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Accurate Computation of Singular Values in Terms of Shifted Integrable Schemes

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A new scheme with a shift of origin for computing singular values σ_k is presented. A shift θ is introduced into the recurrence relation defined by the discrete integrable Lotka–Volterra system with variable step-size. A suitable shift strategy is given so that the singular value computation becomes numerically stable. It is proved that variables in the new scheme converge to $\sigma_k^2 - \sum \theta^2$. A comparison of the zero-shift and the nonzero-shift routines is drawn. With respect to both the computational time and the numerical accuracy, it is shown that the nonzero-shift routine is more accurate and faster than a credible LAPACK routine for singular values at least in four different types of test matrices.

Key words: discrete Lotka–Volterra system, shift of origin, singular value

1. Introduction

In 1965 Golub and Kahan [6] found that a singular value decomposition (SVD) for any rectangular matrix $A \in \mathbf{R}^{l\times m}$ $(l > m)$ can be accomplished by using both the Householder transformation and the QR scheme. First we apply a sequence of Householder transformations to obtain a bidiagonalization B of A such that

$$\begin{pmatrix} B \\ 0 \end{pmatrix} = U^\top AV, \quad B = \begin{pmatrix} b_{11} & b_{12} & & \\ & b_{22} & \ddots & \\ & & \ddots & b_{m-1,m} \\ \mathbf{0} & & & b_{m,m} \end{pmatrix},$$

where U and V are suitable orthogonal matrices and $\top$ denotes the transposed. Then it becomes possible to obtain singular values of B by the QR scheme for the symmetric tridiagonal matrix $B^\top B$. The singular values of B are congruent with those of A. When $l < m$, the Golub-Kahan scheme also acts well through $(B \;\; 0) = U^\top AV$.

Several results based on their idea have been still observed. Especially, the QR scheme part is improved by Golub–Reinsch [5], Demmel–Kahan [3] and so on. Golub–Reinsch introduced a shift of origin into the QR scheme. The Golub-Reinsch version computes an SVD of B much faster than the original QR scheme. In 1990 Demmel–Kahan proposed a definitive version of the QR scheme with shift, and then were awarded the second SIAM prize in numerical linear algebra. The Demmel–Kahan scheme is open to the public as a reliable SVD routine "DBDSQR" in a library of Fortan 77 routines "Linear Algebra PACKage (LAPACK)" [1] for solving the most commonly occurring problems in numerical linear algebra. There are also some LAPACK routines for computing singular values not an SVD of B. One of the LAPACK routines for computing only the singular values is the DLASQ routine. The DLASQ routine is based on the differential quotient difference with shift (dqds) scheme [2, 12]. However, to the best of our knowledge, the convergence of the dqds scheme has not been theoretically proved.

On the other hand singular values of B are shown to be computed [14] by using the discrete integrable Lotka–Volterra system with fixed discrete step-size $\delta = 1$. The convergence speed is accelerated by introduing the discrete Lotka–Volterra system with arbitrary positive constant step-size $\delta > 0$ [9]. Though the convergence speed grows faster as δ becomes larger, numerical accuracy is deteriorated by an inappropriate choice of step-size in some cases. Moreover a numerical scheme [10] for computing the singular values is designed in terms of the discrete Lotka–Volterra system with variable step-size (vdLV) [8, 13]

$$u_k^{(n+1)}\left(1+\delta^{(n+1)}u_{k-1}^{(n+1)}\right) = u_k^{(n)}\left(1+\delta^{(n)}u_{k+1}^{(n)}\right), \quad k = 1, \ldots, 2m-1, \tag{1}$$

$$u_0^{(n)} \equiv 0, \quad u_{2m}^{(n)} \equiv 0, \quad 0 < \delta^{(n)} < M, \quad n = 0, 1, \ldots. \tag{2}$$

where $u_k^{(n)}$ and $\delta^{(n)}$ denote the value of u_k and δ, respectively, at the discrete time $\sum_{i=0}^{n-1} \delta^{(i)}$ and M is some positive constant. In this paper we call this scheme the dLV scheme, for short. The step-size $\delta^{(n)}$ of the dLV scheme can be changed at each step n. A better choice of the stepwise parameter $\delta^{(n)}$ gives a benefit from viewpoint of the convergence speed and the numerical accuracy. However it has not been known how to accelerate the dLV scheme by introducing a shift.

In this paper we design a nonzero-shift version (named *the mdLVs routine*) of the dLV routine and compare it with the zero-shift dLV routine in singular value computation of B. In a numerical test, the mdLVs routine requires the computational time much less than the dLV routine. The singular values computed by the mdLVs routine are shown to have a higher relative accuracy than that of the dLV routine. From viewpoint of both convergence speed and numerical accuracy, the mdLVs routine is remarkably better than DBDSQR routine (without computing singular vectors) at least in four types of test matrices. The mdLVs routine also has a better scalability.

Our goal in this paper is threefold: The first is to introduce a shift of origin into the dLV scheme for accelerating the convergence. The second is to give a shift strategy for avoiding numerical instability. The third is to prove that the mdLVs variable always converges to singular values as $n \to \infty$. In the new scheme, it is possible to find how to determine a suitable shift such that the mdLVs varibles stably converge to shifted singular values. The property of holding the positivity on the discrete Lotka–Volterra system takes an active part in the numerical stability of the shifted scheme.

This paper is organized as follows. In Section 2, we introduce a new system and present two theorems for singular value computation of B. In Section 3, we show how to estimate the amount of shift so that the resulting scheme is numerically stable. In Section 4, we prove a convergence of the new scheme with a shift. Two particular cases where B has zero entries are described in Section 5. In Section 6, we show test results for several examples.

2. The Shifted Integrable Scheme

The main purpose of this section is to introduce a shift of origin into a certain recurrence relation derived from the vdLV system (1). We then investigate an influence of the shift on the singular values of the upper bidiagonal matrix B.

Let us begin our analysis by introducing three mappings $\psi_j^{(n)}$, $j = 1, 2, 3$ and two bijections $\phi_j^{(n)}$, $j = 1, 2$, for some n. Let $\psi_j^{(n)}$, $j = 1, 2, 3$ and $\phi_j^{(n)}$, $j = 1, 2$ be

$$
\begin{aligned}
\psi_1^{(n)}&: \bar{W}^{(n)} = \left\{\bar{w}^{(n)} \,\middle|\, \bar{w}^{(n)} \in \mathbf{R}^{2m-1}\right\} \to U^{(n)} = \left\{u^{(n)} \,\middle|\, u^{(n)} \in \mathbf{R}^{2m-1}\right\},\\
&\quad \bar{w}^{(n)} = \left(\bar{w}_1^{(n)}, \bar{w}_2^{(n)}, \ldots, \bar{w}_{2m-1}^{(n)}\right) \mapsto u^{(n)} = \left(u_1^{(n)}, u_2^{(n)}, \ldots, u_{2m-1}^{(n)}\right),\\
\psi_2^{(n)}&: U^{(n)} \to V^{(n)} = \left\{v^{(n)} \,\middle|\, v^{(n)} \in \mathbf{R}^{2m-1}\right\},\\
&\quad u^{(n)} \mapsto v^{(n)} = \left(v_1^{(n)}, v_2^{(n)}, \ldots, v_{2m-1}^{(n)}\right),\\
\psi_3^{(n)}&: \bar{V}^{(n)} = \left\{\bar{v}^{(n)} \,\middle|\, \bar{v}^{(n)} \in \mathbf{R}^{2m-1}\right\} \to W^{(n+1)} = \left\{w^{(n+1)} \,\middle|\, w^{(n+1)} \in \mathbf{R}^{2m-1}\right\}, \qquad (3)\\
&\quad \bar{v}^{(n)} = \left(\bar{v}_1^{(n)}, \bar{v}_2^{(n)}, \ldots, \bar{v}_{2m-1}^{(n)}\right) \mapsto w^{(n+1)} = \left(w_1^{(n+1)}, w_2^{(n+1)}, \ldots, w_{2m-1}^{(n+1)}\right),\\
\phi_1^{(n)}&: W^{(n)} = \left\{w^{(n)} \,\middle|\, w^{(n)} \in \mathbf{R}^{2m-1}\right\} \to \bar{W}^{(n)},\\
&\quad w^{(n)} = \left(w_1^{(n)}, w_2^{(n)}, \ldots, w_{2m-1}^{(n)}\right) \mapsto \bar{w}^{(n)},\\
\phi_2^{(n)}&: V^{(n)} \to \bar{V}^{(n)}, \quad v^{(n)} \mapsto \bar{v}^{(n)}
\end{aligned}
$$

where $\psi_1^{(n)} : \bar{w}^{(n)} \mapsto u^{(n)}$, $\psi_2^{(n)} : u^{(n)} \mapsto v^{(n)}$ and $\psi_3^{(n)} : \bar{v}^{(n)} \mapsto w^{(n+1)}$ are defined by

$$
\begin{aligned}
&u_k^{(n)} = \frac{\bar{w}_k^{(n)}}{1 + \delta^{(n)} u_{k-1}^{(n)}}, \quad v_k^{(n)} = u_k^{(n)}\left(1 + \delta^{(n)} u_{k+1}^{(n)}\right) \quad \text{and} \quad w_k^{(n+1)} = \bar{v}_k^{(n)},\\
&u_0^{(n)} \equiv 0, \quad u_{2m}^{(n)} \equiv 0, \quad k = 1, 2, \ldots, 2m-1,
\end{aligned} \qquad (4)
$$

respectively. The explicit forms of the mappings $\phi_j^{(n)}$, $j = 1, 2$ will be defined in the subsequent discussion. Under the boundary condition $u_0^{(n)} \equiv 0$ and $u_{2m}^{(n)} \equiv 0$, the variables $u_k^{(n)}$ and $v_k^{(n)}$ in $\psi_j^{(n)}$, $j = 1, 2$ are also given as

$$
\begin{aligned}
&u_1^{(n)} = \bar{w}_1^{(n)},\ u_2^{(n)} = \frac{\bar{w}_2^{(n)}}{1 + \delta^{(n)} \bar{w}_1^{(n)}}, \ldots, \\
&u_{2m-1}^{(n)} = \frac{\bar{w}_{2m-1}^{(n)} \big|}{\big| \ 1} + \frac{\delta^{(n)} \bar{w}_{2m-2}^{(n)} \big|}{\big| \ 1} + \cdots + \frac{\delta^{(n)} \bar{w}_2^{(n)} \big|}{\big| 1 + \delta^{(n)} \bar{w}_1^{(n)}}, \\
&v_1^{(n)} = u_1^{(n)} \left(1 + \delta^{(n)} u_2^{(n)}\right), \ldots,\ v_{2m-2}^{(n)} = u_{2m-2}^{(n)} \left(1 + \delta^{(n)} u_{2m-1}^{(n)}\right),\ v_{2m-1}^{(n)} = u_{2m-1}^{(n)},
\end{aligned}
$$

in terms of $\bar{w}_k^{(n)}$ and $v_k^{(n)}$, respectively. Hence we see that $\psi_j^{(n)}$, $j = 1, 2$ are bijections. It is also obvious that $\psi_3^{(n)}$ is a bijection.

Let us consider that $\psi_j^{(n)}$, $j = 1, 2, 3$ and $\phi_j^{(n)}$, $j = 1, 2$ are defined as (3) and (4) for every n. Moreover, in this section, we assume that $w_k^{(n)} > 0$, $u_k^{(n)} > 0$, $v_k^{(n)} > 0$ and $\bar{w}_k^{(n)} > 0$, $\bar{v}_k^{(n)} > 0$, $k = 1, 2, \ldots, 2m-1$ for every n. A composite mapping

$$\psi^{(n+1)} \equiv \psi_3^{(n)} \circ \phi_2^{(n)} \circ \psi_2^{(n)} \circ \psi_1^{(n)} \circ \phi_1^{(n)} \tag{5}$$

produces a maping $W^{(n)} \to W^{(n+1)}$ shown as in Fig. 1. Similarly, $\psi_1^{(n+1)} \circ \phi_1^{(n+1)} \circ \psi_3^{(n)} \circ \phi_2^{(n)} \circ \psi_2^{(n)} \colon U^{(n)} \to U^{(n+1)}$.

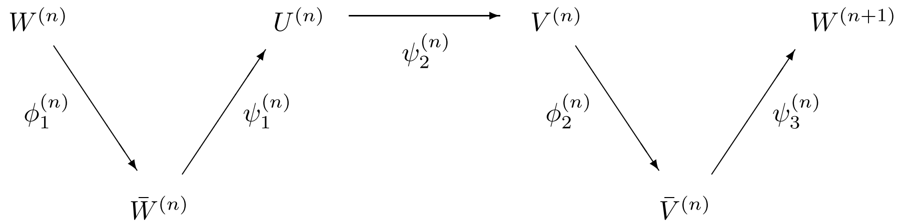

Fig. 1. An evolution $W^{(n)} \to W^{(n+1)}$.

Let us introduce here $\tilde{\phi}_j^{(n)}$, $j = 1, 2$ such that $\bar{w}^{(n)} = \tilde{\phi}_1^{(n)}\left(w^{(n)}\right) = w^{(n)}$ and $\bar{v}^{(n)} = \tilde{\phi}_2^{(n)}\left(v^{(n)}\right) = v^{(n)}$ as a concrete example of the bijections $\phi_j^{(n)}$, $j = 1, 2$, respectively. Then the vdLV system (1) can be also regarded as a dynamical system which generates an evolution from n to $n+1$ of $u^{(n)}$ by a composite mapping $\psi_1^{(n+1)} \circ \tilde{\phi}_1^{(n+1)} \circ \psi_3^{(n)} \circ \tilde{\phi}_2^{(n)} \circ \psi_2^{(n)} \colon u^{(n)} \mapsto u^{(n+1)}$.

Let us replace $\phi_1^{(n)}$ and $\phi_2^{(n)}$ in the mapping (5) with $\tilde{\phi}_1^{(n)}$ and $\tilde{\phi}_2^{(n)}$, respectively. Then the maping $\psi^{(n+1)} \colon W^{(n)} \to W^{(n+1)}$ shown as in Fig. 1 is reduced to

$$\psi_{\mathrm{dLV}}^{(n+1)} \colon W^{(n)} = \bar{W}^{(n)} \xrightarrow{\psi_1^{(n)}} U^{(n)} \xrightarrow{\psi_2^{(n)}} V^{(n)} = \bar{V}^{(n)} \xrightarrow{\psi_3^{(n)}} W^{(n+1)}.$$

In [10], it is shown that the singular values of

$$B^{(n)} = \begin{pmatrix} \sqrt{w_1^{(n)}} & \sqrt{w_2^{(n)}} & & & \\ & \sqrt{w_3^{(n)}} & \ddots & & \\ & & \ddots & \sqrt{w_{2m-2}^{(n)}} \\ 0 & & & \sqrt{w_{2m-1}^{(n)}} \end{pmatrix}, \tag{6}$$

are invariant in n under the evolution (1). Here the sequence $B^{(n)}$ starts from $B^{(0)} = B$ and $\psi_{\mathrm{dLV}}^{(n+1)} \equiv \psi_3^{(n)} \circ \tilde{\phi}_2^{(n)} \circ \psi_2^{(n)} \circ \psi_1^{(n)} \circ \tilde{\phi}_1^{(n)}$ generates an evolution $B^{(n)} \mapsto B^{(n+1)}$. It is also proved in [10] that $\psi_{\mathrm{dLV}}^{(n)} \circ \psi_{\mathrm{dLV}}^{(n-1)} \circ \cdots \circ \psi_{\mathrm{dLV}}^{(1)} : w^{(0)} \mapsto \left(\sigma_1^2(B), 0, \sigma_2^2(B), 0, \ldots, 0, \sigma_m^2(B)\right)$ as $n \to \infty$, where $\sigma_k(B)$ denotes each singular value such that

$$\sigma_1(B) > \sigma_2(B) > \cdots > \sigma_m(B) > 0.$$

It is of significance to note that $\lambda_k \left(\left(B^{(n)}\right)^\top B^{(n)} \right)$ is invariant in n as long as the evolution $B^{(n)} \mapsto B^{(n+1)}$ is produced by $\psi_{\mathrm{dLV}}^{(n+1)}$, where $\lambda_k(T)$ is the k-th eigenvalue of T.

It has been known in matrix eigenvalue problems [2] that a shift of origin

$$\left(\bar{B}^{(n)}\right)^\top \bar{B}^{(n)} = \left(B^{(n)}\right)^\top B^{(n)} - {\theta^{(n)}}^2 I,$$

$$\bar{B}^{(n)} \equiv \begin{pmatrix} \sqrt{\bar{w}_1^{(n)}} & \sqrt{\bar{w}_2^{(n)}} & & & \\ & \sqrt{\bar{w}_3^{(n)}} & \ddots & & \\ & & \ddots & \sqrt{\bar{w}_{2m-2}^{(n)}} \\ 0 & & & \sqrt{\bar{w}_{2m-1}^{(n)}} \end{pmatrix} \tag{7}$$

is useful to accelate the convergence speed, where ${\theta^{(n)}}^2$ denotes the shift at discrete time $\sum_{i=0}^{n-1} \delta^{(i)}$. We here assume that ${\theta^{(n)}}^2$ is a suitable shift for keeping $\bar{w}_k^{(n)} > 0$, $k = 1, 2, \ldots, 2m-1$. Let us introduce a parametric bijection

$$\phi_{1;\theta^{(n)}}^{(n)} : w^{(n)} = \left(w_1^{(n)}, w_2^{(n)}, \ldots, w_{2m-1}^{(n)}\right) \mapsto \bar{w}^{(n)} = \left(\bar{w}_1^{(n)}, \bar{w}_2^{(n)}, \ldots, \bar{w}_{2m-1}^{(n)}\right),$$
$$\begin{cases} \bar{w}_{2k-2}^{(n)} + \bar{w}_{2k-1}^{(n)} = w_{2k-2}^{(n)} + w_{2k-1}^{(n)} - {\theta^{(n)}}^2, \\ \bar{w}_{2k-1}^{(n)} \bar{w}_{2k}^{(n)} = w_{2k-1}^{(n)} w_{2k}^{(n)}, \quad w_0^{(n)} \equiv 0, \quad \bar{w}_0^{(n)} \equiv 0. \end{cases} \tag{8}$$

Uniquely we can compute $\bar{w}^{(n)}$ from $w^{(n)}$ by

$$\bar{w}_{2k-1}^{(n)} = w_{2k-2}^{(n)} + w_{2k-1}^{(n)} - {\theta^{(n)}}^2 - \kappa_{2k-2}^{(n)},\ \bar{w}_{2k-1}^{(n)}\bar{w}_{2k}^{(n)} = w_{2k-1}^{(n)}w_{2k}^{(n)},\ \bar{w}_{2k-2}^{(n)} = \kappa_{2k-2}^{(n)},$$
$$\kappa_{2k-2}^{(n)} \equiv \frac{w_{2k-3}^{(n)}w_{2k-2}^{(n)} \Big|}{\Big| w_{2k-4}^{(n)} + w_{2k-3}^{(n)} - {\theta^{(n)}}^2} - \frac{w_{2k-5}^{(n)}w_{2k-4}^{(n)} \Big|}{\Big| w_{2k-6}^{(n)} + w_{2k-5}^{(n)} - {\theta^{(n)}}^2} - \cdots - \frac{w_1^{(n)}w_2^{(n)} \Big|}{\Big| w_1^{(n)} - {\theta^{(n)}}^2}. \tag{9}$$

It is worth noting that $w_{2k-1}^{(n)} \geq \bar{w}_{2k-1}^{(n)}$ and $w_{2k}^{(n)} \leq \bar{w}_{2k}^{(n)}$ from $w_1^{(n)} \geq \bar{w}_1^{(n)}$. Let us replace $\phi_1^{(n)}$ and $\phi_2^{(n)}$ in (5) with $\phi_{1;\theta^{(n)}}^{(n)}$ and $\tilde{\phi}_2^{(n)}$, respectively. Then $\psi_{\mathrm{dLVs1};\theta^{(n)}}^{(n+1)} : W^{(n)} \to W^{(n+1)}$ is also defined by the composite mapping

$$\psi_{\mathrm{mdLVs1};\theta^{(n)}}^{(n+1)} \equiv \psi_3^{(n)} \circ \tilde{\phi}_2^{(n)} \circ \psi_2^{(n)} \circ \psi_1^{(n)} \circ \phi_{1;\theta^{(n)}}^{(n)} \tag{10}$$

as follows:

$$\psi_{\mathrm{mdLVs1};\theta^{(n)}}^{(n+1)} : W^{(n)} \xrightarrow{\phi_{1;\theta^{(n)}}^{(n)}} \bar{W}^{(n)} \xrightarrow{\psi_1^{(n)}} U^{(n)} \xrightarrow{\psi_2^{(n)}} V^{(n)} = \bar{V}^{(n)} \xrightarrow{\psi_3^{(n)}} W^{(n+1)}.$$

In this paper we call the procedure from $W^{(n)}$ to $W^{(n+1)}$ by the mapping $\psi_{\mathrm{dLVs1};\theta^{(n)}}^{(n+1)}$ *the modified discrete Lotka–Volterra with shift (mdLVs) scheme I*. Let $\psi^{(n+1)}(X)$, for some matrices X, denote the mappings of the entries of X by $\psi^{(n+1)}$. Then $\left(B^{(n+1)}\right)^\top B^{(n+1)} = \psi_3^{(n)} \circ \tilde{\phi}_2^{(n)} \circ \psi_2^{(n)} \circ \psi_1^{(n)} \circ \tilde{\phi}_1^{(n)} \circ \left(\tilde{\phi}_1^{(n)}\right)^{-1} \left(\left(\bar{B}^{(n)}\right)^\top \bar{B}^{(n)}\right) = \psi_{\mathrm{dLV}}^{(n)} \circ \left(\tilde{\phi}_1^{(n)}\right)^{-1} \left(\left(\bar{B}^{(n)}\right)^\top \bar{B}^{(n)}\right)$. It is to be noted that the composite mapping $\psi_{\mathrm{dLV}}^{(n)} \circ \left(\tilde{\phi}_1^{(n)}\right)^{-1}$ generates an evolution from $\bar{B}^{(n)}$ to $B^{(n+1)}$ such that $\lambda_k\left(\left(B^{(n+1)}\right)^\top B^{(n+1)}\right) = \lambda_k\left(\left(\bar{B}^{(n)}\right)^\top \bar{B}^{(n)}\right)$. By relating it to (7), it follows that

$$\lambda_k\left(\left(B^{(n+1)}\right)^\top B^{(n+1)}\right) = \lambda_k\left(\left(B^{(n)}\right)^\top B^{(n)}\right) - {\theta^{(n)}}^2. \tag{11}$$

Therefore we have the following theorem for the mdLVs scheme I.

THEOREM 2.1. *The bidiagonal matrix*

$$B^{(n+1)} = \psi_{\mathrm{mdLVs1};\theta^{(n)}}^{(n+1)} \circ \psi_{\mathrm{mdLVs1};\theta^{(n-1)}}^{(n)} \circ \cdots \circ \psi_{\mathrm{mdLVs1};\theta^{(0)}}^{(1)} \left(B^{(0)}\right)$$

satisfies

$$\lambda_k\left(\left(B^{(0)}\right)^\top B^{(0)}\right) = \lambda_k\left(\left(B^{(n+1)}\right)^\top B^{(n+1)}\right) + \sum_{N=0}^{n} {\theta^{(N)}}^2. \tag{12}$$

Proof. From (11), we have (12). □

We here consider the case where $\phi_1^{(n)}$ is replaced by $\tilde{\phi}_1^{(n)}$ in (5). A composite mapping $\psi_3^{(n)} \circ \phi_2^{(n)} \circ \psi_2^{(n)} \circ \psi_1^{(n)} \circ \tilde{\phi}_1^{(n)}$ produces $W^{(n)} \to W^{(n+1)}$ such that

$$W^{(n)} = \bar{W}^{(n)} \xrightarrow{\psi_1^{(n)}} U^{(n)} \xrightarrow{\psi_2^{(n)}} V^{(n)} \xrightarrow{\phi_2^{(n)}} \bar{V}^{(n)} \xrightarrow{\psi_3^{(n)}} W^{(n+1)}.$$

Simultaneouly, $\psi_3^{(n)} \circ \phi_2^{(n)} \circ \psi_2^{(n)} \circ \psi_1^{(n)} \circ \tilde{\phi}_1^{(n)} : B^{(n)} \mapsto B^{(n+1)}$. Let us define a new parameteric mapping

$$\bar{\psi}_{3;\theta^{(n)}}^{(n)} : v^{(n)} = \left(v_1^{(n)}, v_2^{(n)}, \ldots, v_{2m-1}^{(n)}\right) \mapsto w^{(n+1)} = \left(w_1^{(n+1)}, w_2^{(n+1)}, \ldots, w_{2m-1}^{(n+1)}\right),$$
$$\begin{cases} w_{2k-2}^{(n+1)} + w_{2k-1}^{(n+1)} = v_{2k-2}^{(n)} + v_{2k-1}^{(n)} - {\theta^{(n)}}^2, \\ w_{2k-1}^{(n+1)} w_{2k}^{(n+1)} = v_{2k-1}^{(n)} v_{2k}^{(n)}, \quad w_0^{(n)} \equiv 0, \quad v_0^{(n)} \equiv 0, \end{cases} \tag{13}$$

with the shift ${\theta^{(n)}}^2$ which keeps $w_k^{(n+1)} > 0$, $k = 1, 2, \ldots, 2m-1$. We also see that $\bar{\psi}_{3;\theta^{(n)}}^{(n)}$ is a bijection since $\phi_{1;\theta^{(n)}}^{(n)}$ in (8) coincides with $\bar{\psi}_{3;\theta^{(n)}}^{(n)}$ in (13) by replacing $w_k^{(n)}, \bar{w}_k^{(n)}$ with $v_k^{(n)}, w_k^{(n+1)}$, respectively. Let us call the procedure from $B^{(n)}$ to $B^{(n+1)}$ by a composite mapping

$$\psi_{\mathrm{mdLVs2};\theta^{(n)}}^{(n+1)} \equiv \bar{\psi}_{3;\theta^{(n)}}^{(n)} \circ \psi_2^{(n)} \circ \psi_1^{(n)} \circ \tilde{\phi}_1^{(n)} \tag{14}$$

the mdLVs scheme II. Then we have a theorem for the mdLVs scheme II.

THEOREM 2.2. *The bidiagonal matrix*

$$B^{(n+1)} = \psi_{\mathrm{mdLVs2};\theta^{(n)}}^{(n+1)} \circ \psi_{\mathrm{mdLVs2};\theta^{(n-1)}}^{(n)} \circ \cdots \circ \psi_{\mathrm{mdLVs2};\theta^{(0)}}^{(1)} \left(B^{(0)}\right)$$

satisfies (12).

Proof. Let us introduce a mapping

$$\phi_{2;\theta^{(n)}}^{(n)} : v^{(n)} = \left(v_1^{(n)}, v_2^{(n)}, \ldots, v_{2m-1}^{(n)}\right) \mapsto \bar{v}^{(n)} = \left(\bar{v}_1^{(n)}, \bar{v}_2^{(n)}, \ldots, \bar{v}_{2m-1}^{(n)}\right),$$
$$\begin{cases} \bar{v}_{2k-2}^{(n)} + \bar{v}_{2k-1}^{(n)} = v_{2k-2}^{(n)} + v_{2k-1}^{(n)} - {\theta^{(n)}}^2, \\ \bar{v}_{2k-1}^{(n)} \bar{v}_{2k}^{(n)} = v_{2k-1}^{(n)} v_{2k}^{(n)}, \quad \bar{v}_0^{(n)} \equiv 0, \quad v_0^{(n)} \equiv 0. \end{cases} \tag{15}$$

Then we can regard $\bar{\psi}_{3;\theta^{(n)}}^{(n)}$ in (13) as a composite mapping $\psi_3^{(n)} \circ \phi_{2;\theta^{(n)}}^{(n)}$. Note here that

$$\psi_{\mathrm{mdLVs2};\theta^{(n)}=0}^{(n+1)}\left(\left(B^{(n)}\right)^\top B^{(n)}\right) = \psi_3^{(n)} \circ \phi_{2;\theta^{(n)}=0}^{(n)} \circ \psi_2^{(n)} \circ \psi_1^{(n)} \circ \tilde{\phi}_1^{(n)}\left(\left(B^{(n)}\right)^\top B^{(n)}\right)$$
$$= \psi_{\mathrm{dLV}}^{(n+1)}\left(\left(B^{(n)}\right)^\top B^{(n)}\right).$$

Hence we see that $\lambda_k\left(\psi_{\mathrm{mdLVs2};\theta^{(n)}=0}^{(n+1)}\left(\left(B^{(n)}\right)^\top B^{(n)}\right)\right) = \lambda_k\left(\left(B^{(n)}\right)^\top B^{(n)}\right)$. Moreover a mapping $\bar{\psi}_{3;\theta^{(n)}}^{(n)}$ in (13) implies that

$$\lambda_k\left(\psi_{\mathrm{mdLVs2}}^{(n+1)}\left(\left(B^{(n)}\right)^\top B^{(n)}\right)\right) = \lambda_k\left(\psi_{\mathrm{mdLVs2};\theta^{(n)}=0}^{(n)}\left(\left(B^{(n)}\right)^\top B^{(n)}\right)\right) - {\theta^{(n)}}^2,$$

since $w_k^{(n+1)} = v_k^{(n)}$ if $\theta^{(n)} = 0$. Consequently,

$$\lambda_k \left(\left(B^{(n+1)} \right)^\top B^{(n+1)} \right) = \lambda_k \left(\left(B^{(n)} \right)^\top B^{(n)} \right) - {\theta^{(n)}}^2.$$

This leads to (12). □

In this section two types of shifted integrable schemes, named the mdLVs schemes I and II, are presented. A desirable choice of the shift ${\theta^{(n)}}^2$ which guarantees a numerical stability will be discussed in the next section. A convergence to singular values of the schemes will be proved in Section 4.

3. Shift Strategy

The mapping $\phi^{(n)}_{1;\theta^{(n)}=0}$ in (8) holds $\bar{w}_k^{(n)} > 0$ if $w_k^{(n)} > 0$ for $k = 1, 2, \dots, 2m-1$. However $\bar{w}_k^{(n)}$ is not always nonzero positive when $\theta^{(n)}$ is large. The value of $\bar{w}_k^{(n)}$ does not only become negative but also numerically overflow in the worst case. For some k_0, if $\bar{w}_{2k_0-1}^{(n)} = 0$ by an inappropriate shift, then $\bar{w}_{2k_0}^{(n)}$ diverges to infinity, i.e. we can not compute $\bar{w}_{2k_0}^{(n)}$ numerically. Moreover we do not desire the case where $\bar{w}_1^{(n)} > 0, \dots, \bar{w}_{k_0-1}^{(n)} > 0, \bar{w}_{k_0}^{(n)} < 0, \dots$ by a too large shift. This is because $1 + \delta^{(n)} u_{k_0}^{(n)}$ with $u_{k_0}^{(n)} < 0$ may be zero, i.e. $u_{k_0+1}^{(n)}$ may become numerically uncomputable by the mapping $\psi_1^{(n)} : \bar{w}^{(n)} \mapsto u^{(n)}$. Hence for a rather large shift the mdLVs scheme I may be numerically unstable. There is an intimate relationship among the stability, the shift and the positivity of the variables $\bar{w}_k^{(n)}$. We here present the following fundamental theorem for keeping $\bar{w}_k^{(n)} > 0$.

Theorem 3.1. *Assume that* $w_k^{(n)} > 0$ *for* $k = 1, 2, \dots, 2m-1$. *Then* $\left(B^{(n)}\right)^\top B^{(n)}$ *is positive-definite symmetric. It holds that* $\bar{w}_k^{(n)} > 0$ *for* $k = 1, 2, \dots, 2m-1$ *if and only if* ${\theta^{(n)}}^2 < \lambda_m \left(\left(B^{(n)} \right)^\top B^{(n)} \right)$, *where* $\lambda_m \left(\left(B^{(n)} \right)^\top B^{(n)} \right)$ *is the minimal eigenvalue of* $\left(B^{(n)}\right)^\top B^{(n)}$. *Namely,* $\bar{w}_k^{(n)} > 0$ *if and only if*

$$ {\theta^{(n)}}^2 < \sigma_m^2 \left(B^{(n)} \right). \tag{16}$$

Proof. Let $w_k^{(n)} > 0$, $k = 1, 2, \dots, 2m-1$. Then it is obvious from (6) that $\sigma_k \left(B^{(n)} \right) > 0$, $k = 1, 2, \dots, m$. Simultaneously, $\lambda_k \left(\left(B^{(n)} \right)^\top B^{(n)} \right) > 0$, $k = 1, 2, \dots, m$. Hence we see that $\left(B^{(n)}\right)^\top B^{(n)}$ is positive definite and symmetric.

Let us here consider the case where ${\theta^{(n)}}^2 < \lambda_m \left(\left(B^{(n)} \right)^\top B^{(n)} \right)$. Since it is shown in Section 2 that $\lambda_k \left(\left(\bar{B}^{(n)} \right)^\top \bar{B}^{(n)} \right) = \lambda_k \left(\left(B^{(n)} \right)^\top B^{(n)} \right) - {\theta^{(n)}}^2$, $k = 1, 2, \dots, m$, we see that $\lambda_k \left(\left(\bar{B}^{(n)} \right)^\top \bar{B}^{(n)} \right) > 0$, $k = 1, 2, \dots, m$, i.e. $\left(\bar{B}^{(n)} \right)^\top \bar{B}^{(n)}$ is a positive definite and symmetric. Let $\bar{B}_k^{(n)}$, $k = 1, 2, \dots, m$ denote $k \times k$ matrices defined by

$$\bar{B}_k^{(n)} = \begin{pmatrix} \sqrt{\bar{w}_1^{(n)}} & \sqrt{\bar{w}_2^{(n)}} & & \\ & \sqrt{\bar{w}_3^{(n)}} & \ddots & \\ & & \ddots & \sqrt{\bar{w}_{2k-2}^{(n)}} \\ 0 & & & \sqrt{\bar{w}_{2k-1}^{(n)}} \end{pmatrix}, \tag{17}$$

where $\bar{B}_m^{(n)} = \bar{B}^{(n)}$. Then the positive definite and symmetric matrix $\left(\bar{B}^{(n)}\right)^\top \bar{B}^{(n)}$ satisfies $\det\left(\left(\bar{B}_k^{(n)}\right)^\top \bar{B}_k^{(n)}\right) > 0$, $k = 1, 2, \dots, m$. Note that $\det\left(\left(\bar{B}_k^{(n)}\right)^\top \bar{B}_k^{(n)}\right) = \det\left(\left(\bar{B}_k^{(n)}\right)^\top\right) \det\left(\bar{B}_k^{(n)}\right)$. Hence we derive $\prod_{j=1}^k \bar{w}_{2j-1}^{(n)} > 0$, $k = 1, 2, \dots, m$, i.e. $\bar{w}_{2k-1}^{(n)} > 0$, $k = 1, 2, \dots, m$. Moreover, it is obvious from (8) that $\bar{w}_{2k-1}^{(n)} \bar{w}_{2k}^{(n)} = w_{2k-1}^{(n)} w_{2k}^{(n)}$, $k = 1, 2, \dots, m-1$. From the assumption $w_k^{(n)} > 0$, $k = 1, 2, \dots, 2m-1$, it follows that $\bar{w}_{2k}^{(n)} > 0$, $k = 1, 2, \dots, m-1$.

Conversely, we assume that $\bar{w}_k^{(n)} > 0$, $k = 1, 2, \dots, 2m-1$. Then $\prod_{j=1}^k \bar{w}_{2j-1}^{(n)} > 0$, $k = 1, 2, \dots, m$, i.e. $\det\left(\left(\bar{B}_k^{(n)}\right)^\top \bar{B}_k^{(n)}\right) > 0$, $k = 1, 2, \dots, m$. Since $\left(\bar{B}^{(n)}\right)^\top \bar{B}^{(n)}$ is positive definite and symmetric, we see that $\lambda_k\left(\left(\bar{B}^{(n)}\right)^\top \bar{B}^{(n)}\right) > 0$, $k = 1, 2, \dots$, m. Note here that $\lambda_k\left(\left(\bar{B}^{(n)}\right)^\top \bar{B}^{(n)}\right) = \lambda_k\left(\left(B^{(n)}\right)^\top B^{(n)}\right) - {\theta^{(n)}}^2$, $k = 1, 2, \dots, m$. Hence it follows that ${\theta^{(n)}}^2 < \lambda_m\left(\left(B^{(n)}\right)^\top B^{(n)}\right)$.

Therefore it is concluded that $\bar{w}_k^{(n)} > 0$, $k = 1, 2, \dots, 2m-1$ if and only if ${\theta^{(n)}}^2 < \lambda_m\left(\left(B^{(n)}\right)^\top B^{(n)}\right)$, i.e. ${\theta^{(n)}}^2 < \sigma_m^2\left(B^{(n)}\right)$. □

The Geršgorin-type lower bound proposed by C.R. Johnson [11] helps us to estimate the minimal singular value $\sigma_m\left(B^{(n)}\right)$ in (16) as follows:

$$\sigma_m(B^{(n)}) \geq \max\left\{0, \vartheta_1^{(n)}\right\}, \quad \vartheta_1^{(n)} \equiv \min_k\left\{\sqrt{w_{2k-1}^{(n)}} - \frac{1}{2}\left(\sqrt{w_{2k-2}^{(n)}} + \sqrt{w_{2k}^{(n)}}\right)\right\}. \tag{18}$$

Combining it with Theorem 3.1, we perform a shift strategy for avoiding numerical instability of the mdLVs scheme I.

THEOREM 3.2. *Assume that the initial data is as* $w_k^{(0)} > 0$ *for* $k = 1, 2, \dots$, $2m-1$ *and* ε *is some small positive constant. Then*

$${\theta^{(n)}}^2 = \max\left\{0, \left(\max\{0, \vartheta_1^{(n)}\}\right)^2 - \varepsilon\right\} \tag{19}$$

is a safe choice for numerical stability of the mdLVs scheme I.

Next we consider a different shift stratagy from Theorem 3.2. Let us introduce a new variable

$$\vartheta_2^{(n)^2} = \frac{1}{2}\min_k \left\{ w_{2k-1}^{(n)} - \left(w_{2k-2}^{(n)} + w_{2k}^{(n)} \right) \right\}. \tag{20}$$

Then we obtain the following theorem.

Theorem 3.3. *If $\theta^{(n)^2}$ is computed by*

$$\theta^{(n)^2} = \max\left\{0, \vartheta_2^{(n)^2} - \varepsilon\right\}, \tag{21}$$

instead of (19), *then the mdLVs scheme I is also numerically stable.*

Proof. Let us consider two cases $\vartheta_1^{(n)} \leq 0$ and $\vartheta_1^{(n)} > 0$.

For $x, y \geq 0$, it is well known that $(x+y)/2 \geq \sqrt{xy}$. Note that $w_k^{(n)} > 0$, $k = 1, 2, \ldots, 2m-1$. Then we have

$$\begin{aligned}
\sqrt{w_{2k-1}^{(n)}}\vartheta_1^{(n)} &= \sqrt{w_{2k-1}^{(n)}}\min_k \left\{ \sqrt{w_{2k-1}^{(n)}} - \frac{1}{2}\left(\sqrt{w_{2k-2}^{(n)}} + \sqrt{w_{2k}^{(n)}} \right) \right\} \\
&= \min_k \left\{ w_{2k-1}^{(n)} - \sqrt{ w_{2k-1}^{(n)} \cdot \frac{1}{4}\left(\sqrt{w_{2k-2}^{(n)}} + \sqrt{w_{2k}^{(n)}} \right)^2 } \right\} \\
&\geq \min_k \left\{ \frac{1}{2} w_{2k-1}^{(n)} - \frac{1}{8}\left(\sqrt{w_{2k-2}^{(n)}} + \sqrt{w_{2k}^{(n)}} \right)^2 \right\} \\
&= \frac{1}{2}\min_k \left\{ w_{2k-1}^{(n)} - \frac{1}{4}\left(w_{2k-2}^{(n)} + w_{2k}^{(n)} \right) - \frac{1}{2}\sqrt{ w_{2k-2}^{(n)} w_{2k}^{(n)} } \right\} \\
&\geq \frac{1}{2}\min_k \left\{ w_{2k-1}^{(n)} - \frac{1}{2}\left(w_{2k-2}^{(n)} + w_{2k}^{(n)} \right) \right\} \\
&> \vartheta_2^{(n)^2}
\end{aligned}$$

which implies that $\vartheta_2^{(n)^2} < 0$ if $\vartheta_1^{(n)} \leq 0$. Hence $\max\left\{0, \left(\max\left\{0, \vartheta_1^{(n)}\right\}\right)^2 - \varepsilon\right\} = \max\left\{0, \vartheta_2^{(n)^2} - \varepsilon\right\} = 0$ if $\vartheta_1^{(n)} \leq 0$.

Assume that $\vartheta_1^{(n)} > 0$, then it follows that

$$\begin{aligned}
\vartheta_1^{(n)^2} &= \min_k \left\{ \left(\sqrt{w_{2k-1}^{(n)}} - \frac{1}{2}\left(\sqrt{w_{2k-2}^{(n)}} + \sqrt{w_{2k}^{(n)}} \right) \right)^2 \right\} \\
&= \min_k \left\{ w_{2k-1}^{(n)} + \frac{1}{4}\left(\sqrt{w_{2k-2}^{(n)}} + \sqrt{w_{2k}^{(n)}} \right)^2 - \sqrt{ w_{2k-1}^{(n)} \left(\sqrt{w_{2k-2}^{(n)}} + \sqrt{w_{2k}^{(n)}} \right)^2 } \right\} \\
&\geq \frac{1}{2}\min_k \left\{ w_{2k-1}^{(n)} - \frac{1}{2}\left(\sqrt{w_{2k-2}^{(n)}} + \sqrt{w_{2k}^{(n)}} \right)^2 \right\} \\
&= \frac{1}{2}\min_k \left\{ w_{2k-1}^{(n)} - \frac{1}{2}\left(w_{2k-2}^{(n)} + w_{2k}^{(n)} \right) - \sqrt{ w_{2k-2}^{(n)} w_{2k}^{(n)} } \right\}
\end{aligned}$$

$$\geq \frac{1}{2}\min_k\left\{w_{2k-1}^{(n)}-\left(w_{2k-2}^{(n)}+w_{2k}^{(n)}\right)\right\}$$
$$= {\vartheta_2^{(n)}}^2.$$

Therefore it is concluded that $\sigma_m^2\left(B^{(n)}\right) > \max\left\{0, {\vartheta_1^{(n)}}^2-\varepsilon\right\} \geq \max\left\{0, {\vartheta_2^{(n)}}^2-\varepsilon\right\}$, i.e. $\theta^{(n)}$ in (21) satisfies the condition ${\theta^{(n)}}^2 < \sigma_m^2\left(B^{(n)}\right)$. □

One of the fortunate characteristics in (21) is that any square root computation does not appear at every n. In the case where we compute ${\theta^{(n)}}^2$ by (19), it is necessary to compute the square root of $w_k^{(n)}$, $k = 1, 2, \ldots, 2m-1$.

The mdLVs scheme II with a rather large shift also has the same type of instability as the mdLVs scheme I. Let us recall that $\left(B^{(n+1)}\right)^\top B^{(n+1)} = \psi_{\mathrm{dLV}}^{(n+1)}\left(\left(B^{(n)}\right)^\top B^{(n)}\right) - {\theta^{(n)}}^2 I$ in the mdLVs scheme II. According to Theorem 3.1 we see that

$$w_k^{(n+1)} > 0, \quad k = 1, 2, \ldots, 2m-1, \tag{22}$$

if and only if ${\theta^{(n)}}^2 < \lambda_m\left(\psi_{\mathrm{dLV}}^{(n+1)}\left(\left(B^{(n)}\right)^\top B^{(n)}\right)\right) = \sigma_m^2\left(\psi_{\mathrm{dLV}}^{(n+1)}\left(B^{(n)}\right)\right)$. Since it is obvious that $\sigma_m\left(\psi_{\mathrm{dLV}}^{(n+1)}\left(B^{(n)}\right)\right) = \sigma_m\left(B^{(n)}\right)$, the mdLVs scheme II is also numerically stable if $\theta^{(n)}$ is computed by (19) or (21). Moreover we may estimate a lower bound of the minimal singular value $\sigma_m\left(\psi_{\mathrm{dLV}}^{(n+1)}\left(B^{(n)}\right)\right)$ by

$$\begin{aligned} &\sigma_m\left(\psi_{\mathrm{dLV}}^{(n+1)}\left(B^{(n)}\right)\right) \geq \max\left\{0, \vartheta_3^{(n)}\right\}, \\ &\vartheta_3^{(n)} = \min_k\left\{\sqrt{v_{2k-1}^{(n)}} - \frac{1}{2}\left(\sqrt{v_{2k}^{(n)}} + \sqrt{v_{2k-2}^{(n)}}\right)\right\}. \end{aligned} \tag{23}$$

This is because $\psi_{\mathrm{dLV}}^{(n+1)}\left(B^{(n)}\right) = \psi_{\mathrm{mdLVs2};\theta^{(n)}=0}^{(n+1)}\left(B^{(n)}\right)$ and $w_k^{(n+1)} = v_k^{(n)}$ if $\theta^{(n)} = 0$ in the mdLVs scheme II. Similarly it follows that $\sigma_m^2\left(\psi_{\mathrm{dLV}}^{(n)}\left(B^{(n)}\right)\right) > \max\left\{0, \max\left\{0, \vartheta_3^{(n)}\right\}^2 - \varepsilon\right\} \geq \max\left\{0, {\vartheta_4^{(n)}}^2 - \varepsilon\right\}$ where

$${\vartheta_4^{(n)}}^2 = \frac{1}{2}\min_k\left\{v_{2k-1}^{(n)} - \left(v_{2k-2}^{(n)} + v_{2k}^{(n)}\right)\right\}. \tag{24}$$

The following theorem guarantees a numerical stability of the mdLVs scheme II.

Theorem 3.4. *Numerical stability is always kept in the mdLVs scheme II if the shift* ${\theta^{(n)}}^2$ *is given by* $\max\left\{0, \left(\max\left\{0, \vartheta_1^{(n)}\right\}\right)^2 - \varepsilon\right\}$, $\max\left\{0, {\vartheta_2^{(n)}}^2 - \varepsilon\right\}$, $\max\left\{0, \left(\max\{0, \vartheta_3^{(n)}\}\right)^2 - \varepsilon\right\}$ *or* $\max\left\{0, {\vartheta_4^{(n)}}^2 - \varepsilon\right\}$.

To ensure a convergence of the schemes with the shift we require the following condition

$$\sum_{n=0}^{\infty} {\theta^{(n)}}^2 < \lambda_m\left(\left(B^{(0)}\right)^\top B^{(0)}\right) = \sigma_m^2\left(B^{(0)}\right) \tag{25}$$

for the sequence of shifts. The stability condition (16) is automatically satisfied. The condition (25) guarantees the positivity of the limit $\lim_{n\to\infty}\left(B^{(n)}\right)^\top B^{(n)}$ if it exists, which is discussed in the next section.

We here propose four possible choices of the shift ${\theta^{(n)}}^2$ which keep the mdLVs schemes stable. Two of them are based on the Johnson-type bound. Others are new and do not need any square root computation. An optimal choice of the shift is not found yet. This is because the best choice with respect to the computational time and the accuracy depend on the type of matrices. In Section 6 numerical tests will be given for the purpose in comparing one of the mdLVs schemes and a credible routine of LAPACK.

4. Convergence to Shifted Singular Values

In this section we consider an asymptotic behavior of $w_k^{(n)}$ as $n\to\infty$. Moreover we explain a relationship between the limit of $w_{2k-1}^{(n)}$ as $n\to\infty$ and the singular value of $B^{(0)}$ with the help of the sequence of shifts in Theorems 3.2, 3.3 or 3.4. If $0<\lambda_m\left(\left(B^{(0)}\right)^\top B^{(0)}\right)\le\varepsilon$, then the shift ${\theta^{(n)}}^2$, $n=0,1,\ldots$ becomes 0. It is proved in [10] that $w_{2k-1}^{(n)}\to\sigma_k^2\left(B^{(0)}\right)$ and $w_{2k}^{(n)}\to 0$ as $n\to\infty$ in the zero-shift scheme. It is of significance to note that $\lambda_m\left(\left(B^{(n)}\right)^\top B^{(n)}\right)>\varepsilon$, $n=1,2,\ldots$ if $\lambda_m\left(\left(B^{(0)}\right)^\top B^{(0)}\right)>\varepsilon$. Even if $\theta^{(n_0)}=0$ for some finite n_0, nonzero shift ${\theta^{(n_0+k)}}^2$ may be chosen for any $k=1,2,\ldots$. We here discuss a convergence of the mdLVs schemes for such case.

Let us prepare two lemmas for $w^{(n)}=\left(w_1^{(n)},w_2^{(n)},\ldots,w_{2m-1}^{(n)}\right)$ and $u^{(n)}=\left(u_1^{(n)},u_2^{(n)},\ldots,u_{2m-1}^{(n)}\right)$ given by $\psi_{\mathrm{mdLVs1}}^{(n+1)}\circ\psi_{\mathrm{mdLVs1}}^{(n)}\circ\cdots\circ\psi_{\mathrm{mdLVs1}}^{(1)}\left(w^{(0)}\right)$ or $\psi_{\mathrm{mdLVs2}}^{(n+1)}\circ\psi_{\mathrm{mdLVs2}}^{(n)}\circ\cdots\circ\psi_{\mathrm{mdLVs2}}^{(1)}\left(w^{(0)}\right)$. We assume that the shift ${\theta^{(n)}}^2$ satisfies (25) in the following lemmas, propositions and theorem.

Lemma 4.1. *Let M_0 and M_1 be some positive constants. Then $0<w_k^{(n+1)}<M_1$ and $0<u_k^{(n)}<M_1$, for any n, if $0<w_k^{(0)}<M_0$ and $\sum_{n=0}^{\infty}{\theta^{(n)}}^2<\sigma_m^2\left(B^{(0)}\right)$.*

Proof. It is proved in the previous section that $0<w_k^{(n+1)}$. In Theorems 2.1 and 2.2, we see that $\mathrm{trace}\left(\left(B^{(0)}\right)^\top B^{(0)}\right)=\mathrm{trace}\left(\left(B^{(n+1)}\right)^\top B^{(n+1)}\right)+m\Big({\theta^{(0)}}^2+{\theta^{(1)}}^2+\cdots+{\theta^{(n)}}^2\Big)$. Theorem 3.1 implies that $0\le{\theta^{(0)}}^2+{\theta^{(1)}}^2+\cdots+{\theta^{(n)}}^2<\sigma_m^2\left(B^{(0)}\right)$. Note here that $\mathrm{trace}\left(\left(B^{(0)}\right)^\top B^{(0)}\right)=\sigma_1^2\left(B^{(0)}\right)+\sigma_2^2\left(B^{(0)}\right)+\cdots+\sigma_m^2\left(B^{(0)}\right)$. Hence

$$0<\mathrm{trace}\left(\left(B^{(n+1)}\right)^\top B^{(n+1)}\right)<M_2,$$

or equivalently, $0<w_1^{(n+1)}+w_2^{(n+1)}+\cdots+w_{2m-1}^{(n+1)}<M_2$, where M_2 is some positive constant. Therefore it follows that $0<w_k^{(n+1)}<M_1$. Since it is obvious

from the definition that $u_k^{(n)} \leq w_k^{(n+1)}$ in the mdLVs schemes I, we also have $0 < u_k^{(n)} < M_1$. In the mdLVs scheme II, it follows from (13) that $0 < v_1^{(n)} + v_2^{(n)} + \cdots + v_{2m-1}^{(n)} < M_2 + m\sigma_m^2\left(B^{(0)}\right)$. This implies that $0 < v_1^{(n)} < M_1$ and $u_k^{(n)} = v_k^{(n)} \Big/ \left(1 + \delta^{(n)} u_{k-1}^{(n)}\right) \leq v_k^{(n)} < M_1$. □

Lemma 4.2. *If $\sum_{n=0}^{\infty} {\theta^{(n)}}^2 < \sigma_m^2\left(B^{(0)}\right)$, then the variable $w_k^{(n+1)}$ is written as*

$$w_k^{(n+1)} = \prod_{N=0}^{n} \left(\frac{1}{\gamma_k^{(N)}} \cdot \frac{1 + \delta^{(N)} u_{k+1}^{(N)}}{1 + \delta^{(N)} u_{k-1}^{(N)}} \right) w_k^{(0)}, \tag{26}$$

where $\gamma_k^{(N)}$ are some constants such that $\gamma_{2k-1}^{(N)} \geq 1$ and $0 < \gamma_{2k}^{(N)} \leq 1$ for any N.

Proof. (i) Let us consider the case where $w^{(n+1)} = \psi_{\text{mdLVs1}}^{(n+1)} \circ \psi_{\text{mdLVs1}}^{(n)} \circ \cdots \circ \psi_{\text{mdLVs1}}^{(1)}(w^{(0)})$. Then

$$w_k^{(n)} = \gamma_k^{(n)} \bar{w}_k^{(n)} \tag{27}$$

for some constants such that $\gamma_{2k-1}^{(n)} \geq 1$ and $0 < \gamma_{2k}^{(n)} \leq 1$ for any n and $k = 1, 2, \ldots, 2m-1$, since it follows from (8) and (9) that $w_{2k-1}^{(n)} \geq \bar{w}_{2k-1}^{(n)}$ and $w_{2k}^{(n)} \leq \bar{w}_{2k}^{(n)}$. Hence, in the mapping $\psi_{\text{mdLVs1}}^{(n+1)}$, we derive a time evolution from n to $n+1$ of $w_k^{(n)}$ as follows:

$$\begin{aligned}\frac{1 + \delta^{(n)} u_{k+1}^{(n)}}{1 + \delta^{(n)} u_{k-1}^{(n)}} w_k^{(n)} &= \gamma_k^{(n)} \frac{1 + \delta^{(n)} u_{k+1}^{(n)}}{1 + \delta^{(n)} u_{k-1}^{(n)}} \bar{w}_k^{(n)} = \gamma_k^{(n)} \left(1 + \delta^{(n)} u_{k+1}^{(n)}\right) u_k^{(n)} = \gamma_k^{(n)} v_k^{(n)} \\ &= \gamma_k^{(n)} w_k^{(n+1)}.\end{aligned}$$

(ii) Let $w_k^{(n+1)}$ be given by $w^{(n+1)} = \psi_{\text{mdLVs2}}^{(n+1)} \circ \psi_{\text{mdLVs2}}^{(n)} \circ \cdots \circ \psi_{\text{mdLVs2}}^{(1)}\left(w^{(0)}\right)$. Inequalities $v_{2k-1}^{(n)} \geq \bar{v}_{2k-1}^{(n)}$ and $v_{2k}^{(n)} \leq \bar{v}_{2k}^{(n)}$ in (15) lead

$$v_k^{(n)} = \gamma_k^{(n)} \bar{v}_k^{(n)}. \tag{28}$$

Therefore we see that

$$\frac{1 + \delta^{(n)} u_{k+1}^{(n)}}{1 + \delta^{(n)} u_{k-1}^{(n)}} w_k^{(n)} = \left(1 + \delta^{(n)} u_{k+1}^{(n)}\right) u_k^{(n)} = v_k^{(n)} = \gamma_k^{(n)} \bar{v}_k^{(n)} = \gamma_k^{(n)} w_k^{(n+1)}.$$

Noting that $0 < \delta^{(n)}$ and $0 < u_k^{(n)}$ we have

$$w_k^{(n+1)} = \frac{1}{\gamma_k^{(n)}} \frac{1 + \delta^{(n)} u_{k+1}^{(n)}}{1 + \delta^{(n)} u_{k-1}^{(n)}} w_k^{(n)} \tag{29}$$

in both cases (i) and (ii). This completes the proof of (26). □

It is significant to emphasize that the evolution from n to $n+1$ of $w_k^{(n)}$ given by the mdLVs scheme I has the same properties shown in Lemmas 4.1 and 4.2 as those of the evolution given by the mdLVs scheme II. Lemmas 4.1 and 4.2 lead to the following fundamental propositions on an asymptotic behavior of $\gamma_{2k-1}^{(n)}$ and $w_k^{(n)}$ as $n \to \infty$.

Proposition 4.3. *As $n \to \infty$, $\gamma_{2k-1}^{(n)} \to 1$ if $\sum_{n=0}^{\infty} {\theta^{(n)}}^2 < \sigma_m^2\left(B^{(0)}\right)$.*

Proof. Let us consider $\prod_{k=1}^m w_{2k-1}^{(n)}$ with $0 < \prod_{k=1}^m w_{2k-1}^{(0)} < \infty$. From (26), we derive

$$\prod_{k=1}^{m} w_{2k-1}^{(n+1)} = \prod_{k=1}^{m} w_{2k-1}^{(0)} \left(\prod_{N=0}^{n} \prod_{k=1}^{m} \gamma_{2k-1}^{(N)} \right)^{-1} \tag{30}$$

which implies that $\prod_{k=1}^m w_{2k-1}^{(0)} \geq \prod_{k=1}^m w_{2k-1}^{(1)} \geq \cdots \geq \prod_{k=1}^m w_{2k-1}^{(n)} \geq \cdots \geq 0$. Since $\prod_{k=1}^m w_{2k-1}^{(n)}$, $n = 0, 1, \ldots$, is monotonicly decreasing, we see that $\prod_{k=1}^m w_{2k-1}^{(n)} \to c_{1:m}$ as $n \to \infty$ for some nonnegative constant $c_{1:m} \geq 0$. Note that $\prod_{k=1}^m w_{2k-1}^{(n)} = \det\left(\left(B^{(n)}\right)^\top B^{(n)}\right) = \prod_{k=1}^m \lambda_k\left(\left(B^{(n)}\right)^\top B^{(n)}\right)$. It is here emphasized that $\lim_{n\to\infty} \prod_{k=1}^m w_{2k-1}^{(n)} = \lim_{n\to\infty} \prod_{k=1}^m \lambda_k\left(\left(B^{(n)}\right)^\top B^{(n)}\right) > 0$ if ${\theta^{(n)}}^2 \geq 0$ is the suitable shift shown as (25). Hence it follows that $c_{1:m} = \lim_{n\to\infty} \prod_{k=1}^m w_{2k-1}^m$ is positive. Simultaneously, it is obvious from (30) that for $j = 1, 2, \ldots, m$,

$$\prod_{N=0}^{n} \gamma_{2j-1}^{(N)} \leq \prod_{N=0}^{n} \prod_{k=1}^{m} \gamma_{2k-1}^{(N)} = \left(\prod_{k=1}^{m} w_{2k-1}^{(n)} \right)^{-1} \prod_{k=1}^{m} w_{2k-1}^{(0)} \leq \frac{1}{c_{1:m}} \prod_{k=1}^{m} w_{2k-1}^{(0)} < \infty, \tag{31}$$

$$1 \leq \prod_{N=0}^{1} \gamma_{2j-1}^{(N)} \leq \cdots \leq \prod_{N=0}^{n} \gamma_{2j-1}^{(N)} \leq \cdots. \tag{32}$$

Namely, $\prod_{N=0}^n \gamma_{2j-1}^{(N)}$ converges to some positive constant $\bar{p}_j > 0$ as $n \to \infty$. Therefore, for $\gamma_{2j-1}^{(n)} \geq 1$, it is concluded that $\lim_{n\to\infty} \gamma_{2j-1}^{(n)} = 1$. □

Proposition 4.4. *As $n \to \infty$, $w_{2k-1}^{(n)} \to c_k$, $w_{2k}^{(n)} \to 0$ if $\sum_{n=0}^{\infty} {\theta^{(n)}}^2 < \sigma_m^2(B^{(0)})$, where c_k are some positive constants such that $c_1 > c_2 > \cdots > c_m > 0$.*

Proof. When $k = 1$ in (26), we derive

$$w_1^{(n+1)} = w_1^{(0)} \left(\prod_{N=0}^{n} \gamma_1^{(N)} \right)^{-1} \prod_{N=0}^{n} \left(1 + \delta^{(N)} u_2^{(N)} \right). \tag{33}$$

Let us recall here that $w_1^{(n+1)} < M_1$ and $\prod_{N=0}^n \gamma_1^{(N)} \leq \bar{p}_1$ for any n in Lemma 4.1 and Proposition 4.3, respectively. Then it is obvious from (33) that

$$1 < \prod_{N=0}^{n} \left(1 + \delta^{(N)} u_2^{(N)} \right) = \frac{w_1^{(n+1)}}{w_1^{(0)}} \prod_{N=0}^{n} \gamma_1^{(N)} < \frac{M_1}{w_1^{(0)}} \bar{p}_1 < \infty.$$

Since $\prod_{N=0}^{n}\left(1+\delta^{(n)}u_2^{(N)}\right)$, $n=0,1,\ldots,$ is monotonically increasing, we see that $\prod_{N=0}^{n}\left(1+\delta^{(N)}u_2^{(N)}\right)$ converges to some positive constant p_1 as $n\to\infty$. Substituting $\lim_{n\to\infty}\prod_{N=0}^{n}\gamma_1^{(N)}=\bar{p}_1$ and $\lim_{n\to\infty}\prod_{N=0}^{n}\left(1+\delta^{(N)}u_2^{(N)}\right)=p_1$ into (33) as $n\to\infty$, we have

$$\lim_{n\to\infty} w_1^{(n)}=c_1, \tag{34}$$

where $c_1\equiv w_1^{(0)}p_1/\bar{p}_1>0$ is some positive constant. While $\sum_{N=0}^{n}\delta^{(N)}u_2^{(N)}$ converges to some positive constant as $n\to\infty$ if and only if $\prod_{N=0}^{n}\left(1+\delta^{(N)}u_2^{(N)}\right)$ converges to some positive constant. This implies that $\lim_{n\to\infty}\delta^{(n)}u_2^{(n)}=0$ with $0<\delta^{(n)}<M$ and $\lim_{n\to\infty}u_2^{(n)}=0$. Note here that $w_2^{(n)}=\alpha_2^{(n)}u_2^{(n)}\left(1+\delta^{(n)}u_1^{(n)}\right)$ with $0<\alpha_2^{(n)}\equiv\left\{\gamma_2^{(n)},1\right\}\le 1$ and $0<u_1^{(n)}<M_1$. Hence it follows that

$$\lim_{n\to\infty} w_2^{(n)}=0. \tag{35}$$

Next we consider the case where $k=2,3,\ldots,m-1$ in (26). From Lemma 4.1 and Proposition 4.3 we derive

$$\begin{aligned}1<\prod_{N=0}^{n}\left(1+\delta^{(N)}u_{2k}^{(N)}\right)&=\frac{w_{2k-1}^{(n+1)}}{w_{2k-1}^{(0)}}\left(\prod_{N=0}^{n}\gamma_{2k-1}^{(N)}\right)\left(\prod_{N=0}^{n}\left(1+\delta^{(N)}u_{2k-2}^{(N)}\right)\right)\\&<\frac{M_1}{w_{2k-1}^{(0)}}\bar{p}_k p_{k-1}<\infty,\end{aligned}$$

if $\prod_{N=0}^{n}\left(1+\delta^{(N)}u_{2k-2}^{(N)}\right)$ converges to some positive constant $p_{k-1}>0$ as $n\to\infty$. It is proved that $\lim_{n\to\infty}\prod_{N=0}^{n}\left(1+\delta^{(N)}u_2^{(N)}\right)=p_1$. Along the same line of thought as above we can show the following convergence of infinite product $\prod_{N=0}^{\infty}\left(1+\delta^{(N)}u_{2k}^{(N)}\right)=p_k$ where p_k is some positive constant. Therefore the limit of $w_{2k-1}^{(n)}$ as $n\to\infty$ exists and is a positive constant, namely,

$$\lim_{n\to\infty} w_{2k-1}^{(n)}=w_{2k-1}^{(0)}\frac{p_k}{\bar{p}_k p_{k-1}}=c_k>0. \tag{36}$$

Simultaneously, $u_{2k-2}^{(n)}\to 0$ as $n\to\infty$, and consequently, we have

$$\lim_{n\to\infty} w_{2k-2}^{(n)}=0. \tag{37}$$

Finally let us discuss the asymptotic behavior of

$$\frac{w_{2k}^{(n+1)}}{w_{2k}^{(n)}}=\frac{1}{\gamma_{2k}^{(n)}}\cdot\frac{1+\delta^{(n)}u_{2k+1}^{(n)}}{1+\delta^{(n)}u_{2k-1}^{(n)}}$$

as $n \to \infty$. Since the positive variable $w_{2k}^{(n)}$, $n = 1, 2, \ldots$, converges to 0 and $0 < \gamma_{2k}^{(n)} \leq 1$, we have

$$1 + \delta^{(n)} u_{2k+1}^{(n)} < \gamma_{2k}^{(n)} \left(1 + \delta^{(n)} u_{2k-1}^{(n)}\right) \leq 1 + \delta^{(n)} u_{2k-1}^{(n)}$$

for a large n. Here we remark that $u_{2k-1}^{(n)} = \alpha_{2k-1}^{(n)} w_{2k-1}^{(n)} \Big/ \left(1 + \delta^{(n)} u_{2k-2}^{(n)}\right) \to c_k$ with $\alpha_{2k-1}^{(n)} \equiv \left\{1, 1/\gamma_{2k-1}^{(n)}\right\} \to 1$, $w_{2k-1}^{(n)} \to c_k$ and $u_{2k-2}^{(n)} \to 0$ as $n \to \infty$. We see that the limit c_k satisfies

$$c_{k+1} < c_k. \tag{38}$$

It is concluded that $c_1 > c_2 > \cdots > c_m > 0$. This completes the proof. $\square$

A relationship between the limit of $w_k^{(n)}$ and the square of singular values $\sigma_k^2\left(B^{(0)}\right)$ is now evident by using Theorem 2.1, 2.2 and Proposition 4.4. Note that $\sigma_k^2\left(B^{(0)}\right) = \lambda_k\left(\left(B^{(0)}\right)^\top B^{(0)}\right)$. Then we have the following theorem on asymptotic behavior of the variables $w_k^{(n)}$ by using singular values and shifts.

Theorem 4.5. *As* $n \to \infty$, $w_{2k-1}^{(n)} \to c_k = \sigma_k^2(B^{(0)}) - \sum_{N=0}^{\infty} \theta^{(N)^2}$ *and* $w_{2k}^{(n)} \to 0$ *if* $\sum_{n=0}^{\infty} \theta^{(n)^2} < \sigma_m^2(B^{(0)})$.

A convergence to singular values of the mdLVs schemes is now proved. It is to be remarked that the square of singular values are computed from $\lim_{n\to\infty} w_{2k-1}^{(n)}$ in descendent order as $k = 1, 2, \ldots, m$. By combining Theorem 4.5 with Theorems 3.1, 3.2, 3.3, 3.4 on stability it is concluded that the mdLVs schemes are shown to be credible singular value computation schemes.

All singular values of $B^{(0)}$ are not multiple if and only if $w_{2k}^{(0)} > 0$ for $k = 1, 2, \ldots, m-1$ [16]. Hence it is not nessesary to consider the case where $B^{(0)}$ has some multiple singular values, i.e., $c_{k+1} = c_k$ in Proposition 4.4. When $w_{k_0}^{(0)} = 0$ for some k_0, we may decompose $B^{(n)}$ into some smaller upper bidiagonal matrices whose singular values are simple and nonzero as shown in Section 5.

5. Splitting and Deflation Process

In the previous sections we assume that $w_k^{(0)} > 0$, $k = 1, 2, \ldots, 2m-1$. Note that $w_{2k}^{(n)}$ tends to 0 as n grows. If $B^{(n)}$ in (6) has zero-singular value, then $w_{2k_0-1}^{(n)}$ tends to 0 for some k_0. In computer, the value of $w_k^{(n)}$ is also regarded as 0 if $w_k^{(n)}$ is less than the machine epsilon ε_M, where ε_M denotes the minimal floating number such that $1 + \varepsilon_M > 1$. In this section we consider two cases where $w_{2k_0}^{(n)} = 0$ and $w_{2k_0-1}^{(n)} = 0$.

First, let $w_{2k_0}^{(n)} = 0$, then $B^{(n)}$ is decomposed as

$$B^{(n)} = \begin{pmatrix} B_1^{(n)} & 0 \\ 0 & B_2^{(n)} \end{pmatrix}, \tag{39}$$

where $B_j^{(n)}$ are upper bidiagonal matrices such as $B_1^{(n)} \in \mathbf{R}^{k_0 \times k_0}$ and $B_2^{(n)} \in \mathbf{R}^{(m-k_0)\times(m-k_0)}$. This implies that the singular values of $B^{(n)}$ are equivalent to those of $B_1^{(n)}$ and $B_2^{(n)}$. Both $B_1^{(n)}$ and $B_2^{(n)}$ have nonzero positive diagonal and upper subdiagonal entries. The singular values of $B_1^{(n)}$ and $B_2^{(n)}$ can be computed as shown in the previous sections. Let us call this process a splitting. Especially, $w_{2m-1}^{(n)}$ is just the square of a singular value when $w_{2m-2}^{(n)} = 0$ for some n. And we may computes the singular values of $(m-1)\times(m-1)$ matrix $B_1^{(n)}$ instead of $m \times m$ matrix $B^{(n)}$. This process is called a deflation.

Next we explain a splitting process in the case where $w_{2k_0-1}^{(n)} = 0$. Let us assume that $\left(\tilde{B}^{(n)}\right)^\top \tilde{B}^{(n)} = \left(B^{(n)}\right)^\top B^{(n)}$, where $\tilde{B}^{(n)}$ is an upper bidiagonal matrix with the (k,k)-entry $\sqrt{\tilde{w}_{2k-1}^{(n)}}$ and the $(k,k+1)$-entry $\sqrt{\tilde{w}_{2k}^{(n)}}$. Then it is obvious that $\tilde{w}_{2k_0-1}^{(n)}\tilde{w}_{2k_0}^{(n)} = 0$ since $\tilde{w}_{2k_0-1}^{(n)}\tilde{w}_{2k_0}^{(n)} = w_{2k_0-1}^{(n)}w_{2k_0}^{(n)}$. It is of significance to note that $\tilde{w}_{2k_0}^{(n)}$ may be an arbitrary number. If we set $\tilde{w}_{2k_0}^{(n)} = 0$, then $\tilde{B}^{(n)}$ is decomposed as the same form as in (39), i.e.,

$$\tilde{B}^{(n)} = \begin{pmatrix} \tilde{B}_1^{(n)} & 0 \\ 0 & \tilde{B}_2^{(n)} \end{pmatrix}, \tag{40}$$

where $\tilde{B}_1^{(n)} \in \mathbf{R}^{k_0\times k_0}$ and $\tilde{B}_2^{(n)} \in \mathbf{R}^{(m-k_0)\times(m-k_0)}$ are upper bidiagonal matrices. Note here that $\sigma_k\left(B^{(n)}\right) = \sigma_k\left(\tilde{B}^{(n)}\right)$ and $\sigma_k\left(\left(\tilde{B}_1^{(n)}\right)^\top\right) = \sigma_k\left(\tilde{B}_1^{(n)}\right)$. Hence the singular values of $B^{(n)}$ are equal to those of $\left(\tilde{B}_1^{(n)}\right)^\top$ and $\tilde{B}_2^{(n)}$. Let us here introduce a new upper bidiagonal matrix $\hat{B}_1^{(n)}$ with the same form of $\tilde{B}^{(n)}$ such that $\left(\hat{B}_1^{(n)}\right)^\top \hat{B}_1^{(n)} = \tilde{B}_1^{(n)}\left(\tilde{B}_1^{(n)}\right)^\top$ with $\tilde{w}_{2k_0-1}^{(n)} = 0$. Then we see that $\hat{w}_{2k_0-2}^{(n)} = 0$ and $\hat{w}_{2k_0-1}^{(n)} = 0$. Consequently, without changing the singular values, $B^{(n)}$ can be transformed to

$$\hat{B}^{(n)} = \begin{pmatrix} \hat{B'}_1^{(n)} & & \mathbf{0} \\ & 0 & \\ \mathbf{0} & & \tilde{B}_2^{(n)} \end{pmatrix}, \tag{41}$$

where both $\hat{B'}_1^{(n)} \in \mathbf{R}^{(k_0-1)\times(k_0-1)}$ and $\tilde{B}_2^{(n)}$ have nonzero positive diagonal and upper subdiagonal entries. Namely, we may compute the singular values of both $\bar{B'}_1^{(n)}$ and $\tilde{B}_2^{(n)}$ instead of $B^{(n)}$ with $w_{2k_0-1}^{(n)} = 0$.

By using the mdLVs schemes with the above splitting and deflation process successively, the upper bidiagonal matrix $B^{(n)}$ approaches to a diagonal matrix whose entries are singular values of $B^{(0)}$.

6. Test Results

Tests have been carried out on our computer with CPU: PentiumIII 933 MHz, RAM: 512 MB. As numerical examples, we consider 100×100 and 1000×1000

matrices of four types as in Table 1. Let us set the step-size $\delta^{(n)} = 1$ and the shift ${\theta^{(n)}}^2 = \left(\max\left\{0, \vartheta_1^{(n)}\right\}\right)^2$ for $n = 0, 1, \ldots$ in the mdLVs scheme II. Then, in many cases, ${\theta^{(n)}}^2 < \sigma_m^2\left(B^{(n)}\right)$, $w_k^{(n+1)} > 0$ and the mdLVs scheme II is numerically stable. Only the variable $w_k^{(n+1)}$ is computed as $w_k^{(n+1)} = v_k^{(n)}$ for $k = 1, 2, \ldots, 2m-1$ if $w_k^{(n+1)} \leq 0$ in (13). Namely, we adopt the zero-shift stable version of the mdLVs scheme II. It can be shown that the convergence speed of the mdLVs scheme II is slightly faster than that of the mdLVs scheme I in numerical tests. Hence we demonstrate the computational performance of the mdLVs scheme II in this paper. A variable step-size version without shift is discussed in [10]. The splitting or the deflation shown in Section 5 are performed when $w_{2k_0-1}^{(n)}$ or $w_{2k_0}^{(n)}$ are relatively small for some k_0. We here designed a new trial routine named *the mdLVs routine* in terms of the mdLVs scheme II. *The dLV routine* is just the zero-shift version of the mdLVs routine. The singular values are computed with double precision in our routines. In this section, we compare the mdLVs, the dLV and DBDSQR (without computing singular vectors) routines with respect to both the computational time and the numerical accuracy. Here DBDSQR is well known and is widely used as one of the most credible routines in LAPACK having a stability and a guaranteed convergence. We use a FORTRAN routine of DBDSQR in LAPACK 3.0 downloaded from a web site [1]. Many fundamental linear computations in LAPACK routines are performed by Basic Linear Algebra Subprograms (BLAS).

Table 1. Four types of upper bidiagonal matrices.

	Diagonal $b_{k,k}$	Subdiagonal $b_{k,k+1}$	Distribution of $\hat{\sigma}_k$	Minimal $\hat{\sigma}_m$
Type 1: B_1	2.001	2	sufficiently separated	nonzero
Type 2: B_2	1	10	separated	almost zero
Type 3: B_3	$\begin{cases} 1 & (k=1) \\ 2 & (k \neq 1) \end{cases}$	$\begin{cases} 0.001 & (k=1) \\ 0.002 & (k \neq 1) \end{cases}$	dense (except for $\hat{\sigma}_m$)	nonzero
Type 4: B_4	0.001	2	dense (except for $\hat{\sigma}_m$)	almost zero

First we compare the computational time by the mdLVs, the dLV and DBDSQR routines for computing every singular values of B_k, $k = 1, 2, 3, 4$ in Table 1, where B_k are 100×100 and 1000×1000 matrices. Table 2 gives the computational time. Obviously the mdLVs routine requires the computational time less than the dLV routine. Compare it with DBDSQR routine, there is a little difference in the computational time when every B_k is 100×100. This is such a small-scale computation that the most of data are stored in not main memory but efficient cache memory of computer. In the singular value computation of 1000×1000 matrices, the mdLVs routine is 26–46 % faster than DBDSQR routine. It can be shown that the mdLVs routine has a better scalability than DBDSQR routine. In contrast with the dLV and DBDSQR routines, the mdLVs routine runs in almost the same time independently of matrix type. Moreover DBDSQR routine is not accelerated by using an optimized BLAS "Automatically Tuned Linear Algebra Software (ATLAS) [15]." This is because DBDSQR routine for computing only singular values does not require any vector and matrix operations accelerated by ATLAS. In a full SVD by DBDSQR, ATLAS will demonstrate it's ability.

Table 2. Computational time by the mdLVs, the dLV and DBDSQR routines (sec.).

	100×100			1000×1000	
	mdLVs	dLV	DBDSQR	mdLVs	DBDSQR
Type 1	0.02	0.13	0.02	1.34	2.27
Type 2	0.02	0.88	0.03	1.32	2.43
Type 3	0.02	36.2	0.02	1.30	1.76
Type 4	0.02	174	0.02	1.32	2.00

Next we discuss the numerical accuracy of computed singular values by the mdLVs, the dLV and DBDSQR routines. Fig. 2 describes relative errors $|\sigma_k - \hat{\sigma}_k| / \hat{\sigma}_k$ in the computed singular values σ_k of 100×100 Type 4 matrix B_4, where $\hat{\sigma}_k$ are the verified correct values computed by using Maple [7] with 50-digits. The relative errors themselves were also computed with 50-digits in Maple. Visibly the relative errors of computed singular values by the mdLVs routine are much smaller than those by the dLV routine. Since the roundoff operations in the mdLVs routine are much less than those in the dLV routine, the roundoff errors in the mdLVs routine seems to be smaller. Hence the mdLVs routine is superior to the dLV routine with respect to the numerical accuracy. The computed singular values by the mdLVs routine are also practically with higher accuracy than those by DBDSQR routine. For other type of matrices in Table 1, we also obtain the graphs similar to Fig. 2.

In this paper it is shown that the mdLVs routine is better than DBDSQR routine of LAPACK with respect to both the computational time and the numerical accuracy. The higher relative accuracy of the mdLVs routine will be quite useful to compute singular vectors from the singular values.

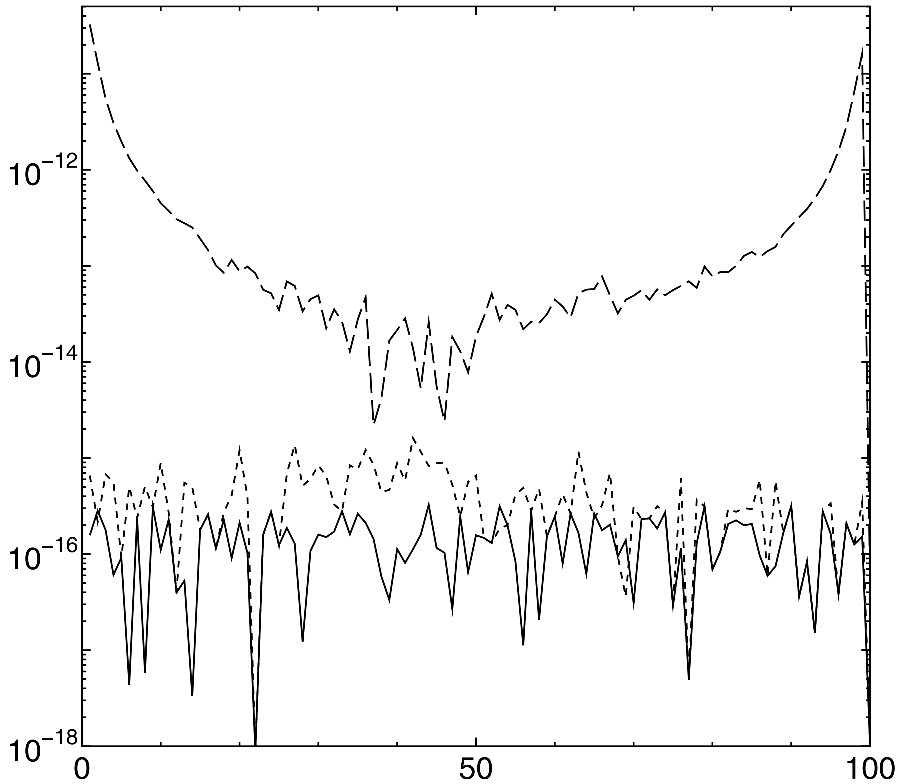

Fig. 2. A graph of the suffix k for ordering singular values σ_k according to magnitude (x-axis) and the relative errors in computed singular values of B_4 by the mdLVs, the dLV and DBDSQR routines (y-axis). The soild, dashed and dotted lines are given by the mdLVs, the dLV and DBDSQR routines, respectively. The relative error of σ_{100} is plotted on x-axis because $|\sigma_{100} - \hat{\sigma}_{100}| \sim 0$. Here the machine epsilon is $\varepsilon_M = 2.22 \times 10^{-16}$.

7. Concluding Remarks

In this paper a new shifted scheme for singular values of matrices is designed. In Section 2, two types of such schemes, named the mdLVs schemes I and II, are presented. In Section 3, four possible choices of the shift which keep the mdLVs schemes numerically stable. In Section 4, a convergence to singular values of the mdLVs schemes is proved. It is concluded that the mdLVs schemes are stable schemes having guaranteed convergence to singular values. In Section 6 a comparison of the mdLVs routine with a credible routine, DBDSQR, of LAPACK. It is shown that the mdLVs routine is more accurate and faster than DBDSQR routine and has a good scalability.

The higher relative accuracy of the mdLVs schemes is quite important to compute orthogonal singular vectors from computed singular values in terms of, for example, a new twisted factorization method. An optimal implementation, the cubic convergence to singular values, a parallelization of the mdLVs schemes and a full SVD scheme will be discussed in subsequent papers. The authors hope that the new shifted schemes for singular values will contribute effectively to large scaled SVD problems.

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