ON SENSITIVITY OF GAUSS-CHRISTOFFEL QUADRATURE ESTIMATES*

DIANNE P. O'LEARY† AND ZDENĚK STRAKOŠ‡

Abstract. In this work, we investigate conditions under which Gauss-Christoffel quadrature estimates are insensitive under perturbation of the distribution function, deriving an error bound that depends on the perturbation and the function to be integrated. We show that for the Riemann-Stieltjes integral even a small perturbation of a discontinuous distribution function can cause large difference of Gauss-Christoffel quadrature estimates.

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1. Introduction. Suppose we have two distribution functions $\omega(x)$ and $\tilde{\omega}(x)$ which are close to each other, nondecreasing, and differentiable on the finite interval $[a, b]$, with $\omega'(x)$ and $\tilde{\omega}'(x)$ Riemann-integrable on $[a, b]$. We are interested in estimating the two integrals

$$I_\omega = \int_a^b f(x)\, d\omega(x) = \int_a^b f(x)\omega'(x)\, dx\,, \tag{1.1}$$

$$I_{\tilde{\omega}} = \int_a^b f(x)\, d\tilde{\omega}(x) = \int_a^b f(x)\tilde{\omega}'(x)\, dx\,. \tag{1.2}$$

Here we have used the fact that under our assumptions, the Riemann-Stieltjes integral with the distribution function $\omega(x)$ reduces to the weighted Riemann integral with the weight function $\omega'(x)$ [3, Sections 1.6.5 and 1.10]), and similarly for $\tilde{\omega}$.

If we use Gauss-Christoffel quadrature [8] [3, Section 2.7] to compute the estimates, then $\omega(x)$ and $\tilde{\omega}(x)$ induce different sequences of orthogonal polynomials. Therefore, the quadrature weights and nodes might be quite different from each other and in fact can be unstable under small perturbations to $\omega(x)$; see [8, pp. 121-125], [6, 5, 7]. Thus, although it is natural to expect that the Gauss-Christoffel quadrature estimates of the same degree will be close, it is not immediately clear that this is true. In this work we prove the result under certain conditions on distribution functions ω and $\tilde{\omega}$ and for sufficiently smooth functions f.

We formulate our problem in terms of Gauss-Christoffel quadrature of a Riemann-Stieltjes integral, even though the assumption on the distribution functions $\omega(x)$ and $\tilde{\omega}(x)$ given above reduces the problem to Gauss quadrature of the weighted Riemann integrals (1.1) and (1.2). We do this for two reasons, different in nature.

The bounds we establish for Gauss quadrature of the weighted Riemann integral can similarly be formulated and proved also for Gauss-Christoffel quadrature of a *general* Riemann-Stieltjes integral. For the latter case, however, the interpretation of the results is, particularly for discontinuous distribution functions, much more complicated due to some subtle properties of orthogonal polynomials. Therefore we consider it convenient to work with the Riemann-Stieltjes formulation (anticipating

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possible generalizations) under strong assumptions on the distribution function which make the situation more transparent. Subsequently we will comment on the general case.

Second, our interest in this problem originated in analysis of the conjugate gradient method for solving linear systems and of the Lanczos method for solving the symmetric eigenvalue problem. The close relationship of these methods of numerical linear algebra with Gauss-Christoffel quadrature of the Riemann-Stieltjes integral has been known since their introduction; see [14, § 14-18], [24, Chapter III]. In particular, the conjugate gradient method generates a sequence of approximations to the piecewise constant distribution function that has jumps at the eigenvalues of the linear operator equal in magnitude to the squared proportions of the initial residual along the corresponding eigenfunctions; see Section 4. Moreover, the size of the A-norm of the error at the kth step of the conjugate gradient method has a natural interpretation as the scaled remainder of the kth order Gauss-Christoffel quadrature approximation of the Riemann-Stieltjes integral.

This last result, published in [2], stimulated extensive work on estimating error norms in the conjugate gradient method [4, 9, 11, 10, 17, 18, 1]. The survey paper [22] compares different approaches and addresses the question of whether these estimates are numerically stable in the presence of rounding errors; see also [11]. This leads to a more general question of how to precisely explain the numerical behavior of the conjugate gradient method, and, in particular, how to model the delay of convergence caused by rounding errors. One algebraic model was introduced in [12, 13]; the description would simplify and also gain some elegance when formulated in the language of the Gauss-Christoffel quadrature of the Riemann-Stieltjes integral. As a part of such reformulation we need to resolve the question of *when the results of the model are insensitive with respect to small perturbations of the distribution function.* This question motivates our work and will be considered further in connection with the model of numerical behavior of the conjugate gradient method in [20].

With this application in mind we therefore need to consider both piecewise constant distribution functions with finite or infinite points of increase, and continuous and differentiable distribution functions with Riemann-integrable derivatives. We present the main tool for our analysis in Section 2 in a general way, and then complete the discussion in Section 3 focusing for clarity of exposition on the latter case. Then we comment in Section 4 on other more complicated cases, illustrating them numerically, and concluding with Section 5.

2. The main tool: a formula for interpolation error. The main tool in our analysis is a slight generalization of a result found in the classic textbook of Isaacson and Keller [15] in Theorem 3 (p. 329) and in the second line of the identity (6) on p. 334. Although the textbook is standard, the result is not, absent even in the very thorough and detailed survey by Gautschi [8]. The standard approach to Gauss quadrature of the Riemann integral and to Gauss-Christoffel quadrature of the Riemann-Stieltjes integral is based on Hermite interpolation and is attributed to Markov; see, e.g. [8, p. 82]. What we need are results based on Lagrange interpolation, and oddly enough, we have found them only in the textbook of Isaacson and Keller [15], the book by Milne-Thomson [19, pp. 173–177] referenced there, and a book by Lanczos [16, Chapter VI, §10]. The idea of using the Lagrange interpolation polynomial $\mathcal{L}_k(x)$ of degree $k-1$ which coincides with $f(x)$ at the points $\lambda_1, \ldots, \lambda_k$ was also used (with $f(x)$ a polynomial of degree at most $2k-1$) in the proof of Theorem 3.4.1 in [23, p. 46]. The use of Lagrange interpolation rather than Hermite is essential to our work – it allows us in the following theorem to retain k free parameters in the remainder term for the kth order quadrature. The proof follows the ideas from [15, pp. 329-330, 334]. We include it here for completeness, and for the subsequent presentation of an interesting consequence of the interpolatory principle.

THEOREM 2.1. *Consider a nondecreasing function $\omega(x)$ on a finite interval $[a, b]$. Let $p_k(x) = (x - \lambda_1) \dots (x - \lambda_k)$ be the kth monic orthogonal polynomial with respect to the inner product defined by the Riemann-Stieltjes integral on the interval $[a, b]$ with the distribution function $\omega(x)$. Choose k distinct points $\mu_1, \dots, \mu_k$ in $[a, b]$ different from the points $\lambda_1, \dots, \lambda_k$. Let*

$$I_\omega = \int_a^b f(x)\, d\omega(x) \,, \tag{2.1}$$

where f' is continuous on $[a, b]$, and let I_ω^k be the approximation to I_ω obtained from the k-point Gauss-Christoffel quadrature rule. Then the error of this approximation is given by

$$E_\omega^k(f) \equiv I_\omega - I_\omega^k = \int_a^b p_k(x)(x - \mu_1) \dots (x - \mu_k) f[\lambda_1, \dots, \lambda_k, \mu_1, \dots, \mu_k, x]\, d\omega(x)$$

where $f[\lambda_1, \dots, \lambda_k, \mu_1, \dots, \mu_k, x]$ is the $(2k)$th divided difference of the function $f(x)$ with respect to the nodes $\lambda_1, \dots, \lambda_k, \mu_1, \dots, \mu_k, x$.

Proof. Let $\mathcal{L}_{2k-1}(x)$ be the Lagrange interpolation polynomial of degree $2k-1$ for the function $f(x)$, with $f(\lambda_j) = \mathcal{L}_{2k-1}(\lambda_j)$, $f(\mu_j) = \mathcal{L}_{2k-1}(\mu_j)$, $j = 1, \dots, k$. Then $f(x)$ can be written as

$$f(x) = \mathcal{L}_{2k-1}(x) + \mathcal{R}_{2k-1}(x) \tag{2.2}$$

where the interpolation error is given by the formula

$$\mathcal{R}_{2k-1}(x) = p_k(x)(x - \mu_1) \dots (x - \mu_k) f[\lambda_1, \dots, \lambda_k, \mu_1, \dots, \mu_k, x] \,.$$

Then

$$\begin{aligned} E_\omega^k(f) = & \int_a^b \mathcal{L}_{2k-1}(x)\, d\omega(x) + \int_a^b \mathcal{R}_{2k-1}(x)\, d\omega(x) \\ & - \sum_{j=1}^k \omega_j \mathcal{L}_{2k-1}(\lambda_j) - \sum_{j=1}^k \omega_j \mathcal{R}_{2k-1}(\lambda_j) \end{aligned}$$

where λ_j, ω_j, $j = 1, \dots, k$ are the nodes and weights of the k-point Gauss-Christoffel quadrature rule. Because $\mathcal{L}_{2k-1}(x)$ has degree at most $2k - 1$, its Gauss-Christoffel quadrature is precise, so

$$\int_a^b \mathcal{L}_{2k-1}(x)\, d\omega(x) \;=\; \sum_{j=1}^k \omega_j \mathcal{L}_{2k-1}(\lambda_j) \,.$$

Moreover, the continuity of $f'(x)$ guarantees the finiteness of $\mathcal{R}_{2k-1}(\lambda_j)$, and, consequently, $\mathcal{R}_{2k-1}(\lambda_j) = 0$ for $j = 1, \dots, k$, by construction. Therefore,

$$E_\omega^k(f) = \int_a^b \mathcal{R}_{2k-1}(x)\, d\omega(x)$$

which completes the proof. □

If we set $\mu_1 = \lambda_1, \dots, \mu_k = \lambda_k$, then replacing the Lagrange interpolant by the Hermite interpolant gives (under the assumption f'' continuous in $[a,b]$) the formula (cf. [19, p. 175] and [15, p. 330]),

$$E_\omega^{(k)}(f) = \int_a^b p^2(x) f[\lambda_1, \dots, \lambda_k, \lambda_1, \dots, \lambda_k, x]\, d\omega(x)\,.$$

The proof of Theorem 2.1 relies on the fact that the k-point Gauss-Christoffel quadrature rule is interpolatory with the nodes of interpolation given by the roots of the corresponding kth orthogonal polynomial $p_k(x)$. Apart from the assumption that $\mu_1, \dots, \mu_k$ are k distinct points in $[a,b]$ different from the points $\lambda_1, \dots, \lambda_k$, the auxiliary nodes $\mu_1, \dots, \mu_k$ are arbitrary. It is easy to see that the proof will follow in the same way also if $\mathcal{L}_{2k-1}(x)$ is replaced by $\mathcal{L}_{k-1}(x)$, where $\mathcal{L}_{k-1}(x)$ denotes the Lagrange interpolation polynomial for $f(x)$ such that $\mathcal{L}_{k-1}(\lambda_j) = f(\lambda_j)$, $j = 1, \dots, k$. Similarly, we can instead replace $\mathcal{L}_{2k-1}(x)$ by $\mathcal{L}_{k+m-1}(x)$, the Lagrange interpolation polynomial for $f(x)$ such that $\mathcal{L}_{k+m-1}(\lambda_j) = f(\lambda_j)$, $j = 1, \dots, k$ and also $\mathcal{L}_{k+m-1}(\mu_j) = f(\mu_j)$, $j = 1, \dots, m$, $m \le k$. Summarizing, we get the following statement.

COROLLARY 2.2. *Let $p_k(x)$, $\lambda_1, \dots, \lambda_k$, and $\mu_1, \dots, \mu_k$ be as in Theorem 2.1, and assume that f' is continuous on $[a,b]$. Then*

$$\begin{aligned} E_\omega^{(k)}(f) &= \int_a^b p_k(x)(x-\mu_1)\dots(x-\mu_k) f[\lambda_1, \dots, \lambda_k, \mu_1, \dots, \mu_k, x]\, d\omega(x) \\ &= \int_a^b p_k(x) f[\lambda_1, \dots, \lambda_k, x]\, d\omega(x) \\ &= \int_a^b p_k(x)(x-\mu_1)\dots(x-\mu_m) f[\lambda_1, \dots, \lambda_k, \mu_1, \dots, \mu_m, x]\, d\omega(x)\,, \end{aligned}$$

where the last equality holds for any m between 1 and k. If f'' is continuous on $[a,b]$, then the statement holds for any distinct $\mu_1, \dots, \mu_k$, even if some of them coincide with some of the points λ_j.

Proof. It remains to comment on the case $\lambda_1 = \mu_1, \dots, \lambda_m = \mu_m, m \le k$. Under the assumed continuity conditions on f'', taking the limit $\mu_j \to \lambda_j$ for $j = 1, \dots, m$ in the divided difference finishes the proof. □

3. The main result: sensitivity of Gauss quadrature estimates of Riemann integrals. We state and prove our result for the weighted Riemann integral with nonnegative weight function that is (for simplicity) continuous on the finite interval $[a,b]$. The continuity assumption is not essential but simplifies the exposition.

THEOREM 3.1. *Let $w(x)$ and $\tilde{w}(x)$ be nonnegative and continuous functions on the finite interval $[a,b]$; let*

$$\omega(x) = \int_a^x w(t)\, dt,\ \tilde{\omega}(x) = \int_a^x \tilde{w}(t)\, dt, \quad x \in [a,b]$$

be the corresponding distribution functions. Consider the weighted Riemann integrals (1.1) and (1.2). Let $p_k(x) = (x-x_1)\dots(x-x_k)$ be the kth orthogonal polynomial with *respect to (1.1), and let $\tilde{p}_k(x) = (x - \tilde{x}_1)\dots(x - \tilde{x}_k)$ be the kth orthogonal polynomial with respect to (1.2). Denote by $\hat{p}_s(x) = (x - z_1)\dots(x - z_s)$ the least common multiple of the polynomials $p_k(x)$ and $\tilde{p}_k(x)$. If f' is continuous on $[a, b]$, then the difference between the approximation I^k_ω to I_ω and the approximation $I^k_{\tilde{\omega}}$ to $I_{\tilde{\omega}}$, obtained from the k-point Gauss quadrature rule, is bounded as*

$$
\begin{aligned}
|I^k_\omega - I^k_{\tilde{\omega}}| \le &\left| \int_a^b \hat{p}_s(x) f[z_1, \dots, z_s, x](w(x) - \tilde{w}(x))\, dx \right| \\
&+ \left| \int_a^b f(x)(w(x) - \tilde{w}(x))\, dx \right| . \qquad (3.1)
\end{aligned}
$$

Proof. Consider the difference between the two Gauss quadrature approximations:

$$
\begin{aligned}
|I^k_\omega - I^k_{\tilde{\omega}}| &= |I^k_\omega - I_\omega + I_{\tilde{\omega}} - I^k_{\tilde{\omega}} + I_\omega - I_{\tilde{\omega}}| \\
&\le |I^k_\omega - I_\omega + I_{\tilde{\omega}} - I^k_{\tilde{\omega}}| + |I_\omega - I_{\tilde{\omega}}| .
\end{aligned}
$$

Assume, for a moment, that the roots $\{x_i\}$ are distinct from the roots $\{\tilde{x}_i\}$. We apply Theorem 2.1 to the first term twice. For $I^k_\omega - I_\omega$, the points $\lambda_1, \dots, \lambda_k$ in Theorem 2.1 are the zeros of the polynomial $p_k(x)$, and we set the points $\mu_1, \dots, \mu_k$ to be the zeros of the polynomial $\tilde{p}_k(x)$. For $I_{\tilde{\omega}} - I^k_{\tilde{\omega}}$, the points $\lambda_1, \dots, \lambda_k$ are the zeros of $\tilde{p}_k(x)$, and we set the points $\mu_1, \dots, \mu_k$ to be the zeros of $p_k(x)$. The result is

$$
\begin{aligned}
|I^k_\omega - I_\omega + I_{\tilde{\omega}} - I^k_{\tilde{\omega}}| &= \Bigg| - \int_a^b p_k(x)\tilde{p}_k(x) f[x_1, \dots, x_k, \tilde{x}_1, \dots, \tilde{x}_k, x] w(x)\, dx \\
&\qquad + \int_a^b \tilde{p}_k(x) p_k(x) f[\tilde{x}_1, \dots, \tilde{x}_k, x_1, \dots, x_k, x] \tilde{w}(x)\, dx \Bigg| \\
&= \left| \int_a^b p_k(x)\tilde{p}_k(x) f[x_1, \dots, x_k, \tilde{x}_1, \dots, \tilde{x}_k, x](\tilde{w}(x) - w(x))\, dx \right|
\end{aligned}
$$

The second term is

$$
|I_\omega - I_{\tilde{\omega}}| = \left| \int_a^b f(x)(w(x) - \tilde{w}(x))\, dx \right| ,
$$

and adding these terms together yields the desired result.

Consider now the general case when $p_k(x)$ and $\tilde{p}_k(x)$ have $k - m$ common zeros, numbered so that $x_{m+1} = \tilde{x}_{m+1}, \dots, x_k = \tilde{x}_k$. Let $s = 2k - m$ and use the last equality of Corollary 2.2 twice. For $I^k_\omega - I_\omega$, set the points $\lambda_1, \dots, \lambda_k$ in the corollary to be the zeros of $p_k(x)$, and set the points $\mu_1, \dots, \mu_m$ to be the first m zeros $\tilde{x}_1, \dots, \tilde{x}_m$ of $\tilde{p}_k(x)$. For $I_{\tilde{\omega}} - I^k_{\tilde{\omega}}$, set the points $\lambda_1, \dots, \lambda_k$ to be the zeros of $\tilde{p}_k(x)$, and set the points $\mu_1, \dots, \mu_m$ to be the first m zeros $x_1, \dots, x_m$ of $p_k(x)$. The rest of the proof follows as above. □

As a consequence of this theorem we obtain, using the same notation, the following sufficient condition:

The Gauss quadrature estimates will be close if the absolute values of the integrands $|\hat{p}_s(x)f[z_1,\ldots,z_s,x](w(x)-\tilde{w}(x))|$ and $|f(x)(w(x)-\tilde{w}(x))|$ are small on $[a,b]$ except possibly on a union of subintervals, denoted J_1, with a small enough total length.

In order to get a simpler condition we consider subintervals on which $w(x)$ differs from $\tilde{w}(x)$, and denote their union by J_2. This leads to the following sufficient condition:

The Gauss quadrature estimates will be close if

$$\int_a^b |w(x)-\tilde{w}(x)|\,dx$$

is small and if $|f(x)|$ and $|\hat{p}_s(x)f[z_1,\ldots,z_s,x]|$ are small on J_2 where $w(x)$ differs from $\tilde{w}(x)$.

It seems, however, difficult to derive nontrivial general statements about the size of

$$\left|\int_a^b \hat{p}_s(x)f[z_1,\ldots,z_s,x](w(x)-\tilde{w}(x))\,dx\right|$$

or about the size of $|\hat{p}_s(x)f[z_1,\ldots,z_s,x]|$ on J_2.

In order to get an idea about the size of the difference $|I_\omega^k - I_{\tilde{\omega}}^k|$ and about the size of the individual terms in the bound (3.1), we present an example illustrating the behavior of quadrature estimates as the size of the perturbation function varies. Consider as an example the weight function

$$w(x) = c_0\sqrt{x-x^2}$$

on the interval $[0,1]$ where c_0 is a constant chosen so that

$$\int_0^1 w(x)\,dx = 1\,.$$

This is the weight function for the shifted Chebyshev polynomials of the second kind. We perturb $w(x)$ to form

$$\tilde{w} = (1-\alpha)\,w(x) + \alpha\,c_1(e^{-16x}-e^{-27x})$$

where c_1 is chosen so that

$$c_1\int_0^1 (e^{-16x}-e^{-27x})\,dx = 1\,.$$

We use Gauss quadrature to estimate the integrals

$$I_\omega \;=\; \int_0^1 \frac{1}{x+\delta}\,w(x)\,dx,\quad I_{\tilde{\omega}} \;=\; \int_0^1 \frac{1}{x+\delta}\,\tilde{w}(x)\,dx,$$

for various values of α. We choose $\delta = 0.1$ to avoid singularity of the integration function.

All experiments in this paper were performed using MATLAB on a computer with machine precision $\approx 10^{-16}$. In this section, the Gauss quadrature nodes and weights were determined from the explicitly generated sequences of orthogonal polynomials.

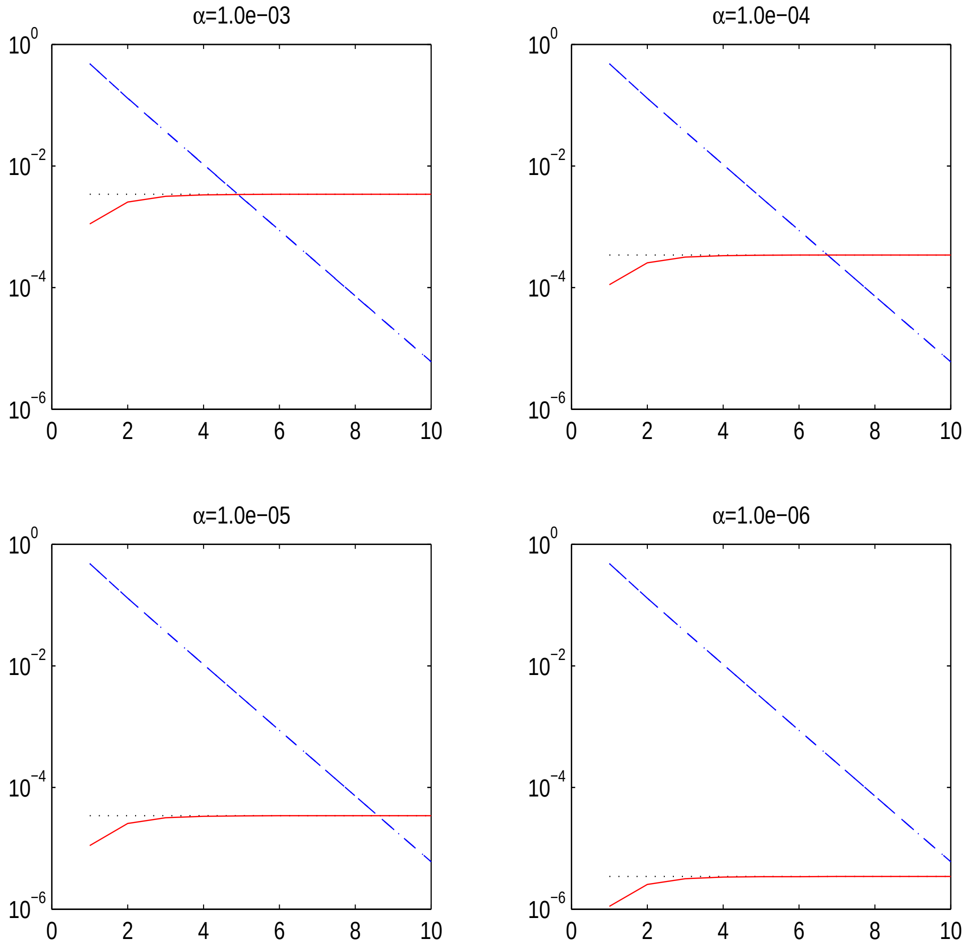

FIG. 3.1. *The error in the quadrature estimates for $w(x) = c_0\sqrt{x - x^2}$ and $\tilde{w}(x)$ (coinciding black dash-dotted line and blue dashed line), and the difference between the original and perturbed estimates (red solid line) as the perturbation parameter α varies for the continuous weight function. The dotted line measures the difference between the true integrals. The horizontal axis is k, the number of nodes in the quadrature estimate.*

The results, which are typical for smooth weight functions, are shown in Figure 3.1. Here we plot the error of the Gauss quadrature approximations $|I_\omega - I_\omega^k|$ (dash-dotted line), $|I_{\tilde{\omega}} - I_{\tilde{\omega}}^k|$ (dashed line) and the difference between the Gauss quadrature approximations $|I_{\tilde{\omega}}^k - I_\omega^k|$ (solid line). The dash-dotted line and the dashed line coincide. Note that for small k (the number of nodes), the errors of the two estimates are much larger than the difference between them. Eventually the two estimates must separate because they aim at approximating different integrals. The value of k at which the difference between the two estimates exceeds the error in each estimate decreases as α increases.

The level on which the two estimates separate is essentially determined by the difference between the original integrals (the second term in (3.1), plotted on Fig. 3.1 by dots). This is further illustrated in Figure 3.2 which shows, using $\alpha = 10^{-3}$, the behavior of the product $p(x)\tilde{p}(x)(w(x)-\tilde{w}(x))$ (the integrand in the first term in (3.1))

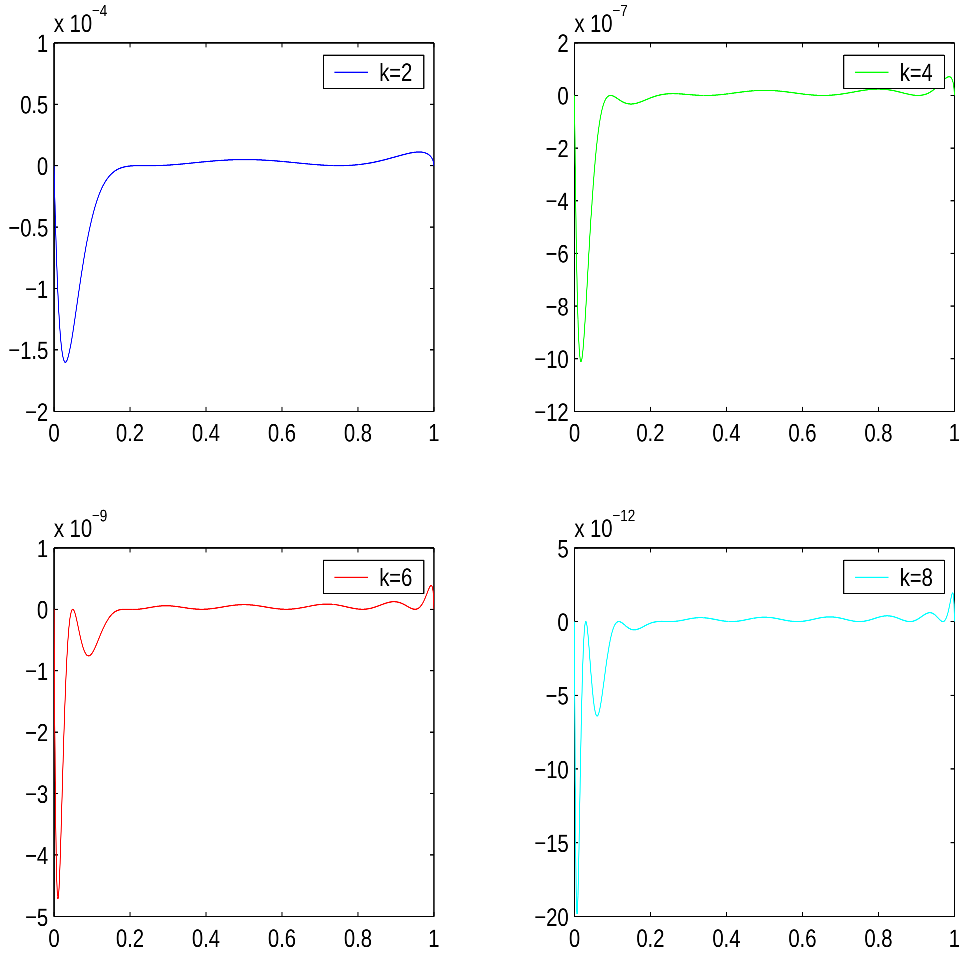

FIG. 3.2. *The product $p(x)\tilde{p}(x)(w(x) - \tilde{w}(x))$ as a function of x for the continuous weight function $w(x) = c_0\sqrt{x - x^2}$, with perturbation parameter $\alpha = 10^{-3}$ and different number of quadrature nodes k.*

as a function of x . Figure 3.3 shows differences between roots of the corresponding orthogonal polynomials. Clearly, the roots are for this example very stable – the maximal change is less then 10^{-4}.

As a second example, we took the highly oscillatory weight function

$$w(x) = 1 + \cos(10\pi x)$$

on the interval $[0, 1]$ and $\tilde{w}(x)$ determined as in the previous example. The results, shown in Figure 3.4 (the other figures analogous to Figures 3.2 and 3.3 are omitted), are very similar to the first example.

Based on experiments it seems that for weighted Riemann integrals with smooth weight functions, the second term in the bound (3.1) dominates the first one. We do not know whether this is true in general. At least it seems difficult to find a counterexample.

The following section will show that for the Gauss-Christoffel quadrature of

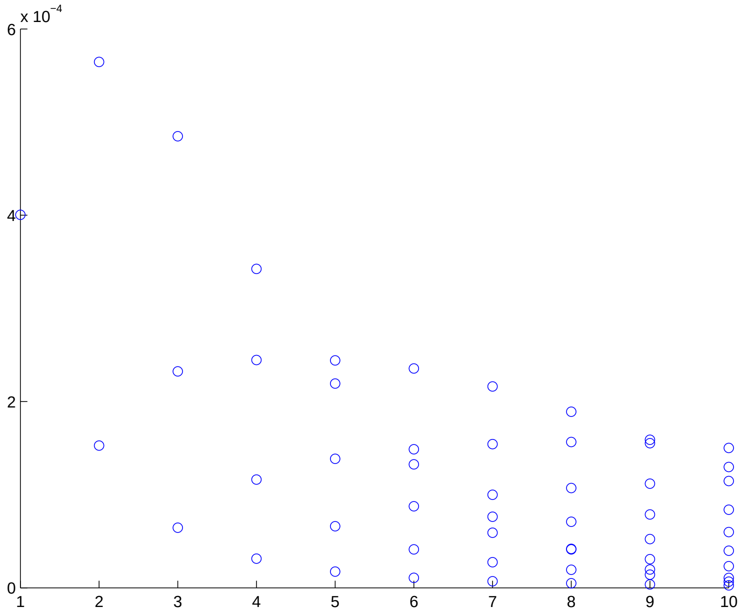

FIG. 3.3. *The change in the polynomial roots for the continuous weight function* $w(x) = c_0\sqrt{x - x^2}$ *with perturbation parameter* $\alpha = 10^{-3}$. *The horizontal axis is* k, *the number of nodes in the quadrature estimate. The vertical axis shows the differences between the sorted roots of the corresponding orthogonal polynomials.*

Riemann-Stieltjes integral with discontinuous distribution function the situation is quite different.

4. Sensitivity of Gauss-Christoffel quadrature estimates for Riemann-Stieltjes integrals. The Riemann-Stieltjes analog of the bound 3.1 is given by

$$\begin{aligned} |I_\omega^k - I_{\tilde\omega}^k| \le & \left| \int_a^b \hat p_s(x) f[z_1,\ldots,z_s,x]\, d\omega(x) \;-\; \int_a^b \hat p_s(x) f[z_1,\ldots,z_s,x]\, d\tilde\omega(x) \right| \\ & + \left| \int_a^b f(x)\, d\omega(x) \;-\; \int_a^b f(x)\, d\tilde\omega(x) \right| . \end{aligned} \tag{4.1}$$

Since (4.1) can be considered a simple consequence of Theorem 2.1 and Corollary 2.2, it is valid for *any functions* $\omega(x)$ and $\tilde\omega(x)$ that are nondecreasing on the interval $[a, b]$. This fact, however, does not immediately yield conditions under which the Gauss-Christoffel quadrature is insensitive to small perturbations to the distribution function. If, however, the first term is insignificant compared to the second term, then (4.1) implies that the difference between the Gauss-Christoffel quadrature approximations $|I_\omega^k - I_{\tilde\omega}^k|$ is bounded from above (with a small inaccuracy) by the size of the difference between the true integrals.

We will present examples of a discontinuous distribution function $\omega(x)$ with finite points of increase and demonstrate the principal difficulties one has to deal with when investigating sensitivity of the Gauss-Christoffel quadrature for a general Riemann-Stieltjes integral. We use a distribution function from [21] with points of increase

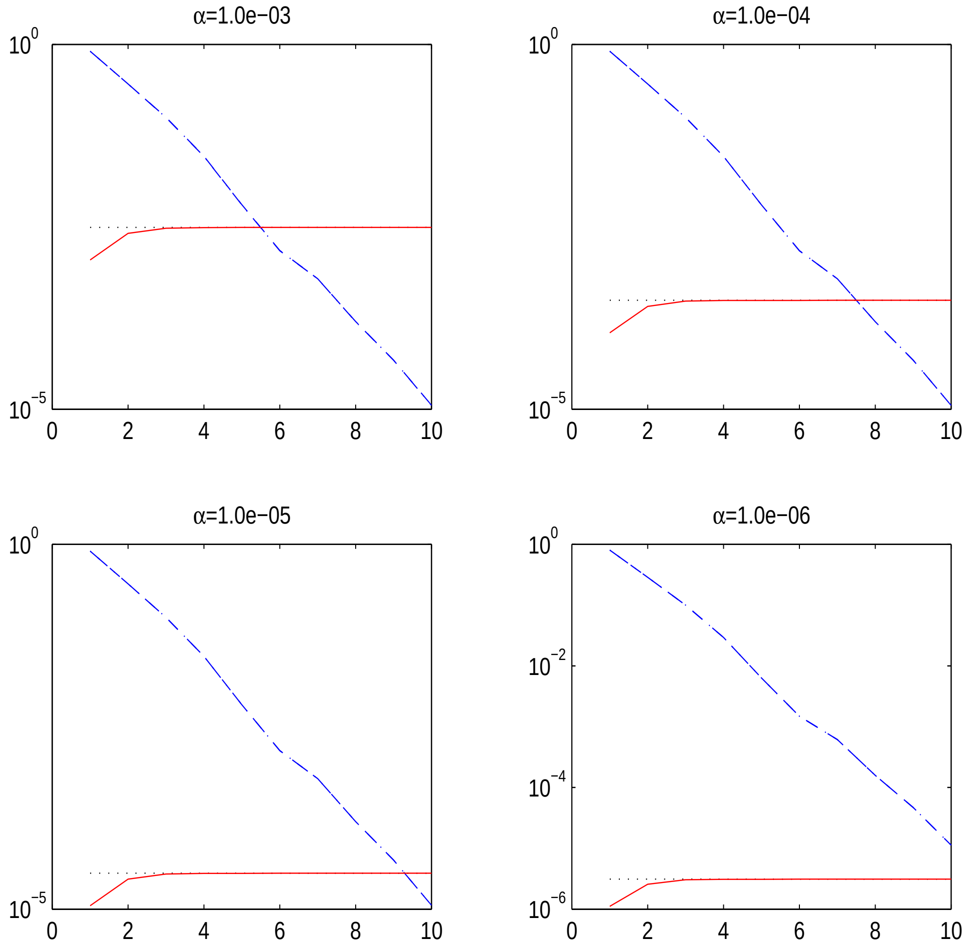

FIG. 3.4. *The error in the quadrature estimates for $w(x) = 1+\cos(10\pi x)$ and $\tilde{w}(x)$ (coinciding black dash-dotted line and blue dashed line), and the difference between the original and perturbed estimates (red solid line) as the perturbation parameter α varies for the continuous weight function. The dotted line measures the difference between the true integrals. The horizontal axis is k, the number of nodes in the quadrature estimate.*

$0 < \gamma_1 \equiv a < \cdots < \gamma_n \equiv b$, with

$$\gamma_i = \gamma_1 + \frac{i-1}{n-1}(\gamma_n - \gamma_1)\,\rho^{n-i}, \quad i = 2, \ldots, n-1,$$

where $\rho \in (0,1)$ is a properly chosen parameter. The size of the individual jumps δ_i, $i = 1, \ldots n-1$ is randomly generated using the MATLAB command *rand* and normalized so that $\omega(\gamma_n) = \sum_{i=1}^{n-1} \delta_i = 1$.

We construct the related distribution $\tilde{\omega}(x)$ to have two points of increase for each single point of increase of $\omega(x)$. Given a positive perturbation parameter ζ, where $\zeta \ll \gamma_1$ and $\zeta \ll \gamma_2 - \gamma_1$, we replace each point of increase γ_i of ω by two close points $\tilde{\gamma}_{2i-1} \equiv \gamma_i - \zeta$ and $\tilde{\gamma}_{2i} \equiv \gamma_i + \zeta$, and proportion the jumps $\tilde{\delta}_{2i-1}$ and $\tilde{\delta}_{2i}$ randomly (using again the MATLAB function *rand*) with scaling so that $\tilde{\delta}_{2i-1} + \tilde{\delta}_{2i} = \delta_i$. Clearly, for a small ζ the distribution functions ω and $\tilde{\omega}$ are close to each other.

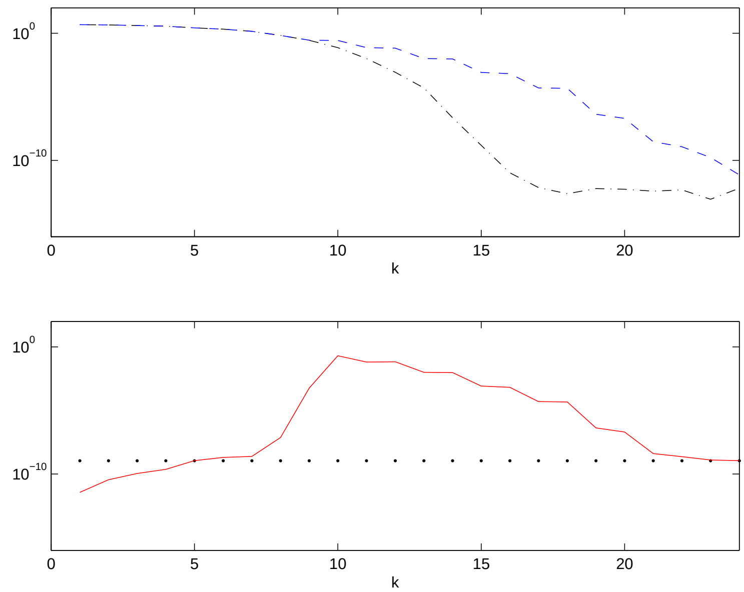

FIG. 4.1. *Sensitivity of the Gauss-Christoffel quadrature, $\zeta = 10^{-8}$. The error of the Gauss-Christoffel quadrature approximation for $f(x) = x^{-1}$ corresponding to the original distribution function ω (dash-dotted line) and to its "perturbation" $\tilde{\omega}$ with doubled points of increase (dashed line), the absolute value of their difference (solid line) and the difference between the approximated integrals (dots).*

Now consider a smooth function $f(x)$ so that the absolute value of the difference

$$\Delta = \left| \int_a^b f(x)\, d\omega(x) - \int_a^b f(x)\, d\tilde{\omega}(x) \right| \tag{4.2}$$

is small. We will demonstrate that the difference between the Gauss-Christoffel quadrature estimates (4.1) can for some values of k become much larger than Δ.

In our experiment we take $f(x) = x^{-1}$, $a = 0.1$, $b = 100$, $n = 24$. In Fig. 4.1 we plot the error of the Gauss-Christoffel quadrature approximations $|I_\omega - I_\omega^k|$ (dash-dotted line) and $|I_{\tilde{\omega}} - I_{\tilde{\omega}}^k|$ (dashed line), the difference between the Gauss-Christoffel approximations $|I_{\tilde{\omega}}^k - I_\omega^k|$ (solid line) and the difference between the approximated integrals $\Delta = |I_\omega - I_{\tilde{\omega}}|$ (dots). For this figure $\rho = 0.55$ and $\zeta = 10^{-8}$, which gives $\Delta \approx 10^{-7}$. We can see that for $k \geq 8$ the Gauss-Christoffel approximations of the integrals $I_{\tilde{\omega}}$ and I_ω start to differ very dramatically, and the size of that difference exceeds 10^{-1} for $k = 10$. After that it is approximately equal to $|I_{\tilde{\omega}} - I_{\tilde{\omega}}^k|$ until that quantity drops below the size of the difference between the approximated integrals.

This observed phenomenon can be explained from the link between the Gauss-Christoffel quadrature and orthogonal polynomials. Though the distribution functions ω and $\tilde{\omega}$ seem very close, the corresponding systems of orthogonal polynomials can become very different. This is illustrated in Fig. 4.2 which shows the quadrature nodes (given by the zeros of the corresponding orthogonal polynomials) for ω and $\tilde{\omega}$. We see that the Gauss-Christoffel quadrature approximations for ω and $\tilde{\omega}$ can for some k be close while several nodes are very different.

Results are similar for different values of ζ, providing that $\zeta \ll \gamma_1$, $\zeta \ll \gamma_2 - \gamma_1$. We illustrate this in Fig. 4.3 – Fig. 4.4, for which $\zeta = 10^{-12}$ with all other parameters

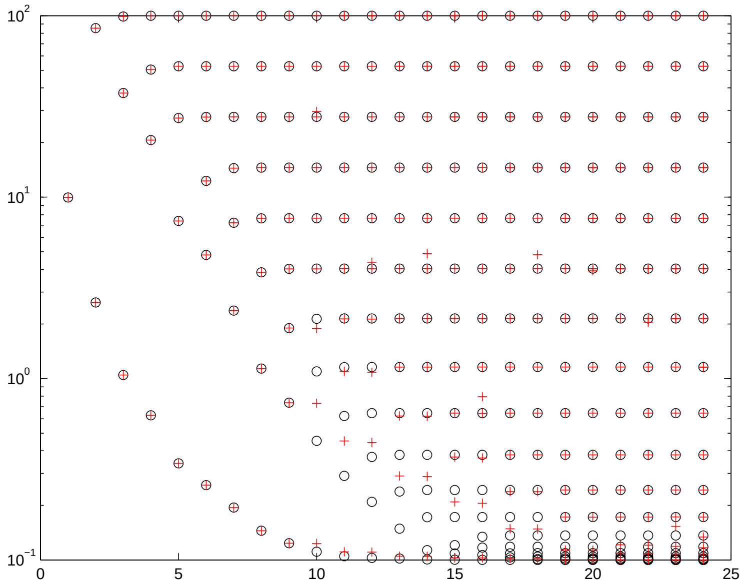

FIG. 4.2. *Quadrature nodes corresponding to the distribution function ω (circles) and $\tilde{\omega}$ (plusses). The horizontal axis is the number of nodes k in the quadrature.*

unchanged.

The Gauss-Christoffel quadrature nodes and weights were computed as the eigenvalues and the squared first components of the corresponding eigenvectors of the symmetric tridiagonal matrices generated via the double-reorthogonalized Lanczos process for the diagonal matrix $A = \mathrm{diag}(\gamma_1, \ldots, \gamma_n)$ resp. $\tilde{A} = \mathrm{diag}(\tilde{\gamma}_1, \ldots, \tilde{\gamma}_{2n})$ with the starting vector $v_1 = [(\delta_1)^{\frac{1}{2}}, \ldots, (\delta_n)^{\frac{1}{2}}]^T$ resp. $\tilde{v}_1 = [(\tilde{\delta}_1)^{\frac{1}{2}}, \ldots, (\tilde{\delta}_{2n})^{\frac{1}{2}}]^T$; see [22]. In this way we exploited the close relationship between the Gauss-Christoffel quadrature and the Lanczos process (the conjugate gradient method).

5. Conclusions. The difference between the quadrature approximations is in (3.1) and (4.1) bounded by sum of two terms where the second one represents the difference between the approximated integrals. In our paper we consider a sufficiently smooth function f so that the investigated phenomena are not affected by its particular behavior.

For the weighted Riemann integral with smooth weight functions it seems difficult to find examples for which the bound in (3.1) is not essentially determined by the difference between the approximated integrals. This suggests that in this case the Gauss quadrature is, under some conditions which are not too restrictive, possibly stable with respect to small perturbations of the weight function. Justification or disproving this conjecture needs further investigation.

In constrast, for the Riemann-Stieltjes integral, even a small perturbation of a discontinuous distribution function can cause dramatic differences between the Gauss-Christoffel quadrature approximations much above the level determined by the difference between the approximated integrals.

The instability of the Gauss-Christoffel quadrature described in this paper is closely related to the behavior of the Lanczos process and the conjugate gradient method, in particular to delay of convergence of the conjugate gradient method due

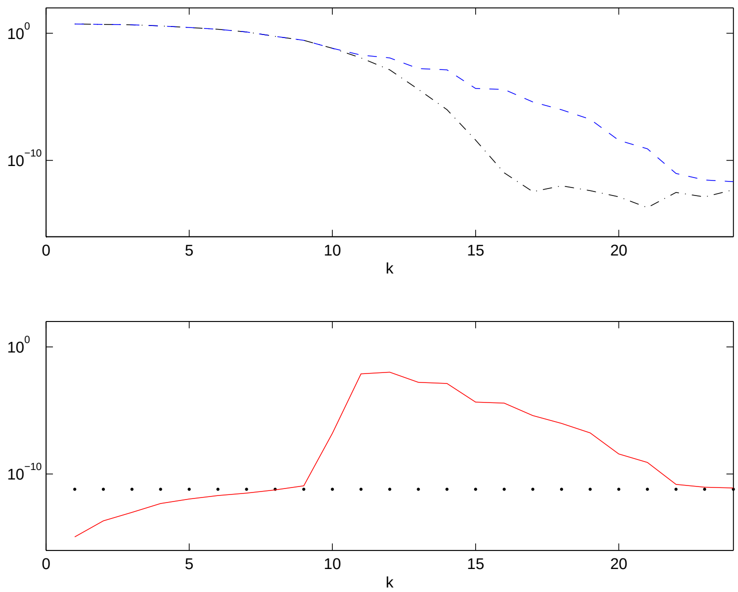

FIG. 4.3. *Sensitivity of the Gauss-Christoffel quadrature, $\zeta = 10^{-12}$. The error of the Gauss-Christoffel quadrature approximation for $f(x) = x^{-1}$ corresponding to the original distribution function ω (dash-dotted line) and to its "perturbation" $\tilde{\omega}$ with doubled points of increase (dashed line), the absolute value of their difference (solid line) and the difference between the approximated integrals (dots).*

to rounding errors. The general results presented in this paper will be used for detailed investigation of this relationship in further work [20].

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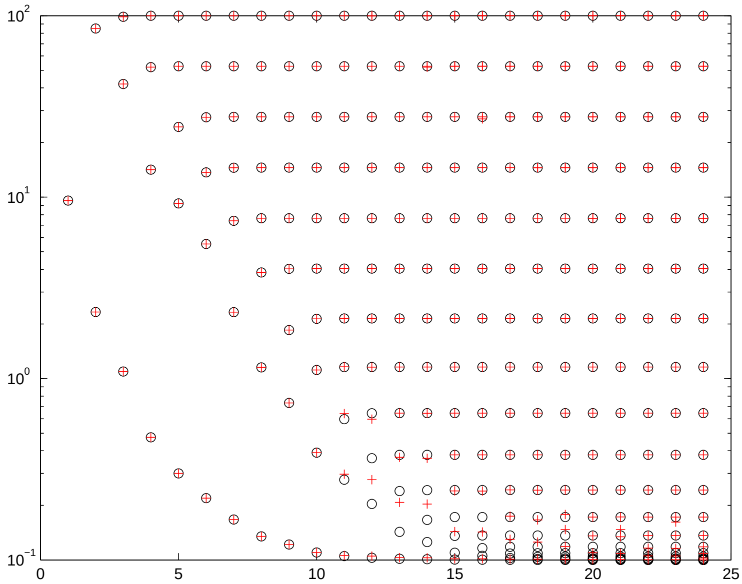

FIG. 4.4. *Quadrature nodes corresponding to the distribution function ω (circles) and $\tilde{\omega}$ (plusses). The horizontal axis is the number of nodes k in the quadrature.*

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