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POSITIVITY OF DLV AND MDLVS ALGORITHMS FOR COMPUTING SINGULAR VALUES*

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Abstract. The discrete Lotka-Volterra (dLV) and the modified dLV with shift (mdLVs) algorithms for computing bidiagonal matrix singular values are considered. Positivity of the variables of the dLV algorithm is shown with the help of the Favard theorem and the Christoffel-Darboux formula of symmetric orthogonal polynomials. A suitable shift of origin also guarantees positivity of the mdLVs algorithm which results in a higher relative accuracy of the computed singular values.

Key words. dLV algorithm, mdLVs algorithm, singular values, relative accuracy

AMS subject classifications. 64F15, 33C45, 15A18, 37K10

1. Introduction.

A close relationship between known numerical algorithms and discrete-time integrable dynamical systems is reviewed in [25]. There, a continuous-time or discrete-time dynamical system is called *integrable*, if it has an explicit solution of determinant form, a Lax form and a sufficient number of conserved quantities. For example, Rutishauser's qd algorithm [27] for computing tridiagonal matrix eigenvalues and continued fraction expansions is equivalent to a discrete-time Toda chain [13]. Wynn's ε-algorithm [35] for accelerating convergence of sequences is a discrete-time KdV equation [26]. Is it possible to formulate a new effective numerical algorithm in terms of some discrete-time integrable system? The answer is yes. A new algorithm for computing bidiagonal matrix singular values is presented in [14, 34] with the help of a discrete-time Lotka-Volterra (dLV, for short) system [12, 29] with constant discrete step size. There is a beautiful expository paper [4] on the dLV system. It is observed in [3] that a solution of a continuous-time finite Lotka-Volterra (LV) system converges to bidiagonal singular values; see also the preceeding works [24, 30] on the connection between a continuous-time finite Toda chain and tridiagonal eigenvalues. The corresponding discrete-time Toda chain is just the recurrence relation of the qd algorithm. Thus, the existence of discrete-time integrable systems is a key to design new numerical algorithms. Though the dLV algorithm itself is subtraction free and has exponential stability [17], its convergence rate to the singular values is only linear [14]. Therefore, a generalization of the dLV to the case with variable step size is discussed in [15]. A modified dLV with shift (mdLVs) algorithm is then designed in [16]. The mdLVs algorithm has a higher order convergence rate and a higher relative accuracy. An implementation of the mdLVs algorithm with the Johnson shift [19] and its evaluation are discussed in [32].

Convergence theorems and stability of the dLV and the mdLVs algorithms are proved in [14, 15, 16, 17] assuming that the free parameter $\delta^{(n)}$ is *positive* and *bounded*, namely, $0 < \delta^{(n)} \leq M$ for some positive constant M. However, this parameter originally appears as a non-zero discrete step-size in [12], where $-\infty < \delta^{(n)} < 0$, or $0 < \delta^{(n)} < \infty$. In other words, the dLV system with non-zero $\delta^{(n)}$ itself is not suitable to design stable numerical algorithms. Since the qd algorithm and the ε-algorithm have no such free parameter and include subtraction, it has been an important problem how to stabilize these algorithms.

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In this paper, it is proved that $\delta^{(n)}$ should be positive and bounded, $0 < \delta^{(n)} \leq M$, by definition of the dLV algorithm in terms of orthogonal polynomials (OPs). Here, the dLV system is derived from the compatibility condition between the Christoffel-Darboux formula and the three-terms recurrence relation of symmetric OPs. As an application of the Favard theorem it is shown in this paper that the positivity and boundedness of $\delta^{(n)}$ result from the positivity of a linear functional of such OPs. Since the dLV system has no subtraction, all the variables are kept positive.

Positivity and convergence of the mdLVs algorithm are also proved in [16] assuming that the shift is less than the minimal singular value together with positivity and boundedness of $\delta^{(n)}$. It is possible to choose such a shift. The generalized Newton shift introduced in [20] is a candidate of a stable shift. Since the positivity and boundedness of $\delta^{(n)}$ is guaranteed by the Favard theorem, positivity of the mdLVs is also proved in this paper. It is shown that the positivity is an inherent property of the mdLVs and brings us high relative accuracy. Numerical experiments of the mdLVs with the generalized Newton shift are given as well. The mdLVs algorithm finds all the singular values, even the tiniest ones, to high relative accuracy.

2. The dLV algorithm and the mdLVs algorithm revised. Here, we give a brief review of the dLV algorithm and the mdLVs algorithm. Let us consider the continuous-time finite Lotka-Volterra (LV) system

$$
\begin{aligned}
&\frac{du_k}{dt} = u_k(u_{k+1} - u_{k-1}), \quad (k = 1, 2, \ldots, 2m-1), \\
&u_0(t) = 0, \quad u_{2m}(t) = 0,
\end{aligned}
\tag{2.1}
$$

where $u_{2m}(t) = 0$ is an additional condition. M. Chu [3] showed that for $k = 1, 2, \ldots, m$ a solution $u_{2k-1}(t)$ of the LV converges to the square of some singular value σ_k of a given upper bidiagonal matrix

$$
B = \begin{bmatrix} b_1 & b_2 & & \\ & b_3 & \ddots & \\ & & \ddots & b_{2m} \\ \text{\Large 0} & & & b_{2m-1} \end{bmatrix}
$$

and $u_{2k}(t)$ goes to 0 as $t \to \infty$: $\lim_{t\to\infty} u_{2k-1}(t) = \sigma_k^2$ and $\lim_{t\to\infty} u_{2k}(t) = 0$. Here, every b_j is assumed to be positive, $b_j > 0$. Such a bidiagonal matrix is derived from a general nonsingular matrix through Householder transformation [9]. Without loss of generality, the singular values of B are arranged as $\sigma_1 > \sigma_2 > \cdots > \sigma_m > 0$. In [3], the initial values of the differential equation (2.1) are given by

$$
u_{2k-1}(0) = b_{2k-1}^2 > 0, \quad u_{2k}(0) = b_{2k}^2 > 0, \quad (k = 1, 2, \ldots, m). \tag{2.2}
$$

A proof is carried out with the help of the asymptotic behavior of the solution of the finite Toda equation [24]. Deift-Demmel-Li-Tomei [5] discussed a Hamiltonian structure and its meaning in the singular value decomposition. However, it has not been clear for a long time how to design an actual numerical algorithm based on the preceding works [3, 5].

Let us consider the recurrence relation

$$
u_k^{(n+1)} = \frac{1 + \delta^{(n)} u_{k+1}^{(n)}}{1 + \delta^{(n+1)} u_{k-1}^{(n+1)}} u_k^{(n)}, \tag{2.3}
$$

$$
\begin{aligned}
&u_0^{(n)} = 0, \quad 0 < u_k^{(n)}, \quad u_{2m}^{(n)} = 0, \quad 0 < \delta^{(n)} \leq M, \\
&(n = 0, 1, \ldots, \quad k = 1, 2, \ldots, 2m-1).
\end{aligned}
\tag{2.4}
$$

$$
\begin{array}{ccccccccc}
 & b_1^2 & \cdots & b_{2k-2}^2 & b_{2k-1}^2 & b_{2k}^2 & \cdots & b_{2m-1}^2 & \\
u_0^{(0)} & u_1^{(0)} & \cdots & u_{2k-2}^{(0)} & u_{2k-1}^{(0)} & u_{2k}^{(0)} & \cdots & u_{2m-1}^{(0)} & u_{2m}^{(0)} \\
u_0^{(1)} & u_1^{(1)} & \cdots & u_{2k-2}^{(1)} & u_{2k-1}^{(1)} & u_{2k}^{(1)} & \cdots & u_{2m-1}^{(1)} & u_{2m}^{(1)} \\
u_0^{(2)} & u_1^{(2)} & \cdots & u_{2k-2}^{(2)} & u_{2k-1}^{(2)} & u_{2k}^{(2)} & \cdots & u_{2m-1}^{(2)} & u_{2m}^{(2)} \\
\vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots \\
0 & \sigma_1^2 & \cdots & 0 & \sigma_k^2 & 0 & \cdots & \sigma_m^2 & 0
\end{array}
$$

FIG. 2.1. *dLV table.*

Let us regard $u_k^{(n)}$ as the value of $u_k = u_k(t)$ at the time $t = \sum_{j=0}^{n-1} \delta^{(j)}$. Keeping t a constant, we take a limit $\delta^{(n)} \to +0$ such that $\delta^{(n+1)}/\delta^{(n)} \to 1$. We then derive (2.1) from (2.3). We call (2.3) the finite discrete LV (dLV) system. In [15] it is shown that a solution of the dLV with the additional condition (2.4) converges to the same limit as the finite LV

$$
\lim_{n\to\infty} u_{2k-1}^{(n)} = \sigma_k^2, \quad (k = 1, 2, \ldots, m), \quad \lim_{n\to\infty} u_{2k}^{(n)} = 0, \quad (k = 1, 2, \ldots, m-1)
$$

under the *assumption of positivity and boundedness* of $\delta^{(n)}$. In Section 5, the dLV system (2.3) is presented as a deformation equation of a finite number of symmetric OPs. It is proved in Theorem 5.2 that the assumption of positivity and boundedness is automatically satisfied by definition.

It is to be remarked that the initial value setting is different from that in the LV case (2.2). The appropriate choice of initial values found in [34] is

$$
\begin{aligned}
u_{2k-1}^{(0)} &= \frac{b_{2k-1}^2}{1 + \delta^{(0)} u_{2k-2}^{(0)}}, \quad (k = 1, 2, \ldots, m), \\
u_{2k}^{(0)} &= \frac{b_{2k}^2}{1 + \delta^{(0)} u_{2k-1}^{(0)}}, \quad (k = 1, 2, \ldots, m-1)
\end{aligned} \tag{2.5}
$$

as well as $u_0^{(0)} = 0$ and $u_{2m}^{(0)} = 0$. Here, $u_{2m}^{(0)} = 0$ corresponds to the case where $a_{2m}^2 = 0$ and $D_{2m+1} = 0$ (cf. Section 3). The computational procedure is indicated by a rhombus rule in Figure 2.1 and will be called the *dLV algorithm* for computing singular values of bidiagonal matrices.

Basic properties of the dLV algorithm such as convergence, convergence rate, error analysis, and stability are discussed in [4, 14, 15, 17, 34]. With respect to accuracy and stability the dLV has the following good properties. There is no subtraction in (2.3). The denominator $1 + \delta^{(n+1)} u_{k-1}^{(n+1)}$ in the division is always greater than 1. Obviously, no underflow occurs in the denominator. Therefore, it is expected that the dLV algorithm has a good relative accuracy. The dLV algorithm is shown to have exponential stability with the help of the existence of a center manifold, in which the positivity of $\delta^{(n)}$ plays a key role.

Next, we discuss a relationship between the dLV algorithm and Rutishauser's qd (quo-

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tient difference) algorithm [11, 27]. Introduce new variables $\{q_k^{(n)}, e_k^{(n)}\}$ by

$$\begin{aligned} q_k^{(n)} &:= \frac{1}{\delta^{(n)}}\left(1+\delta^{(n)}u_{2k-2}^{(n)}\right)\left(1+\delta^{(n)}u_{2k-1}^{(n)}\right), \\ e_k^{(n)} &:= \delta^{(n)}u_{2k-1}^{(n)}u_{2k}^{(n)}, \qquad (n=0,1,\dots,\quad k=1,2,\dots,m). \end{aligned} \tag{2.6}$$

Then it follows from (2.3) that $\{q_k^{(n)}, e_k^{(n)}\}$ satisfy

$$q_k^{(n+1)} = q_k^{(n)} - e_{k-1}^{(n+1)} + e_k^{(n)} - \left(\frac{1}{\delta^{(n)}} - \frac{1}{\delta^{(n+1)}}\right), \quad e_k^{(n+1)} = e_k^{(n)}\frac{q_{k+1}^{(n)}}{q_k^{(n+1)}}. \tag{2.7}$$

This recurrence relation takes the form of the progressive qd algorithm with shift (pqds, for short) [28]. The pqds algorithm (2.7) is expressed in the following matrix form of the LR transformation

$$\begin{gathered} L^{(n+1)}R^{(n+1)} = R^{(n)}L^{(n)} - \left(\frac{1}{\delta^{(n)}} - \frac{1}{\delta^{(n+1)}}\right)I, \\ L^{(n)} := \begin{bmatrix} q_1^{(n)} & & & \mathbf{0} \\ 1 & q_2^{(n)} & & \\ & \ddots & \ddots & \\ & & 1 & q_m^{(n)} \end{bmatrix}, \quad R^{(n)} := \begin{bmatrix} 1 & e_1^{(n)} & & \\ & 1 & \ddots & \\ & & \ddots & e_{m-1}^{(n)} \\ \mathbf{0} & & & 1 \end{bmatrix}, \end{gathered} \tag{2.8}$$

where I is the $m \times m$ unit matrix. Since the matrix $R^{(n)}L^{(n)}$ is positive definite by definition (2.8), the shift $1/\delta^{(n)} - 1/\delta^{(n+1)}$ should be nonnegative, which implies $0 < \delta^{(n)} \le \delta^{(n+1)}$. It follows from (2.4) that $\delta^{(n)}$ tends to some positive constant, say δ_+, as $n \to \infty$. Thus, $1/\delta^{(n)} - 1/\delta^{(n+1)} \to 0$ as $n \to \infty$. When $\delta^{(n)}$ is constant in n, the dLV recurrence relation is reduced to that of the progressive qd algorithm without shift (pqd); see (2.7). A negative constant $\delta^{(n)}$ is allowed in the general pqd algorithm, thus exponential stability of the pqd is not proved [17].

The rate of convergence of the dLV algorithm is then described by a ratio of the closest adjacent singular values (σ_j, σ_{j+1})

$$R_{\mathrm{dLV}} := \frac{\sigma_{j+1}^2 + \dfrac{1}{\delta_+}}{\sigma_j^2 + \dfrac{1}{\delta_+}} = \max_{k=1,\dots,m-1} \frac{\sigma_{k+1}^2 + \dfrac{1}{\delta_+}}{\sigma_k^2 + \dfrac{1}{\delta_+}} < 1. \tag{2.9}$$

This is proved by an asymptotic analysis of explicit solutions [14, 15]. It is shown that the convergence rate of the dLV algorithm is only *linear* since $\delta_+ > 0$. When the limit δ_+ becomes larger, the rate of convergence R_{dLV} becomes slightly faster within linear convergence.

The mdLVs (modified dLV with shift) [16] is a shifted dLV algorithm keeping the positivity of the parameter $\delta^{(n)}$. Let us introduce intermediate variables $\{\bar{w}_k^{(n)}, w_k^{(n)}\}$ by

$$\begin{aligned} \bar{w}_k^{(n+1)} &:= u_k^{(n)}\left(1+\delta^{(n)}u_{k+1}^{(n)}\right), \\ w_k^{(n)} &:= u_k^{(n)}\left(1+\delta^{(n)}u_{k-1}^{(n)}\right), \quad (n=0,1,\dots,\quad k=1,2,\dots,m). \end{aligned}$$

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$$\begin{tikzcd}
\{\bar{w}_k^{(n)}\} \arrow[r, "(2.10),\,(2.11)"] \arrow[d, "\text{mdLVs}"'] & \{w_k^{(n)}\} \arrow[d, "(2.12)"'] \\
\{\bar{w}_k^{(n+1)}\} & \{u_k^{(n)}\} \arrow[l, "(2.13)"]
\end{tikzcd}$$

FIG. 2.2. *mdLVs diagram.*

The initial values (2.5) of the dLV correspond to $w_k^{(0)} = b_k^2$. Let us set

$$B^{(n)} := \begin{bmatrix} \sqrt{w_1^{(n)}} & \sqrt{w_2^{(n)}} & & & \\ & \sqrt{w_3^{(n)}} & \ddots & & \\ & & \ddots & \sqrt{w_{2m}^{(n)}} \\ \mathbf{0} & & & \sqrt{w_{2m-1}^{(n)}} \end{bmatrix}.$$

Obviously, $B^{(0)} = B$. The mdLVs algorithm is defined by the recurrence relations

$$w_{2k-1}^{(n)} = \bar{w}_{2k-1}^{(n)} + \bar{w}_{2k-2}^{(n)} - w_{2k-2}^{(n)} - (\theta^{(n)})^2, \quad \theta^{(0)} = 0, \tag{2.10}$$

$$w_{2k}^{(n)} = \frac{\bar{w}_{2k-1}^{(n)}\bar{w}_{2k}^{(n)}}{w_{2k-1}^{(n)}}, \tag{2.11}$$

$$u_k^{(n)} = \frac{w_k^{(n)}}{1 + \delta^{(n)} u_{k-1}^{(n)}}, \tag{2.12}$$

$$\bar{w}_k^{(n+1)} = u_k^{(n)}\left(1 + \delta^{(n)} u_{k+1}^{(n)}\right), \tag{2.13}$$

where $(\theta^{(n)})^2$ indicates a shift of origin. The mdLVs algorithm is a composition of these mappings as in Figure 2.2.

The mapping from $\{\bar{w}_k^{(n)}\}$ to $\{w_k^{(n)}\}$ defined by (2.10) and (2.11) is expressed in matrix form as

$$\begin{gathered} (B^{(n)})^\top B^{(n)} = (\bar{B}^{(n)})^\top \bar{B}^{(n)} - (\theta^{(n)})^2 I, \\ \bar{B}^{(n)} := \begin{bmatrix} \sqrt{\bar{w}_1^{(n)}} & \sqrt{\bar{w}_2^{(n)}} & & & \\ & \sqrt{\bar{w}_3^{(n)}} & \ddots & & \\ & & \ddots & \sqrt{\bar{w}_{2m-2}^{(n)}} \\ \mathbf{0} & & & \sqrt{\bar{w}_{2m-1}^{(n)}} \end{bmatrix}. \end{gathered} \tag{2.14}$$

Equation (2.14) is similar to (2.8). The difference between the pqds algorithm (2.8) and the mdLVs algorithm is as follows. When $\theta^{(n)} = 0$, the mapping from $\{\bar{w}_k^{(n)}\}$ to $\{w_k^{(n)}\}$ defined by (2.10) and (2.11) is an identity mapping, and the mapping from $\{w_k^{(n)}\}$ to $\{\bar{w}_k^{(n+1)}\}$ defined by (2.12) and (2.13) is just the dLV algorithm (2.3). On the other hand, when $1/\delta^{(n)} - 1/\delta^{(n+1)} = 0$, (2.8) is not an identity mapping but the pqd algorithm.

Since $\theta^{(0)} = 0$, we see that $\bar{w}_k^{(0)} = w_k^{(0)}$ and then $\bar{B}^{(0)} = B^{(0)} = B$. Let us set $\theta^{(n)} \geq 0$, $(n = 1, 2, \ldots)$, for simplicity. For the mapping from $\{\bar{w}_k^{(n)}\}$ to $\{w_k^{(n)}\}$ the following lemma is proved in [16], which implies that the denominator of (2.11) never vanishes.

LEMMA 2.1 (Positivity of $w_k^{(n)}$ for a fixed n). *Let $\bar{w}_k^{(n)} > 0$ for a fixed n and for $k = 1, 2, \ldots, 2m-1$. Let us denote by $\sigma_j(\bar{B}^{(n)})$ the singular values of $\bar{B}^{(n)}$ such that $0 < \sigma_m(\bar{B}^{(n)}) < \sigma_{m-1}(\bar{B}^{(n)}) < \cdots < \sigma_1(\bar{B}^{(n)})$. It holds that*

$$w_k^{(n)} > 0 \quad \textit{if and only if} \quad \theta^{(n)} < \sigma_m(\bar{B}^{(n)}).$$

Moreover, if $\theta^{(n)} < \sigma_m(\bar{B}^{(n)}) - \varepsilon_1$ for some positive constant ε_1, then $w_k^{(n)} > \varepsilon_2$ for some positive constant ε_2.

When the initial values $\bar{w}_k^{(0)}$ have positivity and boundedness, the same property of $\bar{w}_k^{(n)}$ for any n is guaranteed by a successive choice of suitable shifts. Then the target $\{\bar{w}_k^{(n+1)}\}$ of the mdLVs map is positive and bounded given positive initial values $\bar{w}_k^{(0)}$ and suitable shifts.

LEMMA 2.2 (Positivity of $\bar{w}_k^{(n+1)}$ for any n). *Let $\theta^{(\ell)} < \sigma_m(\bar{B}^{(\ell)})$ for $\ell = 0, 1, \ldots, n$. Let M_1 and M_2 be some positive constants. Then $0 < \bar{w}_k^{(n+1)} < M_1$ and $0 < u_k^{(n)} < M_2$ for any n, if $0 < \bar{w}_k^{(0)} < M_1$.*

Now, a convergence theorem [16] of the mdLVs algorithm is given. It follows from Lemma 2.2 that $\sum_{\ell=1}^{\infty}(\theta^{(\ell)})^2 \leq \sigma_m^2$ for $\theta^{(\ell)} < \sigma_m(\bar{B}^{(\ell)})$ for $\ell = 0, 1, \ldots$.

THEOREM 2.3. *Let $0 < \bar{w}_k^{(0)} < M_1$ and $\theta^{(\ell)} < \sigma_m(\bar{B}^{(\ell)})$ for $\ell = 0, 1, \ldots$. Then it follows that*

$$\begin{aligned} &\lim_{n\to\infty} \bar{w}_{2k-1}^{(n)} = \sigma_k^2 - \sum_{\ell=1}^{\infty}(\theta^{(\ell)})^2, \quad (k = 1, 2, \ldots, m) \\ &\lim_{n\to\infty} \bar{w}_{2k}^{(n)} = 0, \quad (k = 1, 2, \ldots, m-1). \end{aligned} \tag{2.15}$$

For an implementation of the mdLVs algorithm the property (2.15) is quite useful to introduce a stopping criteria. The asymptotic rate of convergence of the mdLVs is described by the ratio

$$R_{\mathrm{mdLVs}} := \frac{\sigma_{j+1}^2 - \sum_{\ell=1}^{\infty}(\theta^{(\ell)})^2 + \dfrac{1}{\delta_+}}{\sigma_j^2 - \sum_{\ell=1}^{\infty}(\theta^{(\ell)})^2 + \dfrac{1}{\delta_+}} < R_{\mathrm{dLV}},$$

where (σ_j, σ_{j+1}) is the pair of closest adjacent singular values of $B = \bar{B}^{(0)}$ (see (2.9) for the definition of R_{dLV}). A higher order convergence of the mdLVs [16] results from the inequality $R_{\mathrm{mdLVs}} < R_{\mathrm{dLV}}$. Note that positivity and boundedness of the parameter δ_+ arising from $0 < \delta^{(n)} \leq M$ in (2.4) are still assumed here.

The convergence rate depends on the choice of the shift $\theta^{(n)}$ as well as δ_+. The remaining problem concerns the choice of suitable shifts such that $\theta^{(\ell)} < \sigma_m(\bar{B}^{(\ell)})$ for $\ell = 0, 1, \ldots$. An excellent solution is the p-th generalized Newton bound

$$\Theta_p(\bar{B}^{(\ell)}) := \left(\mathrm{trace}(\bar{B}^{(\ell)\top}\bar{B}^{(\ell)})^{-p}\right)^{-\frac{1}{2p}}, \quad (p = 1, 2, \ldots)$$

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introduced by K. Kimura [20]. We observe that

$$\Theta_p(\bar{B}^{(\ell)}) = \frac{1}{\left(\dfrac{1}{\sigma_1^{2p}} + \cdots + \dfrac{1}{\sigma_m^{2p}}\right)^{\frac{1}{2p}}} < \sigma_m(\bar{B}^{(\ell)}),$$
$$0 < \Theta_1(\bar{B}^{(\ell)}) < \Theta_2(\bar{B}^{(\ell)}) < \cdots < \sigma_m(\bar{B}^{(\ell)}), \quad \lim_{p\to\infty} \Theta_p(\bar{B}^{(\ell)}) = \sigma_m(\bar{B}^{(\ell)}).$$

Obviously, $\Theta_p(\bar{B}^{(\ell)})$ satisfies $\Theta_p(\bar{B}^{(\ell)}) < \sigma_m(\bar{B}^{(\ell)})$ for $\ell = 0, 1, \ldots$. Since it also holds that $\Theta_p(\bar{B}^{(\ell)}) < \sigma_m(\bar{B}^{(\ell)}) - \varepsilon_1$ for some positive constant ε_1, it is obtained from Lemma 2.1 that $w_k^{(n)} > \varepsilon_2$ for some positive ε_2. Thus, we confirm a strict positivity of the denominator $w_{2k-1}^{(n)}$ of (2.11) where the shift is given by the generalized Newton bound.

The generalized Newton bound $\Theta_p(B)$ itself is computed by using a recurrence relation using only $O(pm)$ operations [20]. Recently, Y. Yamamoto [21] proved that the generalized Newton shift yields a weakly $(p+1)$-th order convergence of the mdLVs algorithm. The mdLVs code with the generalized Newton shift ($p = 2, 3, 4$) is shown to be actually faster and more accurate than the mdLVs code [32] with the Johnson shift [19].

3. Orthogonal polynomials.

Let us begin with the Favard theorem ([2, p. 21]). Let $\{s_k\}$, $(k = 0, 1, 2, \ldots)$ be a sequence of real numbers. The sequence $\{s_k\}$ is called positive whenever the bilinear form $\sum_{k,\ell=0}^{m} s_{k+\ell} x_k x_\ell$ is positive for any m. It is known that $\{s_k\}$ is positive if and only if the Hankel determinants

$$D_{m+1} := \begin{vmatrix} s_0 & s_1 & \cdots & s_m \\ s_1 & s_2 & \cdots & s_{m+1} \\ \vdots & \vdots & & \vdots \\ s_m & s_{m+1} & \cdots & s_{2m} \end{vmatrix} = |s_{i+j}|_{0 \le i,j \le 2m}, \quad (m = 0, 1, \ldots)$$

are positive for all $m = 0, 1, \ldots$.

THEOREM 3.1 (Favard). *Let $\{a_k\}$, $\{b_k\}$, $(k = 1, 2, \ldots)$ be sequences of real numbers. Let $\{p_k(\lambda)\}$ be polynomials of λ defined by the three-terms recurrence relation*

$$p_0(\lambda) = 1, \quad p_1(\lambda) = \lambda - b_1, \quad p_{k+1}(\lambda) = (\lambda - b_{k+1})p_k(\lambda) - a_k^2 p_{k-1}(\lambda).$$

Then there exists a unique linear functional J such that

$$J[1] = s_0, \quad J[p_k(\lambda)p_\ell(\lambda)] = 0, \quad (k, \ell = 0, 1, \ldots, \ k \ne \ell)$$

for any positive constant s_0. Moreover, $a_k^2 > 0$ if and only if the sequence of moments defined by

$$s_k := J[\lambda^k], \quad (k = 1, 2, \ldots)$$

is positive.

Proof. We can uniquely introduce a sequence of moments as follows. Set $J[p_k(\lambda)] = 0$, $(k = 1, 2, \ldots)$. The moment $s_0 = J[1]$ is given by $s_0 = a_0^2$. From $J[p_1(\lambda)] = J[\lambda - b_1] = 0$ we find that $s_1 = b_1 s_0$. From $J[p_2(\lambda)] = J[(\lambda - b_2)p_1(\lambda) - a_1^2 p_0(\lambda)] = 0$ we derive $s_2 = (b_1 + b_2)s_1 + (a_1^2 - b_1 b_2)s_0$, and so on. Then, every $s_k = J[\lambda^k]$ is determined by using the recurrence relation. This implies that a linear functions J is defined. It follows from the recurrence relation and $J[p_k(\lambda)] = 0$ that $J[\lambda p_k(\lambda)] = 0$, $(k = 2, 3, \ldots)$. Similarly, we obtain $J[\lambda^j p_k(\lambda)] = 0$, $(j = 0, 1, \ldots, k-1)$ and then $J[p_j(\lambda)p_k(\lambda)] = 0$.

Assume that $a_k^2 > 0$, $(k = 1, 2, \dots)$. Since $J[\lambda^j p_k(\lambda)] = 0$ we have

$$J[\lambda^k p_k(\lambda)] = a_k^2 J[\lambda^{k-1} p_{k-1}(\lambda)] = s_0 a_1^2 \cdots a_k^2.$$

Thus, $J[p_k(\lambda)^2] = s_0 a_1^2 \cdots a_k^2$. On the other hand, the polynomial $p_k(\lambda)$, $(k = 1, 2, \dots)$ takes the determinant form [31]

$$p_k(\lambda) = \frac{1}{D_k} \begin{vmatrix} s_0 & s_1 & \cdots & s_k \\ s_1 & s_2 & \cdots & s_{k+1} \\ \vdots & \vdots & & \vdots \\ s_{k-1} & s_k & \cdots & s_{2k-1} \\ 1 & \lambda & \cdots & \lambda^k \end{vmatrix}.$$

The coefficients a_k^2 of the recurrence relation are

$$a_k^2 = \frac{D_{k-1} D_{k+1}}{D_k^2}.$$

It follows from $a_1^2 \cdots a_k^2 = D_{k+1}/D_k$ that $D_k > 0$ for any k and the corresponding moments are positive. The converse is obvious from the above. $\square$

The Favard theorem says that the polynomials $\{p_k(\lambda)\}$ defined by the three-terms recurrence relation with positive coefficients a_k^2 are orthogonal with respect to the linear functional J, namely, $J[p_k(\lambda)p_\ell(\lambda)] = s_0 a_1^2 \cdots a_k^2 \delta_{k,\ell}$. In this case, the corresponding set of moments $\{s_k\}$ is positive and vice versa. Note that $p_k(\lambda)$ is of degree k and its leading coefficient is 1. The polynomials $\{p_k(\lambda)\}$ are sometimes called the monic orthogonal polynomials (OPs) of the first kind.

OPs have some special features. One of them is the position of zeros. It is known that the zeros of OPs are mutually distinct real numbers and have an interlacing property [1]. Let $\{q_k(\lambda)\}$ be OPs of the second kind defined by

$$q_{-1}(\lambda) = 1, \quad q_0(\lambda) = 0, \quad q_{k+1}(\lambda) = (\lambda - b_{k+1})q_k(\lambda) - a_k^2 q_{k-1}(\lambda),$$

where $q_k(\lambda)$ is of degree $k-1$. Let $\lambda_{j,m}$, $(j = 1, 2, \dots, m)$ and $\mu_{i,m}$, $(i = 1, 2, \dots, m-1)$ be the zeros of $p_m(\lambda)$ and $q_m(\lambda)$, respectively. Then,

$$\lambda_{1,m} < \mu_{1,m} < \lambda_{2,m} < \mu_{2,m} < \cdots < \mu_{m-1,m} < \lambda_{m-1,m}. \tag{3.1}$$

This leads to the following statement. The rational function $q_m(\lambda)/p_m(\lambda)$ of degree m admits a partial fraction expansion

$$\frac{q_m(\lambda)}{p_m(\lambda)} = \sum_{j=1}^{m} \frac{\nu_{j,m}}{\lambda - \lambda_{j,m}}, \quad \nu_{j,m} := \frac{q_m(\lambda_{j,m})}{p'_m(\lambda_{j,m})}. \tag{3.2}$$

From the interlacing property (3.1) it follows that the residues $\nu_{j,m}$ called the Christoffel coefficients satisfy the positivity condition $\nu_{j,m} > 0$.

Here we give two examples of OPs. The Laguerre polynomials correspond to the linear functional $J[f(\lambda)] = \int_0^\infty f(\lambda)\lambda^\alpha e^{-\lambda} d\lambda$, $(\alpha > -1)$. When $\alpha = 0$, the corresponding moments and Hankel determinants are $s_0 = 1$, $s_k = k!$, $(k = 1, 2, \dots)$, and $D_1 = 1$, $D_{m+1} = (\prod_{k=1}^m k!)^2$, $(m = 1, 2, \dots)$, respectively.

The Hermite polynomial is associated with $J[f(\lambda)] = 1/\sqrt{\pi} \int_{-\infty}^\infty f(\lambda) e^{-\lambda^2} d\lambda$. The corresponding moments and Hankel determinants are $s_0 = 1$, $s_{2k-1} = 0$, $s_{2k} = (2k-1)!!/2^k$, $(k = 1, 2, \dots)$, and $D_1 = 1$, $D_{m+1} = \prod_{k=1}^m k!/2^{k(k+1)/2}$, $(m = 1, 2, \dots)$, respectively. Here $(2k-1)!! := (2k-1)(2k-3)\cdots 5 \cdot 3 \cdot 1$. The Hermite polynomials $p_{2k-1}(\lambda)$ are odd and $p_{2k}(\lambda)$ are even functions.

4. Christoffel-Darboux formula for symmetric orthogonal polynomials. For the Hermite, Legendre and Chebyshev polynomials every moment with odd order is zero, $s_{2k-1} = 0$. In the linear functionals of those cases, the measure $d\mu(\lambda)$ is invariant under the exchange $\lambda \to -\lambda$. The linear functional J satisfying

$$s_{2k-1} = J[\lambda^{2k-1}] = 0, \quad (k = 1, 2, \dots)$$

is called symmetric and the corresponding orthogonal polynomial is called a symmetric orthogonal polynomial. When $d\mu(\lambda) = w(\lambda)d\lambda$, the weight function $w(\lambda)$ is an even function over the interval $(-\xi, \xi)$. The coefficients b_k of the recurrence relation are zero for symmetric OPs: $b_k = 0$, $(k = 1, 2, \dots)$. In this section, we restrict ourselves to symmetric OPs.

Let us consider the three-terms recurrence relation of symmetric OPs

$$p_0(\lambda) = 1, \quad p_1(\lambda) = \lambda, \quad p_{k+1}(\lambda) = \lambda p_k(\lambda) - a_k^2 p_{k-1}(\lambda).$$

For simplicity, we write

$$\begin{aligned} y_{k+1} &= \lambda y_k - a_k^2 y_{k-1}, \quad y_k = p_k(\lambda), \\ z_{k+1} &= \kappa z_k - a_k^2 z_{k-1}, \quad z_k = p_k(\kappa), \end{aligned}$$

where κ is a constant. Using the recurrence relation twice, we derive

$$\begin{aligned} y_{k+2} &= (\lambda^2 - a_{k+1}^2) y_k - \lambda a_k^2 y_{k-1}, \\ z_{k+2} &= (\kappa^2 - a_{k+1}^2) z_k - \kappa a_k^2 z_{k-1}. \end{aligned}$$

From the first and the second relations, we have

$$(\kappa^2 - \lambda^2) y_k z_k = y_k z_{k+2} - y_{k+2} z_k - a_k^2 (\lambda y_{k-1} z_k - \kappa y_k z_{k-1}).$$

Then, the following bilinear formula results.

$$\begin{aligned} &\lambda y_{k-1} z_k - \kappa y_k z_{k-1} \\ &= -a_{k-1}^2 (\lambda y_{k-1} z_{k-2} - \kappa y_{k-2} z_{k-1}) \\ &= a_{k-1}^2 (\kappa^2 - \lambda^2) y_{k-2} z_{k-2} + a_{k-1}^2 a_{k-2}^2 (\lambda y_{k-3} z_{k-2} - \kappa y_{k-2} z_{k-3}) \\ &= a_{k-1}^2 (\kappa^2 - \lambda^2) y_{k-2} z_{k-2} + a_{k-1}^2 a_{k-2}^2 a_{k-3}^2 (\kappa^2 - \lambda^2) y_{k-4} z_{k-4} \\ &\quad + a_{k-1}^2 a_{k-2}^2 a_{k-3}^2 a_{k-4}^2 (\lambda y_{k-5} z_{k-4} - \kappa y_{k-4} z_{k-5}). \end{aligned}$$

(i) When $k = 2m - 1$, noting that $y_0 = z_0 = 1$, $y_1 = \lambda$, $z_1 = \kappa$, we see that

$$\begin{aligned} &(\kappa^2 - \lambda^2) y_{2m-1} z_{2m-1} \\ &= -y_{2m-1} z_{2m+1} - y_{2m+1} z_{2m-1} - a_{2m-1}^2 a_{2m-2}^2 (\kappa^2 - \lambda^2) y_{2m-3} z_{2m-3} \\ &\quad - a_{2m-1}^2 a_{2m-2}^2 a_{2m-3}^2 a_{2m-4}^2 (\kappa^2 - \lambda^2) y_{2m-5} z_{2m-5} \\ &\quad - \cdots - a_{2m-1}^2 \cdots a_2^2 (\kappa^2 - \lambda^2) y_1 z_1. \end{aligned}$$

Therefore, we obtain

$$(\kappa^2 - \lambda^2) \sum_{k=1}^{m} \left(\prod_{j=0}^{2m-2k} a_{2m-j}^2 y_{2k-1} z_{2k-1} \right) = y_{2m-1} z_{2m+1} - y_{2m+1} z_{2m-1}.$$

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(ii) When $k = 2m$, noting that $a_0 = 0$, we have

$$(\kappa^2 - \lambda^2) \sum_{k=0}^{m} \left(\prod_{j=0}^{2m-2k-1} a_{2m-j}^2 y_{2k} z_{2k} \right) = y_{2m} z_{2m+2} - y_{2m+2} z_{2m}.$$

In conclusion, we present the Christoffel-Darboux formula for symmetric OPs as follows. In contrast to the case of usual OPs [1, 2, 31], a parity emerges as follows

$$a_1^2 \cdots a_{2m-1}^2 \left(\sum_{j=1}^{m} \frac{p_{2j-1}(\lambda) p_{2j-1}(\kappa)}{a_1^2 \cdots a_{2j-1}^2} \right) = \frac{p_{2m-1}(\lambda) p_{2m+1}(\kappa) - p_{2m+1}(\lambda) p_{2m-1}(\kappa)}{\kappa^2 - \lambda^2} \quad \text{for } k = 2m-1,$$

$$a_1^2 \cdots a_{2m}^2 \left(\sum_{j=1}^{m} \frac{p_{2j}(\lambda) p_{2j}(\kappa)}{a_1^2 \cdots a_{2j}^2} + p_0(\lambda) p_0(\kappa) \right) = \frac{p_{2m}(\lambda) p_{2m+2}(\kappa) - p_{2m+2}(\lambda) p_{2m}(\kappa)}{\kappa^2 - \lambda^2} \quad \text{for } k = 2m.$$

The Christoffel-Darboux formula is useful, for example, to discuss the convergence of series of OPs.

5. Discrete Lotka-Volterra and positivity.

In this section, we first define a kernel polynomial $p_k^*(\lambda)$ corresponding to the original symmetric orthogonal polynomial $p_k(\lambda)$. To this end, we assume $p_k(\kappa) \neq 0$.

$$p_k^*(\lambda) := \begin{cases} -\dfrac{a_1^2 \cdots a_{2m-1}^2}{p_{2m-1}(\kappa)} \displaystyle\sum_{j=1}^{m} \frac{p_{2j-1}(\lambda) p_{2j-1}(\kappa)}{a_1^2 \cdots a_{2j-1}^2} & \text{for } k = 2m-1, \\[2ex] -\dfrac{a_1^2 \cdots a_{2m}^2}{p_{2m}(\kappa)} \left(\displaystyle\sum_{j=1}^{m} \frac{p_{2j}(\lambda) p_{2j}(\kappa)}{a_1^2 \cdots a_{2j}^2} + p_0(\lambda) p_0(\kappa) \right) & \text{for } k = 2m \end{cases}$$

Then, the Christoffel-Darboux formula leads to

$$p_k^*(\lambda) = \frac{1}{\kappa^2 - \lambda^2} \left(p_{k+2}(\lambda) + A_k p_k(\lambda) \right), \quad A_k := -\frac{p_{k+2}(\kappa)}{p_k(\kappa)}.$$

When $k = 2m-1$, $p_k(\lambda)$ is an odd function. When $k = 2m$, $p_k(\lambda)$ is even. The poles $\lambda = \pm\kappa$ are removable poles. Hence, $p_k^*(\lambda)$ is a polynomial of degree k. The transformation

$$\{p_k(\lambda)\} \longrightarrow \{p_k^*(\lambda)\}$$

is just the Christoffel transformation for the symmetric OPs $\{p_k(\lambda)\}$. Let us introduce a new linear functional J^* by

$$J^*[A(\lambda)] := J[(\kappa^2 - \lambda^2) A(\lambda)]$$

for any polynomial $A(\lambda)$ and a suitable constant $\kappa < 0$. The corresponding weight function and moments are $w^*(\lambda) := (\kappa^2 - \lambda^2) w(\lambda)$ and $s_k^* := \kappa^2 s_k - s_{k+2}$, respectively. Let us note a theorem ([2], p.36) on the positivity of the linear functional J^*.

THEOREM 5.1. (Chihara) *Let the linear functional J be positive definite over the interval $[-\xi, \xi,]$ with $\xi > 0$. Then J^* is positive over $[-\xi, \xi,]$, if and only if $\kappa \le -\xi$.*

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Proof. If $\kappa \le -\xi$, then J^* is obviously positive over $[-\xi,\xi,]$. Conversely, let us assume that J^* is positive over $[-\xi,\xi,]$. Let $\lambda_{j,m}$, $(j=1,2,\dots,m)$ be the zeros of the symmetric OP $p_m(\lambda)$ such that $\lambda_{j,m} < \lambda_{j+1,m}$. Note that $\lambda_{1,m} < 0$. Set $r(\lambda) := p_m(\lambda)/(\lambda - \lambda_{1,m})$. Using the Gauss-Jacobi formula we have

$$\begin{aligned} 0 < J^*[r^2(\lambda)] &= J[(\kappa^2-\lambda^2)r^2(\lambda)] \\ &= \sum_{j=1}^{m} \nu_{j,m}(\kappa^2 - (\lambda_{j,m})^2) r^2(\lambda_{j,m}), \end{aligned}$$

where $\nu_{j,m}$ (>0) are the Christoffel coefficients (3.2). Since $r(\lambda_{j,m}) = 0$, $(j=2,\dots,m)$, we obtain $\kappa < \lambda_{1,m}$ from $\kappa^2 - (\lambda_{1,m})^2 > 0$ and $\kappa < 0$, thus, $\kappa \le -\xi$. $\square$

We now consider a successive $(n=0,1,\dots)$ use of the Christoffel transformations

$$(5.1) \qquad p_k^{(n+1)} = \frac{1}{(\kappa^{(n)})^2 - \lambda^2}\left(A_k^{(n)} p_k^{(n)} + p_{k+2}^{(n)}\right), \qquad A_k^{(n)} := -\frac{p_{k+2}^{(n)}(\kappa^{(n)})}{p_k^{(n)}(\kappa^{(n)})}$$

to generate a sequence of kernel polynomials

$$\{p_k^{(0)} := p_k(\lambda)\} \to \{p_k^{(1)} := p_k^*(\lambda)\} \to \{p_k^{(2)}\} \to \cdots,$$

where $p_k^{(n)}(\kappa^{(n)}) \ne 0$ follows from $\kappa^{(n)} < \lambda_{1,k}^{(n)}$ for the zeros $\{\lambda_{j,k}^{(n)}\}$ of $p_k^{(n)}(\lambda)$. Let us consider the compatibility condition of the system of linear equations

$$P^{(n+1)} = \frac{1}{(\kappa^{(n)})^2 - \lambda^2}\begin{bmatrix} A_1^{(n)} & 0 & 1 & 0 & \\ 0 & A_2^{(n)} & 0 & 1 & \ddots \\ & \ddots & \ddots & \ddots & \ddots \end{bmatrix} P^{(n)},$$

$$\begin{bmatrix} 0 & 1 & 0 & \\ (a_1^{(n)})^2 & 0 & 1 & \ddots \\ 0 & (a_2^{(n)})^2 & 0 & \ddots \\ & \ddots & \ddots & \ddots \end{bmatrix} P^{(n)} = \lambda P^{(n)}, \qquad P^{(n)} := \begin{bmatrix} p_1^{(n)} \\ p_2^{(n)} \\ p_3^{(n)} \\ \vdots \end{bmatrix}.$$

The first equation is the system of the Christoffel transformations. The second one is that of the three-terms recurrence relation. Inserting the Christoffel transformations to the three-terms recurrence relation we have

$$\left((a_k^{(n+1)})^2 A_{k-1}^{(n)} - (a_k^{(n)})^2 A_k^{(n)}\right) p_{k-1}^{(n)} + \left(A_{k+1}^{(n)} - (a_{k+2}^{(n)})^2 - A_k^{(n)} + (a_k^{(n+1)})^2\right) p_{k+1}^{(n)} = 0.$$

Hence, as the first compatibility condition we obtain

$$\begin{aligned} (a_k^{(n+1)})^2 &= (a_k^{(n)})^2 \frac{A_k^{(n)}}{A_{k-1}^{(n)}} \\ &= (a_k^{(n)})^2 \frac{p_{k-1}^{(n)}(\kappa^{(n)})}{p_k^{(n)}(\kappa^{(n)})} \frac{p_{k+2}^{(n)}(\kappa^{(n)})}{p_{k+1}^{(n)}(\kappa^{(n)})}. \end{aligned}$$

Let us set

$$(5.2) \qquad \hat{u}_k^{(n)} := (a_k^{(n)})^2 \frac{p_{k-1}^{(n)}(\kappa^{(n)})}{p_k^{(n)}(\kappa^{(n)})}.$$

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It follows from $p_{-1}^{(n)} = 0$ that $\hat{u}_0^{(n)} = 0$. Let $\lambda_{j,k}^{(n)}$, $(j = 1, \ldots, k)$ be the zeros of the OP $p_k^{(n)}(\lambda)$. Note that in the partial fraction expansion

$$\frac{p_{k-1}^{(n)}(\kappa^{(n)})}{p_k^{(n)}(\kappa^{(n)})} = \sum_{j=1}^{k} \frac{\rho_{j,k}^{(n)}}{\kappa^{(n)} - \lambda_{j,k}^{(n)}}, \qquad \rho_{j,k}^{(n)} := \frac{p_{k-1}^{(n)}(\lambda_{j,k}^{(n)})}{p_k'^{(n)}(\lambda_{j,k}^{(n)})}$$

the residues $\rho_{j,k}^{(n)}$ are positive. This is proved by using the interlacing property

$$\lambda_{1,k}^{(n)} < \lambda_{1,k-1}^{(n)} < \lambda_{2,k}^{(n)} < \lambda_{2,k-1}^{(n)} < \cdots < \lambda_{k-1,k-1}^{(n)} < \lambda_{k,k}^{(n)}.$$

It follows from the positivity of the linear functional J^* (Theorem 5.1) that $\kappa^{(n)} - \lambda_{1,k}^{(n)} < 0$. Thus, $p_{k-1}^{(n)}(\kappa^{(n)})/p_k^{(n)}(\kappa^{(n)}) < 0$ and hence $\hat{u}_k^{(n)} < 0$.

Inserting $\hat{u}_k^{(n)}$ into the three-terms recurrence relation we derive

$$(a_{k+1}^{(n)})^2 = \hat{u}_{k+1}^{(n)} \left(\kappa^{(n)} + \hat{u}_k^{(n)}\right).$$

Similarly we have $(a_k^{(n+1)})^2 = \hat{u}_k^{(n)} \left(\kappa^{(n)} + \hat{u}_{k+1}^{(n)}\right)$. We eliminate $(a_k^{(n+1)})^2$ to obtain

$$\hat{u}_k^{(n+1)}(\kappa^{(n+1)} + \hat{u}_{k-1}^{(n+1)}) = \hat{u}_k^{(n)}(\kappa^{(n)} + \hat{u}_{k+1}^{(n)}), \tag{5.3}$$

$$\hat{u}_0^{(n)} = 0, \quad \hat{u}_k^{(n)} < 0, \quad \kappa^{(n)} \le -\xi < 0, \quad (n = 0, 1, \ldots, \quad k = 1, 2, \ldots). \tag{5.4}$$

Equation (5.3) is equivalent to the first compatibility condition. Spiridonov-Zhedanov [29] derived (5.3) with a negative free parameter $\kappa^{(n)} < 0$. In our case, $\kappa^{(n)}$ should satisfy $\kappa^{(n)} \le -\xi < 0$ as in (5.4) to guarantee the positivity of the linear functional and the Hankel determinants $D_k^{(n)}$. Define

$$u_k^{(n)} := \kappa^{(n)} \hat{u}_k^{(n)}, \qquad \delta^{(n)} := \frac{1}{(\kappa^{(n)})^2}. \tag{5.5}$$

By a scale change $u_k^{(n)} \to 1/(\xi^2 M) u_k^{(n)}$, we can relax the condition $0 < \delta^{(n)} \le 1/\xi^2$ to $0 < \delta^{(n)} \le M$ for some positive constant M. Thus, we obtain the following result.

THEOREM 5.2. *Let $u_k^{(n)}$ and $\delta^{(n)}$ be defined by (5.2) and (5.5). Then the Christoffel transformations (5.1) for symmetric OPs induce the recurrence relation*

$$u_k^{(n+1)} = \frac{1 + \delta^{(n)} u_{k+1}^{(n)}}{1 + \delta^{(n+1)} u_{k-1}^{(n+1)}} u_k^{(n)}, \quad (n = 0, 1, \ldots, \quad k = 1, 2, \ldots) \tag{5.6}$$

with the additional conditions

$$u_0^{(n)} = 0, \quad 0 < u_k^{(n)}, \quad 0 < \delta^{(n)} \le M.$$

This implies that the parameter $\delta^{(n)}$ is positive and bounded.

R. Hirota [12] derived the same recurrence relation (5.6) with a non-zero constant $\delta^{(n)}$, namely, $-\infty < \delta^{(n)} < 0$ or $0 < \delta^{(n)} < \infty$. The positivity and boundedness of $\delta^{(n)}$ has not been considered in [12, 29]. It is to be noted that the positivity and boundedness of $\delta^{(n)}$ will be important to prove convergence and stability of the resulting numerical algorithm.

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The condition $u_{2m}^{(n)} = 0$ in (2.4) is satisfied in the case where the successive Christoffel transformations of moments hold $|s_{2i+2j}^{(n)}|_{0\le i,j\le m} = 0$. Here, Equation (2.3) describes a deformation of a finite number of symmetric OPs.

Keeping t a constant, we take a limit $\delta^{(n)} \to +0$ such that $\delta^{(n+1)}/\delta^{(n)} \to 1$. We then derive the semi-infinite LV

$$\frac{du_k}{dt} = u_k(u_{k+1} - u_{k-1}), \quad u_0(t) = 0, \quad (k = 1, 2, \dots) \tag{5.7}$$

for the variable $u_k = u_k(t)$ from the recurrence relation. This process corresponds to the limit $\kappa^{(n)} \to -\infty$ and does not violate the positivity of linear functionals.

The system (5.7) is called the LV system in mathematical biology, the Langmuir lattice in statistical physics, a discrete KdV equation in integrable systems [23]. Conversely, the recurrence relation (5.6) is a discrete-time version of the LV system with a variable step size $\delta^{(n)}$. The most important common feature is the existence of an explicit solution $u_k^{(n)}$ and $u_k(t)$ expressed as ratio of Hankel determinants [12, 14, 15]. Equation (5.6) is rather different from the usual Euler scheme

$$v_k^{(n+1)} + \delta^{(n)} v_k^{(n)} v_{k-1}^{(n)} = v_k^{(n)}(1 + \delta^{(n)} v_{k+1}^{(n)})$$

of (5.7).

The second compatibility condition of the Christoffel transformations and the three-terms recurrence relation

$$A_{k+1}^{(n)} - (a_{k+2}^{(n)})^2 - A_k^{(n)} + (a_k^{(n+1)})^2 = 0$$

is automatically satisfied given (5.3). Indeed, we see

$$\begin{aligned}
&A_{k+1}^{(n)} - A_k^{(n)} \\
&= -\frac{p_{k+3}^{(n)}(\kappa^{(n)})}{p_{k+1}^{(n)}(\kappa^{(n)})} + \frac{p_{k+2}^{(n)}(\kappa^{(n)})}{p_k^{(n)}(\kappa^{(n)})} = \frac{p_{k+1}^{(n)}(\kappa^{(n)})/p_k^{(n)}(\kappa^{(n)}) - p_{k+3}^{(n)}(\kappa^{(n)})/p_{k+2}^{(n)}(\kappa^{(n)})}{p_{k+1}^{(n)}(\kappa^{(n)})/p_{k+2}^{(n)}(\kappa^{(n)})} \\
&= \frac{(\kappa^{(n)} + \hat{u}_k^{(n)}) - (\kappa^{(n)} + \hat{u}_{k+2}^{(n)})}{1/(\kappa^{(n)} + \hat{u}_{k+1}^{(n)})} = (\hat{u}_k^{(n)} - \hat{u}_{k+2}^{(n)})(\kappa^{(n)} + \hat{u}_{k+1}^{(n)}) \\
&= -\hat{u}_{k+2}^{(n)}(\kappa^{(n)} + \hat{u}_{k+1}^{(n)}) + \hat{u}_k^{(n+1)}(\kappa^{(n+1)} + \hat{u}_{k-1}^{(n+1)}) = (a_{k+2}^{(n)})^2 - (a_k^{(n+1)})^2.
\end{aligned}$$

In this section, it is shown that the successive Christoffel transformations (5.1) of symmetric OPs induce a deformation of the coefficients $\{a_k^{(n)}\}$ of the three-terms recurrence relation. The resulting deformation equation (5.6) is the dLV system having the positivity and boundedness of the parameter $\delta^{(n)}$.

6. Numerical experimentations. Finally, we give some numerical examples on the relative accuracy of the computed singular values by the mdLVs algorithm and other today's standard algorithms for the bidiagonal singular value problem with double-precision floating point arithmetic.[1] Here, we use the DBDSLV code of the I-SVD Library [18] for the mdLVs algorithm with the second generalized Newton shift $\Theta_2(B)$, the DBDSQR code of LAPACK [22] for the Demmel-Kahan QR algorithm [7], the DLASQ code [22] for the differential qd algorithm with the aggressive shift (dqds) [8], the DBDSDC code [22] for the

[1] CPU: Intel Core 2 Extreme X9650 3.00 GHz, Memory: 8 GB, OS: Linux kernel 2.6.29, Compiler: gfortran 4.3.2, Library: LAPACK 3.2.1 [22], I-SVD Library [18], Machine epsilon: $\varepsilon = 2.220446049250313 \times 10^{-16}$.

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divide and conquer algorithm (D&C) [10], the DSTEBZ code [22] for the bisection method. The bisection method is highly accurate but very slow. To evaluate these algorithms we need bidiagonal test matrices whose singular values are randomly or artificially given in an interval, for example $(0,\ 1]$, but are exactly known. In this paper, we generate such bidiagonal test matrices by the Golub-Kahan-Lanczos method [33] through multiple-precision floating point arithmetic.

In Figure 6.1, we compare the relative errors in the computed singular values by the mdLVs (DBDSLV code) with the Demmel-Kahan QR (DBDSQR code), the dqds (DLASQ code), the D&C (DBDSDC code). The Demmel-Kahan QR uses QR iteration without shift to compute tiny singular values to high relative accuracy [6]. In the final stage of convergence, DLASQ calls the dqds iteration with a zero shift, while DBDSLV calls the dLV iteration (2.3). The reason why the dLV algorithm computes even the tiniest singular values to high relative accuracy is related to the property $1+\delta^{(n+1)}u_{k-1}^{(n+1)} > 1$ in (2.3). The 1000×1000 bidiagonal random matrix B_1 has singular values such that

$$\sigma_{1000} = 1/888.504408243616 < \sigma_{999} < \cdots < \sigma_2 < \sigma_1 = 1.00000000000000.$$

The condition number of B_1 is then σ_1/σ_{1000}. The sum E_{sum1} of the relative errors of the 1000 singular values is computed as

$$\begin{aligned}
E_{\text{sum1}} &= 2.66529621185386 \times 10^{-13} && \text{for the mdLVs (DBDSLV)},\\
E_{\text{sum1}} &= 1.56457359160163 \times 10^{-12} && \text{for the QR (DBDSQR)},\\
E_{\text{sum1}} &= 6.45198203659775 \times 10^{-13} && \text{for the dqds (DLASQ)},\\
E_{\text{sum1}} &= 2.33427683024027 \times 10^{-13} && \text{for the D\&C (DBDSDC)}.
\end{aligned}$$

The maximal relative error E_{max1} with respect to the 1000 singular values is

$$\begin{aligned}
E_{\text{max1}} &= 2.28258949369991 \times 10^{-15} && \text{for the mdLVs (DBDSLV)},\\
E_{\text{max1}} &= 9.47911409172151 \times 10^{-14} && \text{for the QR (DBDSQR)},\\
E_{\text{max1}} &= 3.81199853522746 \times 10^{-15} && \text{for the dqds (DLASQ)},\\
E_{\text{max1}} &= 1.34754253759979 \times 10^{-15} && \text{for the D\&C (DBDSDC)}.
\end{aligned}$$

In Figure 6.2, we compare the relative errors in the computed singular values obtained by the mdLVs (DBDSLV) with those of the Demmel-Kahan QR (DBDSQR), the dqds (DLASQ), the D&C (DBDSDC). Here, we introduce a 50×50 bidiagonal matrix B_2 having singular values $1,\ \ \varepsilon^{1/49},\ \ \varepsilon^{2/49},\ \ \ldots,\ \varepsilon^{48/49},\ \varepsilon$, where ε is the machine epsilon. The condition number of B_2 is then $\sigma_1/\sigma_{50} = 1/\varepsilon = 4.50359962737050 \times 10^{15}$. According to [6], the D&C does not guarantee that the tiny singular values are computed to high relative accuracy. The sum E_{sum2} of the relative errors of the 50 singular values is computed as

$$\begin{aligned}
E_{\text{sum2}} &= 9.30226226185777 \times 10^{-15} && \text{for the mdLVs (DBDSLV)},\\
E_{\text{sum2}} &= 2.39019061564147 \times 10^{-14} && \text{for the QR (DBDSQR)},\\
E_{\text{sum2}} &= 1.39452380691172 \times 10^{-14} && \text{for the dqds (DLASQ)},\\
E_{\text{sum2}} &= 1.28173379248682 \times 10^{-1} && \text{for the D\&C (DBDSDC)}.
\end{aligned}$$

The maximal relative error E_{max2} with respect to the 50 singular values is

$$\begin{aligned}
E_{\text{max2}} &= 5.87427280192174 \times 10^{-16} && \text{for the mdLVs (DBDSLV)},\\
E_{\text{max2}} &= 1.83578543181057 \times 10^{-15} && \text{for the QR (DBDSQR)},\\
E_{\text{max2}} &= 8.35327903600726 \times 10^{-16} && \text{for the dqds (DLASQ)},\\
E_{\text{max2}} &= 6.25196422083310 \times 10^{-2} && \text{for the D\&C (DBDSDC)}.
\end{aligned}$$

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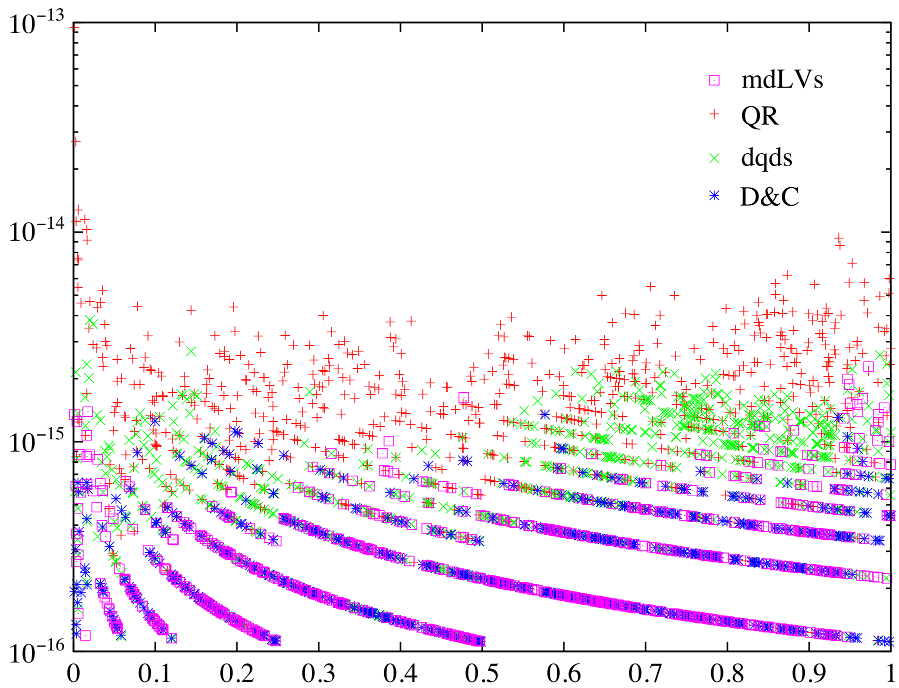

FIG. 6.1. *A graph of the magnitude of the computed singular values of a* 1000×1000 *bidiagonal random matrix* B_1 *(x-axis) and the relative errors in the corresponding singular values (y-axis) computed by mdLVs (DBDSLV), Demmel-Kahan QR (DBDSQR), dqds (DLASQ), D&C (DBDSDC).*

The third test matrix B_3 is a 301×301 bidiagonal matrix having singular values

$$1, \ 10^{-1/6}, \ 10^{-2/6}, \ \ldots, \ 10^{-299/6}, \ 10^{-300/6}.$$

Several large and tiny singular values of B_3 are

$$\begin{aligned}
&\sigma_1(B_3) = 1.00000000000000 \times 10^{0},\\
&\sigma_2(B_3) = 6.81292069057961 \times 10^{-1},\\
&\sigma_3(B_3) = 4.64158883361277 \times 10^{-1},\\
&\cdots\\
&\sigma_{299}(B_3) = 2.15443469003189 \times 10^{-50},\\
&\sigma_{300}(B_3) = 1.46779926762206 \times 10^{-50},\\
&\sigma_{301}(B_3) = 1.00000000000000 \times 10^{-50}.
\end{aligned}$$

The condition number of B_3 is then 10^{50}. The sum E_{sum3} of the relative errors of the 301 singular values computed by the mdLVs (DBDSLV), the Demmel-Kahan QR (DBDSQR), the dqds (DLASQ), the D&C (DBDSDC), the bisection (DSTEBZ) is computed as follows

$$\begin{aligned}
E_{\text{sum3}} &= 8.25112141717703 \times 10^{-14} && \text{for the mdLVs (DBDSLV)},\\
E_{\text{sum3}} &= 1.59645456456799 \times 10^{-13} && \text{for the QR (DBDSQR)},\\
E_{\text{sum3}} &= 8.22908954851692 \times 10^{-14} && \text{for the dqds (DLASQ)},\\
E_{\text{sum3}} &= 1.51104134213085 \times 10^{34} && \text{for the D\&C (DBDSDC)},\\
E_{\text{sum3}} &= 2.85925285862472 \times 10^{-14} && \text{for the bisection (DSTEBZ)}.
\end{aligned}$$

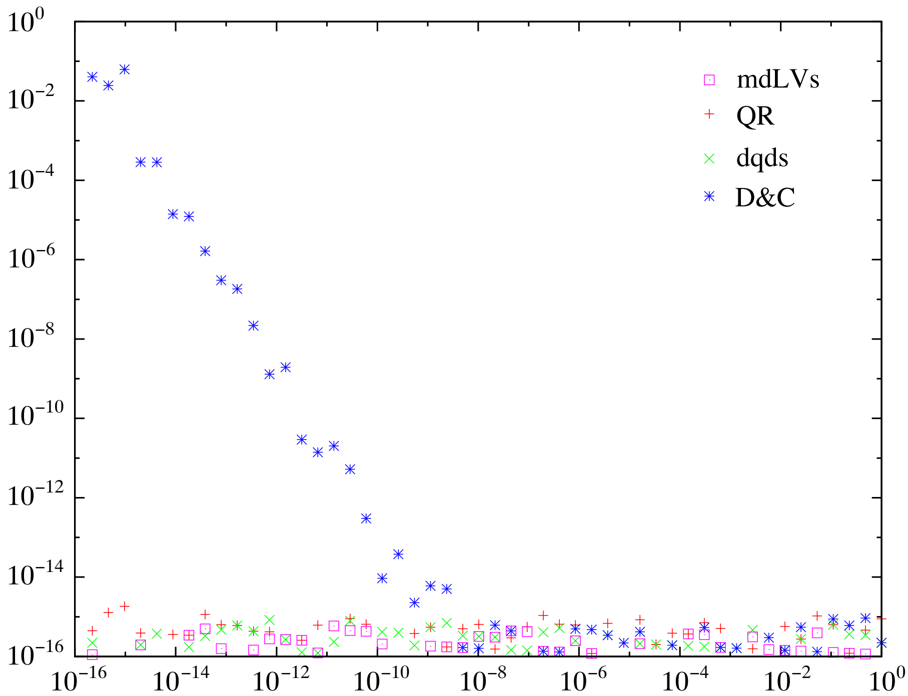

FIG. 6.2. *A graph of the magnitude of the computed singular values of a* 50×50 *bidiagonal matrix* B_2 *(*x*-axis) and the relative errors in the corresponding singular values (*y*-axis) computed by mdLVs (DBDSLV), Demmel-Kahan QR (DBDSQR), dqds (DLASQ), D&C (DBDSDC).*

The maximal relative error $E_{\max 3}$ with respect to the 301 singular values is

$$\begin{aligned}
E_{\max3} &= 1.08902767362569 \times 10^{-15} && \text{for the mdLVs (DBDSLV)},\\
E_{\max3} &= 2.19692596703967 \times 10^{-15} && \text{for the QR (DBDSQR)},\\
E_{\max3} &= 1.35525271560688 \times 10^{-15} && \text{for the dqds (DLASQ)},\\
E_{\max3} &= 4.54473724050997 \times 10^{33} && \text{for the D\&C (DBDSDC)},\\
E_{\max3} &= 3.59168891967719 \times 10^{-16} && \text{for the bisection (DSTEBZ)}.
\end{aligned}$$

7. Concluding remarks. The dLV and the mdLVs are new algorithms for computing singular values of regular bidiagonal matrices. The origin of these algorithm is in the theory of discrete-time integrable systems. Convergence of the algorithms to the singular values is proved in the sequence of papers [14, 15, 16] under the assumption of positivity and boundedness of the discrete step-size $\delta^{(n)}$. In this paper, we reconsider the derivation of the dLV iteration (2.3) as a deformation equation of symmetric OPs and prove that the parameter $\delta^{(n)}$ is positive and bounded *by definition*, namely, $0 < \delta^{(n)} < \delta_+$. Therefore, the positivity of the mdLVs algorithm follows.

As a natural consequence of the positivity of the dLV and the mdLVs algorithms, high relative accuracy of the computed singular values is observed. The mdLVs algorithm is a fast algorithm and will be effective in some numerical problems in chemistry and material science where the smallest singular values are very important.

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