Stabilized linear modification algorithms

Author(s):
Chinellato, Oscar

Publication Date:
2005

Permanent Link:
https://doi.org/10.3929/ethz-a-006775639

STABILIZED LINEAR MODIFICATION ALGORITHMS

OSCAR CHINELLATO

Abstract. Given the recurrence coefficients associated with a given weight function, the problem in question is to find the change in these coefficients if the weight is modified by a linear factor or divisor. In this paper we present two algorithms performing these computations in a stable and accurate way by working directly on the known coefficient sequences.

We show how these results can be applied in the evaluation of particular integrals occurring in finite element models.

Key words. Gaussian quadrature, three term recurrence, Szegö type, orthogonal polynomial sequence, finite elements

1. Introduction. It is well known that every sequence of monic, orthogonal polynomials $\{\pi_k\}$ associated with a weight function $\omega(t)$ can be constructed by means of a three term recurrence involving certain coefficients, see [23]. The knowledge of these coefficients plays a central role in numerous algorithms and their accurate and efficient computation is thus of great importance.

Unfortunately, the processes of accurately determining these quantities are quite involved and elaborate in general, mainly depending on the nature of the underlying weight function $\omega(t)$. However, if the distribution at hand $\omega(t)$ is similar to a weight function $\hat{\omega}(t)$, whose associated recurrence coefficients are known, a remedy can be found. Instead of carrying out the computation of the desired recurrence coefficients from scratch, so called *modification algorithms* can then be used. These algorithms calculate the change of the original recurrence coefficients depending on the given *modification* $\omega(t)/\hat{\omega}(t)$.

The class of modifications which will be considered in this article is the one of rational functions. More precisely, we will investigate two algorithms which compute the new coefficient sequences arising after a modification by a *linear factor* and a *linear divisor*, respectively. The influence of a modification by a rational function can then be quantified by repeated application of these methods.

In order to allow for some theoretical statements about accuracy and stability of our new algorithms, we require the original weight distribution $\omega(t)$ to be of Szegö type [23], i.e. to belong to a special class of weight functions. Fortunately, this limitation is not too restrictive, since it still entails the better part of the popular weight distributions defined over a finite interval. However, more details about this shall be given in Section 2.

The foundations for modification algorithms dealing with polynomial factors and divisors were developed by Christoffel [4] and Uvarov [25, 26]. Unfortunately, the results presented were too theoretical and thus hardly useful for a numerical treatment of the aforementioned problems. Nonetheless, the results served as starting point for the development of several algorithms. Galant was one of the first to devise a scheme which was able to handle linear factors, see [6]. An extension of this scheme to quadratic factors as well as a derivation of "inverted" methods in order to handle linear and quadratic divisors was then given by Gautschi [11]. The fact that these inverted schemes were recognised to be unstable lead other authors to search for alternative methods, such as the ones presented by Golub [12], Kautsky [16] and Fischer [5].

In this article we propose a method which circumvents the aforementioned instability, without having to compute indirectly related quantities like modified moments or matrix polynomials, as it is the case in [12, 16, 5]. To this end we start by giving the necessary preliminaries about Szegö type weight functions in Section 2. These will then be needed in Section 3, for the analysis of the original linear modification algorithms presented by Gautschi [11]. We have taken these as starting point due to both their shortness and their simplicity. The results obtained will extend the *"... strong plausibility argument for the inherent instability..."* given in [7]. Moreover, the localisation of the instability source will then lead to improvements discussed in Section 4. Two new variants of linear modification algorithms will be presented in Section 5. In order to assess the suggested improvements a numerical experiment will be carried out in Section 6. The applicability of modification algorithms to the evaluation of certain integrals arising in finite element models will be shown. Finally, some concluding remarks will be given in Section 7.

2. Szegö type weight functions and their influences. Before we begin with the investigation of the aforementioned modification algorithms, some preliminaries about the theory of *orthogonal polynomial sequences* and their asymptotic behaviour shall be given. We thereto start by specifying a class of weight functions whose associated orthogonal polynomial sequences exhibit advantageous asymptotic properties, see [23].

Let $\mathcal{F}$ and $\mathcal{W}$ denote the sets of nonnegative functions having infinitely many points of increase and satisfying

$$\mathcal{F} = \{f(\theta) : \int_{-\pi}^{\pi} |\log f(\theta)|\, d\theta < \infty\} \quad \text{and} \quad \mathcal{W} = \{w(t) : \, w(\cos\theta)|\sin\theta| \in \mathcal{F}\},$$

where the integral above has to be understood in the Lebesgue sense. In the following we will be concerned with *weight functions* $\omega(t)$ defined over the interval $[-1, 1]$ such that $\omega(t) \in \mathcal{W}$, i.e. Szegö type weight functions. Note, that many popular weight distributions are contained in $\mathcal{W}$, e.g. the distributions associated with Chebyshev polynomials (first and second kind), Legendre polynomials, Gegenbauer polynomials, Jacobi polynomials, etc.

It is well known, that a *monic* orthogonal polynomial sequence $\{\pi_k\}$ associated with a weight function $\omega(t)$ obeys a *three term recurrence* relation of the form

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \quad \pi_0(t) = 1 \quad \text{and} \quad \pi_{-1}(t) = 0,$$

where the recurrence coefficients can be expressed by means of inner products of the type $\langle f, g\rangle_\omega = \int_{-1}^{1} \omega(t) f(t) g(t)\, dt$ leading to

$$\alpha_k = \frac{\langle t\pi_k, \pi_k\rangle_\omega}{\langle \pi_k, \pi_k\rangle_\omega} \quad \text{and} \quad \beta_k = \frac{\langle \pi_k, \pi_k\rangle_\omega}{\langle \pi_{k-1}, \pi_{k-1}\rangle_\omega}. \tag{2.1}$$

Notice, that it is customary to define $\beta_0 = \langle 1, 1\rangle_\omega$ to be the *order zero moment*.

The fact that $\omega(t) \in \mathcal{W}$ has favourable implications on the asymptotic behaviour of the induced orthogonal polynomial sequence, more precisely on its associated recurrence coefficients and its zeroes. Firstly, according to [23, Theorem 12.7.1], the recurrence coefficients defined in (2.1) have the limits

$$\bar{\alpha} = \lim_{k\to\infty} \alpha_k = 0 \quad \text{and} \quad \bar{\beta} = \lim_{k\to\infty} \beta_k = \frac{1}{4}. \tag{2.2}$$

Secondly, according to [23, Theorem 12.7.2], the limiting distribution of the zeroes $t_{kn} = \cos\theta_{kn}$ of the nth orthogonal polynomial $\pi_n(t)$ is such that

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} F(\theta_{kn}) = \frac{1}{\pi} \int_0^\pi F(\theta)\, d\theta. \tag{2.3}$$

for any Riemann–integrable function $F(\theta)$.

We conclude this section by deferring the reader to [23], where more asymptotic properties of orthogonal polynomial sequences can be found.

3. Analysis of the linear modification algorithms. We start our investigation by introducing the *linear factor modification algorithm* (LFM) and the *linear divisor modification algorithm* (LDM) presented in [11] and shown in Table 3.1.

$\{\hat\alpha_k, \hat\beta_k\} \leftarrow \mathrm{LFM}(\{\alpha_k, \beta_k\})$	$\{\hat\alpha_k, \hat\beta_k\} \leftarrow \mathrm{LDM}(\{\alpha_k, \beta_k\})$
$\hat\beta_0 = \langle 1, (t-z)\rangle_\omega = (\alpha_0 - z)\beta_0$	$\rho = \langle 1, (z-t)^{-1}\rangle_\omega$
$q_0 = \alpha_0 - z$	$\hat\beta_0 = -\rho$
$e_0 = \beta_1 / q_0$	$q_0 = -\beta_0/\rho$
$\hat\alpha_0 = \alpha_0 + e_0$	$\hat\alpha_0 = z + q_0$
for $k = 1, 2, \ldots$ do	for $k = 1, 2, \ldots$ do
$\quad q_k = \alpha_k - z - e_{k-1}$	$\quad e_{k-1} = \alpha_{k-1} - z - q_{k-1}$
$\quad \hat\beta_k = q_k e_{k-1}$	$\quad \hat\beta_k = q_{k-1} e_{k-1}$
$\quad e_k = \beta_{k+1}/q_k$	$\quad q_k = \beta_k / e_{k-1}$
$\quad \hat\alpha_k = q_k + z + e_k$	$\quad \hat\alpha_k = q_k + z + e_{k-1}$
end	end

TABLE 3.1
The linear modification algorithms described in [11].

In exact arithmetic, these algorithms compute the recurrence coefficients $\{\hat\alpha_k, \hat\beta_k\}$ associated with a modified weight function $\hat\omega(t)$ given the coefficients $\{\alpha_k, \beta_k\}$ corresponding to an original weight $\omega(t)$. The modifications addressed by the two algorithms comprise linear factors and divisors, i.e.

$$\hat\omega(t) = \omega(t)\, |t - z| \quad \text{and} \quad \hat\omega(t) = \omega(t)\, |t - z|^{-1}$$

with $z \in \mathbb{R} \setminus [-1, 1]$.

As explained in [11], the LDM method can be derived by “inverting” the LFM algorithm. It is thus not surprising that the following theorem holds.

THEOREM 3.1. *Let $\{\alpha_k, \beta_k\}$ be the sequence of recurrence coefficients associated with a weight function $\omega(t)$ and $z \in \mathbb{R} \setminus [-1, 1]$ be a given shift. Then the following holds:*

$$\mathrm{LDM}(\mathrm{LFM}(\{\alpha_k, \beta_k\})) = \{\alpha_k, \beta_k\} = \mathrm{LFM}(\mathrm{LDM}(\{\alpha_k, \beta_k\}))$$

Moreover, the sequences $\{q_k, e_k\}$ generated during the execution of LFM *and* LDM *are identical.*

Proof. Both properties can be verified by carrying out the single steps and comparing the quantities obtained in the two algorithms. ∎

A first point to note is, that the auxiliary sequences $\{q_k\}$ and $\{e_k\}$ arising during the execution of the LFM and the LDM method, can be computed in advance in a sort of preprocessing step. The desired recurrence coefficient sequences $\{\hat\alpha_k, \hat\beta_k\}$ can then be deduced from the auxiliary ones, according to the rules dictated by the respective algorithm.

Indeed, the recurrence relations describing the auxiliary sequences can be isolated from the coefficient sequences $\{\hat\alpha_k, \hat\beta_k\}$. Some simple transformations then suffice to obtain

$$\text{LFM}: \quad q_k = \alpha_k - z - \frac{\beta_k}{q_{k-1}}, \quad q_0 = \alpha_0 - z \tag{3.1}$$

$$\text{LDM}: \quad e_k = \alpha_k - z - \frac{\beta_k}{e_{k-1}}, \quad e_0 = \alpha_0 - z + \frac{\beta_0}{\rho} \tag{3.2}$$

Thus, applying the LFM and the LDM algorithm to the same input sequences $\{\alpha_k, \beta_k\}$ leads to two equivalent recurrence relations (3.1) and (3.2), yet initiated with different values. This fact can be rendered even more evident by applying the variable transform $q_k = u_{k+1}/u_k$ and $e_k = u_{k+1}/u_k$ to the relations (3.1) and (3.2), respectively. The results are so called *linear homogeneous difference equations* of second order having the structure

$$u_{k+1} = (\alpha_k - z)u_k - \beta_k u_{k-1}, \quad u_1 = \begin{cases} \alpha_0 - z & \text{(LFM)} \\ \alpha_0 - z + \beta_0/\rho & \text{(LDM)} \end{cases}, \quad u_0 = 1. \tag{3.3}$$

In general, expressions for the recurrence coefficients α_k and β_k are very complicated and thus hardly known which is why usually little can be said about the sequences $\{u_k\}$. But, according to (2.2), the recurrence coefficients associated with a weight function $\omega(t) \in \mathcal{W}$ will converge towards a limit which suggests to consider the *characteristic equation* associated with (3.3)

$$\sigma^2 - (\bar\alpha - z)\sigma + \bar\beta = \sigma^2 + z\sigma + \frac{1}{4} = (\sigma + \frac{z}{2})^2 + \frac{1}{4}(1 - z^2) = 0. \tag{3.4}$$

As can be seen, its roots $\sigma_{1,2} = \frac{1}{2}(-z \pm \sqrt{z^2 - 1})$ have distinct moduli due to the restriction $z \in \mathbb{R} \setminus [-1, 1]$ and thus Poincaré's difference equation theorem [17, 19] applies, i.e.

$$\lim_{k\to\infty} \frac{u_{k+1}}{u_k} = \sigma_i, \tag{3.5}$$

without specifying which one of the two limits $i = 1, 2$ is attained. In other words, the sequence $\{q_k\}$ as well as the sequence $\{e_k\}$ will attain one of the two possible limits σ_i, each. More precisely, we have

THEOREM 3.2. *Let $\omega(t) \in \mathcal{W}$ be a given weight function, $\{\alpha_k, \beta_k\}$ its associated recurrence coefficient sequences and $z \in \mathbb{R} \setminus [-1, 1]$ a given shift. Let further $\{q_k\}$ and $\{e_k\}$ be the auxiliary sequences computed by either the* LFM *or the* LDM *algorithm. Finally, let σ_1 and σ_2 be the roots of the underlying characteristic equation* (3.4)*. Then*

$$\lim_{k\to\infty} q_k = \sigma_{max} \quad \textit{and} \quad \lim_{k\to\infty} e_k = \sigma_{min},$$

where σ_{max} (σ_{min}) is the root with larger (smaller) modulus.

Proof. According to Theorem 3.1, applying the LDM algorithm to the given data yields the same sequences $\{q_k\}$, $\{e_k\}$ as applying the LFM method to the recurrence coefficients associated with the weight function $\omega(t)\,|t-z|^{-1}$. But since under the given assumptions the latter weight function is also element of $\mathcal{W}$, we can restrict our attention to the behaviour of the LFM method alone.

Performing one LFM step is equivalent to performing a so called *shifted LU–transform* on the *Jacobian* $\mathbf{J}_n$, as has been shown in [6]. In particular, the sequences $\{q_k\}$ and $\{e_k\}$ obtained during the execution of LFM can be used to construct upper and lower triangular matrices $\mathbf{U}_n$ and $\mathbf{L}_n$ such that $\mathbf{J}_n - \mathbf{zI} = \mathbf{L}_n\mathbf{U}_n$ holds, i.e.

$$\begin{pmatrix} \alpha_0 - z & 1 & & \\ \beta_1 & \alpha_1 - z & \ddots & \\ & \ddots & \ddots & 1 \\ & & \beta_n & \alpha_n - z \end{pmatrix} = \begin{pmatrix} 1 & & & \\ e_0 & 1 & & \\ & \ddots & \ddots & \\ & & e_{n-1} & 1 \end{pmatrix} \begin{pmatrix} q_0 & 1 & & \\ & q_1 & \ddots & \\ & & \ddots & 1 \\ & & & q_n \end{pmatrix}$$

The eigenvalues $\lambda_{k,n+1}$ of the Jacobian $\mathbf{J}_n$ are the zeros $t_{k,n+1}$ of the orthogonal polynomial $\pi_{n+1}(t)$ and as such, they do lie in the interval $(-1,1)$, see [23]. Computing the absolute value of the determinants on both sides then yields

$$\prod_{k=1}^{n+1} |t_{k,n+1} - z| = \prod_{k=0}^{n} |q_k| \quad \Leftrightarrow \quad \sum_{k=1}^{n+1} \log|t_{k,n+1} - z| = \sum_{k=0}^{n} \log|q_k|.$$

We define $t_{k,n+1} = \cos\theta_{k,n+1}$ and $F(\theta, z) = \log|\cos\theta - z|$ and apply (2.3) in order to obtain

$$\frac{1}{\pi}\int_0^\pi F(\theta,z)\,d\theta = \lim_{n\to\infty} \frac{1}{n+1}\sum_{k=1}^{n+1} F(\theta_{k,n+1}, z) = \lim_{n\to\infty}\frac{1}{n+1}\sum_{k=0}^{n}\log|q_k|.$$

According to [1], this integral can be bounded from below

$$-\log 2 = \frac{1}{\pi}\int_0^\pi F(\theta,\pm 1)\,d\theta < \frac{1}{\pi}\int_0^\pi F(\theta,z)\,d\theta = \lim_{n\to\infty}\frac{1}{n+1}\sum_{k=0}^{n}\log|q_k|,$$

and since the sequence $\{q_k\}$ is convergent, we know that $\lim_{k\to\infty}|q_k| > 1/2$ holds. As can easily be verified $|\sigma_{min}| < 1/2$ holds and concludingly, the sequence $\{q_k\}$ must converge towards σ_{max}.

To prove the second limit, we have a closer look at the LFM algorithm, especially envisaging the $\hat{\beta}_k = q_k e_{k-1}$ assignment. Since $\omega(t)|t-z| \in \mathcal{W}$ we know from (2.2) that $\lim_{k\to\infty}\hat{\beta}_k = 1/4$ and hence

$$\lim_{k\to\infty}|e_k| = \lim_{k\to\infty}\frac{\hat{\beta}_{k+1}}{|q_{k+1}|} < \frac{1}{2}$$

which, together with property (3.5), completes the proof. □

We conclude this first investigative part by pointing out, that in the theory of *difference equations* the sequence $\{u_k\}$ related to the sequence $\{q_k\}$ is referred to as *dominant solution* and the sequence $\{u_k\}$ related to the sequence $\{e_k\}$ is referred to as *minimal solution* of recurrence equation (3.3), see [9].

So far we have assumed, that all the computations are carried out in exact arithmetic. Of course, this assumption is no longer valid when executing the LFM and the LDM method on real machines with finite precision arithmetic where rounding and cancellation errors unavoidably arise. The influence of these errors on the accuracy of the results obtained by both the LFM and the LDM method is thus the next point to be investigated.

It is known, see e.g. [19], [17], [9], that the naïve forward iteration of a given second order linear difference equation is unproblematic in terms of accuracy as long as a dominant solution has to be computed. Hence, the forward iteration carried out by the LFM algorithm in order to recover the auxiliary sequence $\{q_k\}$, which in turn is associated with the dominant solution sequence $\{u_k\}$, is expected to be accurate as well.

Unfortunately, such a simple forward iteration scheme can not be used for the computation of minimal solutions. Due to the structure of the solution set, any small perturbation arising during the computation will accumulate such as to make the follow up sequence exponentially converge towards a dominant solution sequence, as shown in [9], [17], [21], [14], [24], [15]. Since these perturbations occur whenever finite precision arithmetic is used, the scheme is doomed to fail on every real machine. Indeed, the forward iteration carried out by the LDM algorithm in order to calculate the auxiliary sequence $\{e_k\}$, which in turn is associated with the minimal solution sequence $\{u_k\}$, exhibits a highly unstable behaviour, as pointed out by Gautschi [11].

4. Backward recurrence. According to Theorem 3.2 and the remarks thereafter, the stable and efficient computation of minimal solution sequences, in contrast to dominant solution sequences, is a delicate task. Thus, in order to accurately compute minimal solutions, special algorithms have to be used, such as Miller's backward recurrence algorithm [2], Olver's algorithm [20], Gautschi's continued fraction algorithm [10], etc.

Due to its simplicity we opt for the last one. Applied to our problem, we then have to compute the coefficient sequence $\{e_{k,N}\}$ defined by the recurrence relation

$$e_{k-1,N} = \frac{\beta_k}{\alpha_k - z - e_{k,N}}, \tag{4.1}$$

where an "initial" value $e_{N,N}$ is assumed to be given.

As a matter of fact, relation (4.1) can be obtained by inverting the iteration order in relation (3.2). Consequently, the former minimal solution now becomes the dominant one. Due to numerical errors arising during the computations in finite precision arithmetic, the contributions of the new minimal solution associated with (4.1) will be gradually eliminated and the sequence will thus stably converge towards a new dominant solution, see [10].

Indeed, machine arithmetic artifacts will ensure that the obtained leading subsequence $\mathbf{e}_n = [e_{0,N}, \ldots, e_{n,N}]$ for a desired order n will be accurate enough, depending primarily on the choice of N and only secondarily on the one of $e_{N,N}$. Unfortunately, the rate of decay of the aforementioned contributions corresponds to $|\sigma_{min}/\sigma_{max}|$ which might be low if z is close to the interval $[-1, 1]$. This in turn requires that, in order to yield good approximations, N must be large.

Obviously, the choice of the index N also depends on the behaviour of the parameters $\{\alpha_k\}$ and $\{\beta_k\}$, and if nothing more than our initial assumption $\omega(t) \in \mathcal{W}$ is known, good estimates for the index are hard to find. For some weight functions however, e.g. for Jacobi, Gegenbauer and Legendre distributions, reasonable estimates N_{est} for N are known, see [10].

Assuming such an estimate N_{est} to be known, the subsequence $\mathbf{e}_n$ can then be computed by means of the *backward recurrence method* (BRM) shown in Table 4.1.

$\mathbf{e}_n \leftarrow \mathrm{BRM}(\{\alpha_k, \beta_k\}, \varepsilon)$

```
e'  = 0
e   = 0
N   = N_est
while (‖e_n − e'_n‖ ≥ ε) do
   e'      = e
   N       = N + s
   e_{N,N} = σ_min
   for k = N, ..., 1 do
      e_{k−1,N} = β_k/(α_k − z − e_{k,N})
   end
end
```

TABLE 4.1

Stable computation of the sequence $\{e_{k,N}\}$ by means of backward recursion. The step size s and the tolerance ε should be chosen according to the underlying problem, the initial estimate N_{est} is assumed to be given. Note, that it is essential that all the computations be performed in finite precision arithmetic. The initial assignment

Notice, that the knowledge of good estimates for the index N is imperative for the BRM method to be effective.

The subsequence $\mathbf{e}_n$ obtained by the BRM algorithm is not just an approximation of any of the possible dominant solutions of relation (4.1) but it approximates the desired sequence $\{e_k\}$ defined by relation (3.2) directly. We refrain from giving a proof of this property and defer the interested reader to [9, 20] and references therein.

5. Stabilised and more accurate variants of the LFM/LDM algorithms. As we have shown in the preceeding sections, the instability of the LDM algorithm stems from the naïve approach of computing a minimal solution to a recurrence problem by means of forward iteration. This difficulty has been overcome by introducing the BRM method, one possibility to accurately compute minimal solutions.

Incorporating both the preprocessing split mentioned in Section 3 and the BRM step into the LFM and the LDM method then leads to the *modified* LFM *algorithm* (MLFM) and the *modified* LDM *algorithm* (MLDM). These improved variants are shown in Table 5.1.

Both methods differ from their unmodified counterparts. In case of the MLDM algorithm the unstable computation of the sequence $\{e_k\}$ has been replaced by the stable but more expensive BRM iteration. In addition, both modified variants have different assignment statements for the computation of the sequence $\{\hat{\alpha}_k\}$.

If the shifts z have large moduli, these new assignments avoid the strong cancellation exhibited by the original ones. The reason for this cancellation can be found by considering Theorem 3.2, where we have shown that the limit $\lim_{k\to\infty} q_k = \sigma_{max}$ holds and thus q_k approaches $-z$ for shifts of large magnitude. Hence, the computation of $q_k + z$ performed in both the LFM and the LDM method will unavoidably be inaccurate in finite precision arithmetic.

In cases where the shifts have small moduli, the instabilities originating from the forward iteration used in the LDM method aren't noticed except for large orders n. Moreover, the cancellation problem just addressed will not manifest itself. Therefore, if the desired orders n and the moduli of the shifts are moderate, the original algorithms LFM and LDM may be used.

Modified LFM (MLFM)	Modified LDM (MLDM)
$q_0 = \alpha_0 - z$	$\mathbf{e} = \mathrm{BRM}(\{\alpha_k, \beta_k\}, \epsilon)$
$e_0 = \beta_1/q_0$	$\rho = \langle 1, (z-t)^{-1}\rangle_{\hat{\omega}}$
for $k = 1, 2, \ldots$ do	$q_0 = -\beta_0/\rho$
$\quad q_k = \alpha_k - z - e_{k-1}$	for $k = 1, 2, \ldots$ do
$\quad e_k = \beta_{k+1}/q_k$	$\quad q_k = \beta_k/e_{k-1}$
end	end
$\hat{\beta}_0 = \langle 1, (t-z)\rangle_\omega = (\alpha_0 - z)\beta_0$	$\hat{\beta}_0 = -\rho$
$\hat{\alpha}_0 = \alpha_0 + e_0$	$\hat{\alpha}_0 = z + q_0$
for $k = 1, 2, \ldots$ do	for $k = 1, 2, \ldots$ do
$\quad \hat{\beta}_k = q_k e_{k-1}$	$\quad \hat{\beta}_k = q_{k-1} e_{k-1}$
$\quad \hat{\alpha}_k = \alpha_k - e_{k-1} + e_k$	$\quad \hat{\alpha}_k = \alpha_k - e_k + e_{k-1}$
end	end

TABLE 5.1

Modified variant of both the LFM *and the* LDM *algorithm. The program fragments above the middle line correspond to the preprocessing phases mentioned in Section 3.*

6. A numerical example. Modification algorithms are often used to compute special integrals having peculiar weight functions, as shown in [12, 5, 16, 11]. A different type of application can be found in the evaluation of bilinear forms arising in *finite element* (FE) discretisations. The example which will be considered in the following is taken from [3].

Let $\triangle$ be a triangle with nonnegative vertex coordinates but arbitrary shape and $p(x, y)$ be a given bivariate polynomial of high order. Suppose that the aforementioned bilinear forms to be evaluated possess the structure

$$\int_\triangle x \cdot p(x, y)\, d\triangle \qquad \text{and} \qquad \int_\triangle x^{-1} \cdot p(x, y)\, d\triangle.$$

Due to the huge number of terms arising in the closed form expressions for these integrals, a direct evaluation of the latter unduly suffers from cancellation and thus leads to inaccurate results. The application of simple quadrature rules instead, yields more accurate results, yet at the price of a very large number of function evaluations. Finally, the application of a suited Gaussian quadrature rule is cheap and accurate, yet, almost impossible to obtain, see [18].

One way to circumvent all of these problems consists in recasting the above integrals into line integrals along the triangle boundary by applying Greens's theorem. After having transformed the integrals, for details see [3], we obtain

$$\sum_{k=1}^{3} u_k \int_{-1}^{1} |t - v_k|\, \tilde{p}_k(t)\, dt \qquad \text{and} \qquad \sum_{k=1}^{3} u_k \int_{-1}^{1} |t - v_k|^{-1}\, \tilde{p}_k(t)\, dt \tag{6.1}$$

for the bivariate pendant given above, where the polynomials $\tilde{p}_k(t)$ are not explicitly constructed but may cheaply be evaluated at any point. It is now evident, that each of these one dimensional integrals can by computed by constructing and evaluating the corresponding Gaussian quadrature rule.

As can be seen, evaluating the integrals occurring in the sums (6.1) is structurally equivalent to computing the moment integrals μ_m and ν_m defined as

$$\mu_m = \int_{-1}^{1} |t-z|\, t^m\, dt \qquad \text{and} \qquad \nu_m = \int_{-1}^{1} |t-z|^{-1}\, t^m\, dt$$

where $z \in \mathbb{R} \setminus [-1,1]$. For the sake of simplicity, we will therefore restrict our attention to the latter. Note, that the weight functions of these integrals, similar to the ones given in (6.1), can be obtained by a linear modification of the Legendre weight distribution $\omega(t) = 1$, whose associated recurrence coefficients are known explicitly.

It is well known, that the exact computation of the moments μ_m and ν_m by means of Gauss quadrature requires at least $n = \lfloor m/2 \rfloor + 1$ points, see [22]. The recurrence coefficients required to construct these quadrature rules are computed using the modified modification algorithms. Finally, the quadrature rules are compiled using the Golub–Welsch method described in [13].

Table 6.1 shows two comparisons of relative errors that arise during the computation of the sequence $\{\hat{\alpha}_k\}$ associated with the weight function $|t-z|$. Two cases are presented, one with a relatively large and one with a relatively small shift z. As can be seen, the MLFM method produces smaller errors than then LFM method for increasing shift magnitudes. The reason for this is the different $\hat{\alpha}_k$ assignment statements discussed in Section 5.

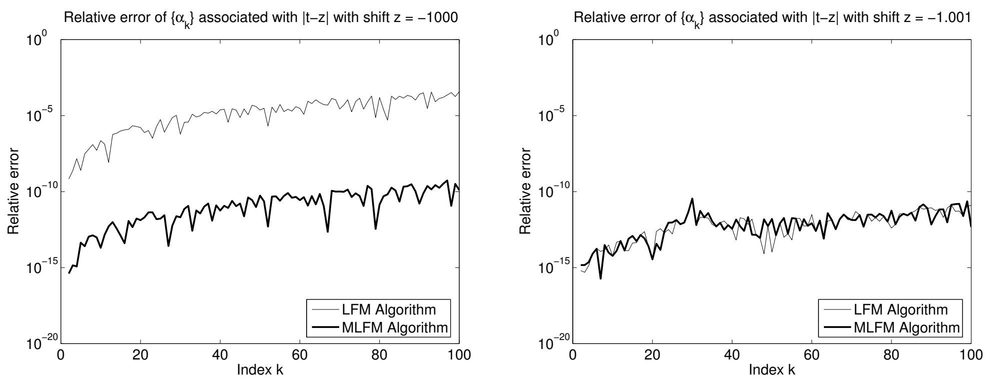

Table 6.1

Comparisons of relative errors arising during the computation of the coefficient sequence $\{\hat{\alpha}_k\}$, $k = 0, \ldots, 100$ *associated with the weight function* $|t-z|$. (left) *The larger errors stemming from the* LFM *method are due to cancellation effects explained in Section 5. These become more evident if a large shift is chosen.* (right) *Comparable behaviour of the methods can be observed.*

The numbers in Table 6.2 show, that the associated sequence $\{\hat{\beta}_k\}$ is computed to high relative accuracy independent from the underlying method or shift.

	±1'000	±100	±10	±1.1	±1.01	±1.001
LFM	2.2 [-16]	2.2 [-16]	4.4 [-16]	2.2 [-16]	2.2 [-16]	2.5 [-16]
MLFM	2.2 [-16]	2.2 [-16]	4.4 [-16]	2.2 [-16]	2.2 [-16]	2.5 [-16]

Table 6.2

Maximum relative error of the coefficients $\hat{\beta}_0, \ldots, \hat{\beta}_{100}$ *for different shifts. Note that both methods yield sequences with high relative accuracy.*

Table 6.3 depicts a comparison of relative errors arising in the computation of the $\{\hat{\alpha}_k\}$ sequence associated with the weight distribution $|t-z|^{-1}$. Again, two cases are presented, one with a relatively large and one with a relatively small shift. As expected, the LDM algorithm fails in recovering the sequence as soon as the index k or the shift modulus are large. As in the linear factor case, the altered assignment statements further improve the results for increasing shift magnitudes.

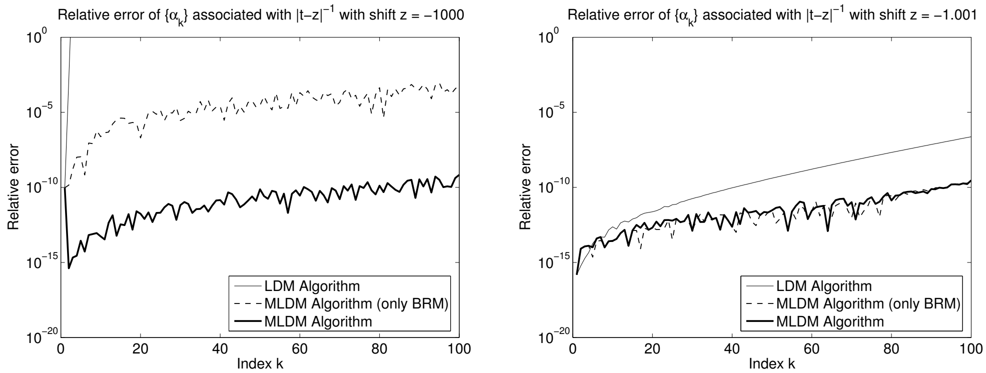

TABLE 6.3
Comparison of relative errors arising during the computation of the coefficient sequence $\{\hat{\alpha}_k\}$ *associated with the weight function* $|t-z|^{-1}$. (left) *As expected, the* LDM *method fails in recovering the minimal solution and hence the coefficient sequence. Note the improvement when altering the assignment statement.* (right) *The computation of the minimal solution is inaccurate but yields still reasonable results as long as the index* k *and the shift are kept small.*

The behaviour of the computed $\{\hat{\beta}_k\}$ sequence is similar in that its relative error is smaller if the MLDM method is used instead of the LDM algorithm, see Table 6.4. Notice, that the indices N occurring in the BRM algorithm satisfactorily correspond to the estimates mentioned in Section 4 and taken from [8].

	±1'000	±100	±10	±1.1	±1.01	±1.001
LDM	-	-	-	2.1 [-01]	2.9 [-05]	9.9 [-13]
MLDM	4.4 [-16]	4.4 [-16]	2.2 [-16]	4.4 [-16]	2.3 [-16]	5.1 [-15]

TABLE 6.4
Maximum relative error of the coefficients $\hat{\beta}_0, \ldots, \hat{\beta}_{100}$ *associated with the weight function* $|t-z|^{-1}$ *for different shifts. The inability of the* LDM *method in stably computing the minimal solution becomes evident.*

The coefficient sequences obtained with the original LFM and LDM algorithms exhibit larger relative errors than the ones obtained by means of their modified counterparts. This is even more the case for the linear divisor algorithms. Consequently, the quadrature rules associated with the respective coefficient sequences and computed with the Golub–Welsch algorithm lead to slightly better results for the moments μ_m and considerably better ones for the moments ν_m, as shown in Tables 6.5 and 6.6.

Finally, in accordance with Section 5, it can be observed that the sequences and the quadrature rules for shifts close to the interval $[-1, 1]$ can quite accurately be computed using the original LDM method, as long as both the order n and the shift z are of moderate moduli.

7. Concluding remarks. In this article we have presented two new linear modification algorithms, namely the MLFM and the MLDM method. Both improve the well known LFM and LDM methods introduced by Galant and Gautschi and

	±1’000	±100	±10	±1.1	±1.01	±1.001
0	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]
10	1.3 [-15]	2.1 [-15]	1.8 [-15]	1.8 [-15]	1.1 [-15]	6.1 [-16]
20	1.5 [-15]	2.6 [-15]	7.0 [-16]	3.2 [-15]	1.4 [-16]	3.5 [-15]
30	9.7 [-15]	3.2 [-15]	1.9 [-15]	1.2 [-14]	1.3 [-15]	6.9 [-15]
40	7.1 [-15]	7.8 [-15]	4.8 [-15]	8.7 [-15]	6.2 [-15]	2.8 [-16]
50	3.3 [-15]	1.0 [-14]	1.2 [-14]	1.6 [-15]	2.9 [-14]	8.3 [-15]
100	1.6 [-14]	2.7 [-14]	2.2 [-14]	3.9 [-14]	2.4 [-14]	1.3 [-14]
200	7.6 [-14]	8.0 [-14]	8.6 [-14]	6.6 [-14]	1.0 [-13]	1.2 [-13]

	±1’000	±100	±10	±1.1	±1.01	±1.001
0	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]
10	7.8 [-16]	1.4 [-15]	1.2 [-16]	1.9 [-15]	0.0 [-]	9.2 [-16]
20	6.0 [-16]	9.7 [-15]	4.4 [-15]	4.2 [-15]	2.0 [-15]	4.9 [-15]
30	4.4 [-15]	8.9 [-15]	1.0 [-15]	2.7 [-15]	7.5 [-15]	5.8 [-15]
40	5.0 [-15]	1.8 [-16]	1.8 [-15]	3.9 [-15]	0.0 [-]	1.4 [-15]
50	1.0 [-14]	1.6 [-14]	1.3 [-14]	9.2 [-15]	1.3 [-14]	7.2 [-15]
100	5.0 [-14]	2.8 [-14]	2.8 [-16]	2.0 [-14]	2.5 [-14]	3.4 [-14]
200	5.7 [-14]	1.1 [-13]	8.3 [-14]	3.2 [-14]	1.7 [-13]	1.3 [-14]

TABLE 6.5

Relative errors of the computed moments μ_m for different orders $m = 0, 10, \ldots$ and shifts $z = \pm 1'000, \pm 100, \ldots$. (top) *The recurrence coefficients where computed using the* LFM *algorithm.* (bottom) *The recurrence coefficients where computed using the* MLFM *algorithm.*

derivates presented by Fischer and Golub. Moreover, an explanation for the unstable behaviour of the LDM method and alikes has been given.

The fact that the new methods succeed in computing the modified sequences $\{\hat{\beta}_k\}$ to high relative accuracy, see Section 6, shows that both sequences $\{q_k\}$ and $\{e_k\}$ are computed accurately, as well. Yet, this implies that the inaccuracy exhibited in the sequences $\{\hat{\alpha}_k\}$ is due to cancellation alone. Its avoidance should be further investigated.

Finally, the applicability of these methods to certain integrals arising in the finite element domain has been shown. Our new methods allow for an efficient and accurate evaluation of the latter.

Acknowledgements. The author would like to express his gratitude to Walter Gautschi and Peter Arbenz for useful discussions on some aspects of this article.

REFERENCES

[1] M. ABRAMOWITZ AND I. A. STEGUN, eds., *Handbook of Mathematical Functions*, Dover Publications, Inc., New York, 1970.
[2] BRITISH ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE, *Mathematical Tables, Vol. X, Bessel Functions*, Part II, Functions of positive integer Order, Cambridge University Press, 1952.
[3] O. CHINELLATO, P. ARBENZ, M. STREIFF, AND A. WITZIG, *Computation of optical modes inside axisymmetric open cavity resonators*, Tech. Rep. 402, ETH Zürich, Institute of Computational Science, June 2003.
[4] E. B. CHRISTOFFEL, *Über die Gaußische Quadratur und eine Verallgemeinerung derselben*, J. Reine Angew. Math., 55 (1858), pp. 61–82.
[5] B. FISCHER AND G. H. GOLUB, *How to generate unknown orthogonal polynomials out of known orthogonal polynomials*, J. Comput. Appl. Math., (1992), pp. 99–115.

	±1'000	±100	±10	±1.1	±1.01	±1.001
0	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]
10	-	-	3.2 [-06]	2.7 [-15]	2.2 [-16]	2.8 [-15]
20	-	-	-	1.3 [-14]	1.0 [-15]	4.2 [-15]
30	-	-	-	4.3 [-14]	1.7 [-14]	8.6 [-15]
40	-	-	-	1.9 [-13]	0.0 [-]	1.8 [-14]
50	-	-	-	5.6 [-13]	1.3 [-14]	8.2 [-15]
100	-	-	-	1.2 [-10]	2.2 [-14]	1.5 [-14]
200	-	-	-	3.2 [-06]	4.4 [-14]	3.9 [-14]

	±1'000	±100	±10	±1.1	±1.01	±1.001
0	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]	0.0 [-]
10	1.6 [-15]	0.0 [-]	1.9 [-15]	1.8 [-15]	0.0 [-]	3.5 [-15]
20	2.0 [-15]	0.0 [-]	2.9 [-15]	4.5 [-16]	4.9 [-15]	4.0 [-15]
30	0.0 [-]	2.9 [-15]	5.1 [-15]	6.1 [-16]	7.2 [-16]	1.4 [-14]
40	9.0 [-15]	9.1 [-15]	2.3 [-15]	5.6 [-15]	7.4 [-15]	6.0 [-15]
50	5.2 [-15]	2.5 [-15]	1.2 [-14]	1.3 [-14]	1.3 [-14]	3.0 [-14]
100	9.2 [-14]	3.9 [-14]	4.0 [-14]	2.8 [-14]	4.1 [-15]	5.2 [-14]
200	9.3 [-14]	3.0 [-14]	7.2 [-14]	8.6 [-14]	3.6 [-14]	1.0 [-13]

TABLE 6.6

Relative errors of the computed moments ν_m *for different orders* $m = 0, 10, \ldots$ *and shifts* $z = \pm 1'000, \pm 100, \ldots$. (top) *The recurrence coefficients where computed using the* LDM *algorithm. Notice the high relative accuracy in the last columns.* (bottom) *The recurrence coefficients where computed using the* MLDM *algorithm.*

[6] D. GALANT, *An implementation of Christoffel's theorem in the theory of orthogonal polynomials*, Math. Comp., 25 (1971), pp. 111–113.

[7] ———, *Algebraic methods for modified orthogonal polynomials*, Math. Comp., 59 (1992), pp. 541–546.

[8] W. GAUTSCHI, *Orthogonal polynomials: Computation and approximation.* To appear in Clarendon Press, Oxford.

[9] ———, *Computational aspects of three–term recurrence relations*, SIAM Rev., 9 (1967), pp. 24–82.

[10] ———, *Minimal solutions of three–term recurrence relations and orthogonal polynomials*, Math. Comp., 36 (1981), pp. 547–554.

[11] ———, *An Algorithmic Implementation of the Generalized Christoffel Theorem*, vol. 57 of Internat. Ser. Numer. Math., Birkhäuser, Basel, 1982, pp. 89–106.

[12] G. H. GOLUB AND J. KAUTSKY, *Calculation of Gauss quadratures with multiple free and fixed knots*, Numer. Math., 41 (1983), pp. 147–163.

[13] G. H. GOLUB AND J. H. WELSCH, *Calculation of Gauss quadrature rules*, Math. Comp., 23 (1969), pp. 221–230.

[14] P. HENRICI, *Discrete Variable Methods in Ordinary Differential Equations*, John Wiley & Sons., Inc., New York, 1962.

[15] E. ISAACSON AND H. B. KELLER, *Analysis of Numerical Methods*, John Wiley & Sons., Inc., New York, 1966.

[16] J. KAUTSKY AND G. H. GOLUB, *On the calculation of Jacobi matrices*, Linear Algebra Appl., 52/53 (1983), pp. 439–455.

[17] V. LAKSHMIKANTHAM AND D. TRIGIANTE, *Theory of Difference Equations: Numerical Methods and Applications*, vol. 181 of Mathematics in Science and Engineering, Academic Press, Inc., San Diego, CA, 1988.

[18] J. N. LYNESS AND R. COOLS, *A survey of numerical cubature over triangles*, Proc. of Symposia in Applied Mathematics, (1994), pp. 127–150.

[19] N. E. NÖRLUND, *Differenzenrechnung*, Springer Verlag, Berlin, 1924.

[20] F. W. J. OLVER AND D. J. SOOKNE, *Note on backward recurrence algorithms*, Math. Comp.,

26 (1972), pp. 941–947.
[21] H. R. Schwarz, *Numerische Mathematik*, B. G. Teubner, Stuttgart, 1986.
[22] A. H. Stroud and D. Secrest, *Gaussian Quadrature Formulas*, Prentice–Hall, Englewood Cliffs, N. J., 1966.
[23] G. Szegö, *Orthogonal Polynomials*, American Mathematical Society, Providence, Rhode Island, 4th ed., 1975.
[24] J. Todd, *Basic Numerical Mathematics*, vol. 1 of International Series of Numerical Mathematics, Birkhäuser, Basel, 1979.
[25] V. B. Uvarov, *Relation between polynomials orthogonal with different weights*, Dokl. Akad. Nauk SSSR, 126 (1959), pp. 33–36.
[26] ———, *The connection between systems of polynomials that are orthogonal with respect to different distribution functions*, U.S.S.R. Computational Math. and Phys., 9 (1969), pp. 25–36.