970(-14) | 3.579(-28) | 1.646(-27) |
| 1.275 | 142 | 204 | 6.252(-14) | 1.287(-13) | 4.562(-7) | 6.162(-7) |
| | | | 6.554(-14) | 1.279(-13) | 1.541(-27) | 3.061(-27) |
| | | | 2.295(-14) | 8.970(-14) | 3.579(-28) | 1.646(-27) |
| 1.5 | 117 | 154 | 3.991(-14) | 7.966(-14) | 4.906(-1) | 2.339(0) |
| | | | 4.207(-14) | 9.064(-14) | 6.932(-28) | 1.676(-27) |
| | | | 3.805(-14) | 8.971(-14) | 4.351(-28) | 1.744(-27) |

TABLE 5.5. Performance of \texttt{gchri} and \texttt{chri} for elementary divisors \((t - x)^2 + y^2\) of the Legendre measure \(d\lambda(t)\) with \(z = x + iy\) on \(\mathcal{E}_\rho\).
6. GAUSS-TYPE QUADRATURE RULES

One of the important uses of orthogonal polynomials is in the approximation of integrals involving a positive measure \(d\lambda\) by quadrature rules of maximum, or nearly maximum, algebraic degree of exactness. In this context, it is indispensable to know the recursion coefficients for the respective orthogonal polynomials \(\{\pi_k(\cdot;d\lambda)\}\), since they allow us to generate the desired quadrature rules accurately and effectively via eigenvalue techniques. The software developed in the previous sections thus finds here a vast area of application.

6.1. Gaussian quadrature. Given the (positive) measure \(d\lambda\) (having an infinite number of support points), there exists, for each \(n \in \mathbb{N}\), a quadrature rule

\[
\int_{\mathbb{R}} f(t)d\lambda(t) = \sum_{k=1}^{n} w_k f(x_k) + R_n(f)
\]

having algebraic degree of exactness \(2n - 1\), i.e., zero error, \(R_n(f) = 0\), whenever \(f\) is a polynomial of degree \(\leq 2n - 1\). The nodes \(x_k\) indeed are the zeros of the \(n\)th-degree orthogonal polynomial \(\pi_n(\cdot;d\lambda)\), and the weights \(w_k\), which are all positive, are also expressible in terms of the same orthogonal polynomials. Alternatively, and more importantly for computational purposes, the nodes \(x_k\) are the eigenvalues of the \(n\)th-order Jacobi matrix

\[
J_n(d\lambda) = 
\begin{pmatrix}
\alpha_0 & \sqrt{\beta_1} & 0 \\
\sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} \\
& \sqrt{\beta_2} & \ddots & \ddots \\
& & \ddots & \ddots \\
0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1}
\end{pmatrix},
\]

(6.2)

where \(\alpha_k = \alpha_k(d\lambda), \beta_k = \beta_k(d\lambda)\) are the recurrence coefficients for the (monic) orthogonal polynomials \(\{\pi_k(\cdot;d\lambda)\}\), and the weights \(w_k\) are expressible in terms of the associated eigenvectors. Specifically, if

\[
J_n(d\lambda)v_k = x_k v_k, \quad v_k^T v_k = 1, \quad k = 1, 2, \ldots, n,
\]

(6.3)

i.e., \(v_k\) is the normalized eigenvector of \(J_n(d\lambda)\) corresponding to the eigenvalue \(x_k\), then

\[
w_k = \beta_0 v_{k,1}^2, \quad k = 1, 2, \ldots, n,
\]

(6.4)
where $\beta_0 = \beta_0(d\lambda)$ is defined in (1.4) and $v_{k,1}$ is the first component of $v_k$ (cf. [40]). There are well-known and efficient algorithms, such as the $QR$ algorithm, to compute eigenvalues and (part of the) eigenvectors of symmetric tridiagonal matrices. These are used in the routine $\texttt{gauss}$, whose calling sequence is

$$\texttt{gauss}(n,\alpha,\beta,\epsilon,\text{zero},\text{weight},\text{ierr},e).$$

On entry,

- $n$ is the number of terms in the Gauss formula; type integer
- $\alpha,\beta$ are arrays of dimension $n$ assumed to hold the recursion coefficients $\alpha(k) = \alpha_{k-1}$, $\beta(k) = \beta_{k-1}$, $k = 1, 2, \ldots, n$
- $\epsilon$ is a relative error tolerance, for example, the machine precision.

On return,

- $\text{zero},\text{weight}$ are arrays of dimension $n$ containing the nodes (in increasing order) and the corresponding weights of the Gauss formula, $\text{zero}(k) = x_k$, $\text{weight}(k) = w_k$, $k = 1, 2, \ldots, n$
- $\text{ierr}$ is an error flag equal to 0 on normal return, equal to $i$ if the $QR$ algorithm does not converge within 30 iterations on evaluating the $i$th eigenvalue, equal to $-1$ if $n$ is not in range, and equal to $-2$ if one of the $\beta$’s is negative.

The array e of dimension n is used for working space. The double precision routine has the name $\texttt{dgauss}$.

We refrain here from giving numerical examples, since the use of the routine $\texttt{gauss}$, and the routines yet to be described, is straightforward.

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3This routine was kindly supplied to the author by Professor G.H. Golub.
Some use of \texttt{gauss} and \texttt{dgauss} has already been made in Examples 4.2, 4.3, 4.4 and 5.2.

6.2. Gauss-Radau quadrature. We now assume that \(d\lambda\) is a measure whose support is either bounded from below, or bounded from above, or both. Let, then, \(x_0\) be either the infimum or the supremum of supp \(d\lambda\), so long as it is finite. (Typically, if supp \(d\lambda = [-1, 1]\), then \(x_0\) could be either \(-1\) or \(+1\); if supp \(d\lambda = [0, \infty]\), then \(x_0\) would have to be 0; etc.). By Gauss-Radau quadrature we then mean a quadrature rule of maximum degree of exactness that contains among the nodes the point \(x_0\). It thus has the form

\[
\int_{\mathbb{R}} f(t) d\lambda(t) = w_0 f(x_0) + \sum_{k=1}^{n} w_k f(x_k) + R_n(f),
\]

and, as is well known, can be made to have degree of exactness \(2n\), i.e., \(R_n(f) = 0\) for all polynomials of degree \(\leq 2n\). Interestingly, all nodes \(x_0, x_1, \ldots, x_n\) and weights \(w_0, w_1, \ldots, w_n\) can again be interpreted in terms of eigenvalues and eigenvectors, exactly as in the case of Gaussian quadrature rules, but now relative to the matrix (cf. [39])

\[
J^*_n(d\lambda) = \begin{bmatrix}
\alpha_0 & \sqrt{\beta_1} & 0 \\
\sqrt{\beta_1} & \alpha_1 & \cdots \\
& \ddots & \ddots \\
& & \sqrt{\beta_{n-1}} & \alpha_{n-1} & \sqrt{\beta_n} \\
0 & & & \sqrt{\beta_n} & \alpha_n^*
\end{bmatrix} \in \mathbb{R}^{(n+1)\times(n+1)},
\]

where \(\alpha_k = \alpha_k(d\lambda)\) \((0 \leq k \leq n-1)\), \(\beta_k = \beta_k(d\lambda)\) \((1 \leq k \leq n)\) as before, but

\[
\alpha_n^* = \alpha^*_n(d\lambda) = x_0 - \beta_n \frac{\pi_{n-1}(x_0; d\lambda)}{\pi_n(x_0; d\lambda)}.
\]

Hence, we can use the routine \texttt{gauss} to generate the Gauss-Radau formula. This is done in the following subroutine.

```
subroutine radau(n, alpha, beta, end, zero, weight, ierr, e, a, b)
dimension alpha(*), beta(*), zero(*), weight(*), e(*), a(*), b(*)
c c The arrays alpha, beta, zero, weight, e, a, b are assumed to have
```
c dimension n+1.
c
epsma=r1mach(3)
c
c epsma is the machine single precision.
c
np1=n+1
do 10 k=1,np1
   a(k)=alpha(k)
   b(k)=beta(k)
10 continue
p0=0.
p1=1.
do 20 k=1,n
   pm1=p0
   p0=p1
   p1=(end-a(k))*p0-b(k)*pm1
20 continue
a(np1)=end-b(np1)*p0/p1
call gauss(np1,a,b,epsma,zero,weight,ierr,e)
return
end

The input variables are n, alpha, beta, end representing, respectively, n, two arrays of dimension n + 1 containing the \( \alpha_k(d\lambda) \), \( \beta_k(d\lambda) \), \( k = 0, 1, 2, \ldots, n \), and the “endpoint” \( x_0 \). The nodes (in increasing order) of the Gauss-Radau formula are returned in the array zero, the corresponding weights in the array weight. The arrays e, a, b are working space, and ierr an error flag inherited from the routine gauss. The double-precision routine has the name dradau.

We remark that \( x_0 \) could also be outside the support of \( d\lambda \), in which case the routine would generate a “Christoffel-type” quadrature rule.

6.3. Gauss-Lobatto quadrature. Assuming now the support of \( d\lambda \) bounded on either side, we let \( x_0 = \inf \text{ supp } (d\lambda) \) and \( x_{n+1} = \sup \text{ supp } (d\lambda) \) and consider a quadrature rule of the type

\[
\int_{\mathbb{R}} f(t)d\lambda(t) = w_0 f(x_0) + \sum_{k=1}^{n} w_k f(x_k) + w_{n+1} f(x_{n+1}) + R_n(f) \quad (6.8)
\]
having maximum degree of exactness $2n+1$. This is called the \textit{Gauss-Lobatto quadrature rule}. Its nodes $x_0, x_1, \ldots, x_{n+1}$ and weights $w_0, w_1, \ldots, w_{n+1}$ again admit the same spectral representation as in the case of Gauss and Gauss-Radau formulae, only this time the matrix in question has order $n+2$ and is given by (cf. [39])

\[
J^\ast_{n+2}(d\lambda) = \begin{bmatrix}
\alpha_0 & \sqrt{\beta_1} & 0 \\
\sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} \\
& \sqrt{\beta_2} & \ddots & \ddots \\
& & \ddots & \sqrt{\beta_n} \\
0 & & & \sqrt{\beta_n} & \alpha_n \\
& & & & \sqrt{\beta^\ast_{n+1}} \\
\end{bmatrix}.
\] (6.9)

Here, as before, $\alpha_k = \alpha_k(d\lambda) \ (0 \leq k \leq n)$, $\beta_k = \beta_k(d\lambda) \ (1 \leq k \leq n)$, and $\alpha^\ast_{n+1}, \beta^\ast_{n+1}$ are the unique solution of the linear $2 \times 2$ system

\[
\begin{bmatrix}
\pi_{n+1}(x_0; d\lambda) & \pi_{n}(x_0; d\lambda) \\
\pi_{n+1}(x_{n+1}; d\lambda) & \pi_{n}(x_{n+1}; d\lambda) \\
\end{bmatrix} \begin{bmatrix}
\alpha^\ast_{n+1} \\
\beta^\ast_{n+1} \\
\end{bmatrix} = \begin{bmatrix}
x_0\pi_{n+1}(x_0; d\lambda) \\
x_{n+1}\pi_{n+1}(x_{n+1}; d\lambda) \\
\end{bmatrix}.
\] (6.10)

Hence, we have the following routine for generating Gauss-Lobatto formulae:

```fortran
subroutine lob(n,alpha,beta,aleft,right,zero,weight,ierr,e,a,b)
dimension alpha(*),beta(*),zero(*),weight(*),e(*),a(*),b(*)
c The arrays alpha,beta,zero,weight,e,a,b are assumed to have
c dimension n+2.
c epsma=r1mach(3)
c epsma is the machine single precision.
c np1=n+1
np2=n+2
do 10 k=1,np2
   a(k)=alpha(k)
   b(k)=beta(k)
d 10 continue
```

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10 continue
   p0l=0.
   p0r=0.
   p1l=1.
   p1r=1.
   do 20 k=1,np1
      pm1l=p0l
      p0l=p1l
      pm1r=p0r
      p0r=p1r
      p1l=(aleft-a(k))*p0l-b(k)*pm1l
      p1r=(right-a(k))*p0r-b(k)*pm1r
   20 continue
   det=p1l*p0r-p1r*p0l
   a(np2)=(aleft*p1l*p0r-right*p1r*p0l)/det
   b(np2)=(right-aleft)*p1l*p1r/det
   call gauss(np2,a,b,epsma,zero,weight,ierr,e)
   return
end

The meaning of the input and output variables is as in the routine radau,
the variable aleft standing for $x_0$ and right for $x_{n+1}$. The double-precision
routine is named dlob.

A remark analogous to the one after the routine radau applies to the
routine lob.

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