A Differential Equation Approach to the Singular Value Decomposition of Bidiagonal Matrices

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ABSTRACT

We consider the problem of approximating the singular value decomposition of a bidiagonal matrix by a one-parameter family of differentiable matrix flows. It is shown that this approach can be fully expressed as an autonomous, homogeneous, and cubic dynamical system. Asymptotic behavior is justified by the established theory of the Toda lattice.

1. INTRODUCTION

One of the most important decompositions in matrix computations is the singular value decomposition (SVD), i.e.

THEOREM 1.1. *If $A \in \mathbb{R}^{m\times n}$, then there exist orthogonal matrices $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ such that U^TAV assumes one of the two following forms*:

$$U^TAV = \begin{bmatrix} \Sigma \\ 0 \end{bmatrix} \quad \text{if} \quad m \geqslant n,$$
$$U^TAV = [\Sigma, 0] \quad \text{if} \quad m \leqslant n, \tag{1.1}$$

where

$$\Sigma = \operatorname{diag}(\sigma_1, \sigma_2, \ldots, \sigma_p), \tag{1.2}$$

$p = \min\{m, n\}$, *and* $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_p \geqslant 0$.

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It is also well known that the SVD of a matrix A is closely related to the Schur decompositions of the symmetric matrices A^TA and AA^T. Indeed,

THEOREM 1.2. *Suppose that* $A \in \mathbb{R}^{m\times n}$ (*we shall assume that* $m \geq n$ *henceforth*) *has the SVD as in* (1.1). *Then*

$$V^T(A^TA)V = \operatorname{diag}(\sigma_1^2, \sigma_2^2, \dots, \sigma_n^2) \in \mathbb{R}^{n\times n} \tag{1.3}$$

and

$$U^T(AA^T)U = \operatorname{diag}(\sigma_1^2, \sigma_2^2, \dots, \sigma_n^2, 0, \dots, 0) \in \mathbb{R}^{m\times m}. \tag{1.4}$$

These connections allow us to adapt the mathematical and algorithmic developments for symmetric eigenvalue problems to this singular value problem. For example, (1.3) suggests that the SVD of A can be calculated through the following steps [8]:

(1) Form $C = A^TA$.

(2) Use the symmetric QR algorithm to compute $V_1^TCV_1 = \operatorname{diag}(\sigma_1^2, \dots, \sigma_n^2)$.

(3) Use QR with column pivoting to upper-triangularize $B = AV_1$, i.e. $U^T(AV_1)T = R$.

In actual practice, however, one does not want to form the matrix C explicitly nor apply the QR algorithm directly. Various reasons for not doing so can be found in [5, 8]. A preferable method, proposed by Golub and Kahan [6], is then composed of two distinct parts:

(1) Reduce A to upper bidiagonal form using a sequence of Householder transformations, i.e.

$$U_B^TAV_B = \begin{bmatrix} B \\ 0 \end{bmatrix} = \left[\begin{array}{cccccc} b_{11} & b_{12} & & & & \bigcirc \\ & b_{22} & b_{23} & & & \\ & & \ddots & \ddots & & \\ & & & \ddots & \ddots & \\ & & & & \ddots & b_{n-1,n} \\ \bigcirc & & & & & b_{n,n} \\ \hdashline & & & \bigcirc & & \end{array}\right]. \tag{1.5}$$

(2) Compute the SVD of B by *implicitly* applying the symmetric QR algorithm to A^TA.

The algorithmic details of this method are discussed in [6, 8] and documented in [5, 7].

In this note we shall assume that the bidiagonalization process has been accomplished somehow. We are interested in developing a continuous approximation to the SVD of B. It turns out that such an approach is totally feasible and can be fully expressed as an autonomous ordinary differential system. The derivation of this homogeneous cubic differential system is presented in the next section. It is related to the Golub-Kahan SVD algorithm almost in the same way as the Toda lattice is related to the QR algorithm. Therefore, conclusions on its asymptotic behavior can be drawn from the knowledge of the Toda lattice. This result is presented in the last section together with a summary theorem.

2. DERIVATION OF THE O.D.E.

Consider the one-parameter family of matrices

$$X(t)=U(t)\cdot B\cdot V(t), \tag{2.1}$$

where both $U(t)$ and $V(t)$ are families of orthogonal matrices to be specified and are assumed to be differentiable with respect to the parameter t. Differentiating with respect to t yields

$$\begin{aligned}\dot{X}&=\dot{U}\cdot B\cdot V+U\cdot B\cdot\dot{V}=(\dot{U}\cdot U^{T})\cdot X+X\cdot(V^{T}\cdot\dot{V})\\&=X\cdot N-M\cdot X,\end{aligned} \tag{2.2}$$

where we have defined

$$M(t)=-\dot{U}(t)\cdot U^{T}(t) \tag{2.3}$$

and

$$N(t)=V^{T}(t)\cdot\dot{V}(t). \tag{2.4}$$

Since both $U(t)$ and $V(t)$ are orthogonal, it is clear that both $M(t)$ and $N(t)$ are skew-symmetric. Furthermore, we note that the above argument can be reversed, namely

THEOREM 2.1. *Let $M(t)$ and $N(t)$ be two one-parameter families of skew-symmetric matrices (both continuous in t). Suppose $U(t)$ and $V(t)$ solve the initial value problems*

$$\dot{U}(t) = -M(t)\cdot U(t), \qquad U(0) = I, \tag{2.5}$$

$$\dot{V}(t) = V(t)\cdot N(t), \qquad V(0) = I, \tag{2.6}$$

respectively. Then

(1) *both $U(t)$ and $V(t)$ are orthogonal matrices;*
(2) *the solution $X(t)$ to (2.2) with initial value $X(0) = B$ can be expressed as (2.1).*

Proof. Assertion (1) follows from the observation that $[U^T(t)\cdot U(t)]^{\cdot} = 0$ for all t and that $U^T(0)\cdot U(0) = I$. Assertion (2) follows from the direct substitution and the uniqueness theorem. ∎

Apparently not all choices of $M(t)$ and $N(t)$ would lead to nice asymptotic behavior for the resulting $X(t)$. We now describe a specific selection of this pair.

Denote the components of a given matrix by the associated lowercase letter, e.g. $X = [x_{ij}]$, $M = [m_{ij}]$, and so on. We insist on the following two conditions throughout the continuous transition:

(C1) In addition to being skew-symmetric, both $M(t)$ and $N(t)$ are further required to be tridiagonal.
(C2) $X(t)$ maintains the bidiagonal form for all t.

To fulfill these requirements, it is not difficult to derive from (2.2) that the following equality constraints must be satisfied:

$$x_{i+1,i+1}n_{i+1,i} - m_{i+1,i}x_{i,i} = 0 \qquad \text{for all} \quad n-1 \geqslant i \geqslant 1, \tag{2.7}$$

$$-x_{i,i+1}n_{i+2,i+1} + m_{i+1,i}x_{i+1,i+2} = 0 \qquad \text{for all} \quad n-2 \geqslant i \geqslant 1. \tag{2.8}$$

This is an underdetermined system of $2n-3$ equations in $2n-2$ unknowns. In matrix form, this system may be represented as

$$\mathscr{A}x = 0, \tag{2.9}$$

where $\mathscr{A}$ is the $(2n-3)\times(2n-2)$ bidiagonal matrix

$$\mathscr{A} = \begin{bmatrix} x_{22} & -x_{11} & & & & & & & \\ & x_{33} & -x_{12} & & & & & \bigcirc & \\ & & x_{33} & -x_{22} & & & & & \\ & & & \ddots & \ddots & & & & \\ & & & & x_{n-1,n-1} & -x_{n-2,n-2} & & & \\ & \bigcirc & & & & x_{n-1,n} & -x_{n-2,n-1} & & \\ & & & & & & x_{nn} & -x_{n-1,n-1} \end{bmatrix}. \tag{2.10}$$

and x is the $(2n-2)\times 1$ column vector

$$x = \left[n_{21}, m_{21}, n_{32}, \ldots, m_{n-1,n-2}, n_{n,n-1}, m_{n,n-1}\right]^T. \tag{2.11}$$

Substituting (2.8) into (2.7) yields the following relationships:

$$\frac{n_{i+1,i}}{n_{i+2,i+1}} = \frac{x_{i,i}x_{i,i+1}}{x_{i+1,i+1}x_{i+1,i+2}}, \tag{2.12}$$

$$\frac{m_{i+1,i}}{m_{i+2,i+1}} = \frac{x_{i+1,i+1}x_{i,i+1}}{x_{i+2,i+2}x_{i+1,i+2}} \tag{2.13}$$

for all $n-2 \geqslant i \geqslant 1$. Therefore, a particular solution of (2.9) is given by

$$n_{i+1,i} = x_{i,i}x_{i,i+1}, \tag{2.14}$$

$$m_{i+1,i} = x_{i+1,i+1}x_{i,i+1} \tag{2.15}$$

for all $n-1 \geqslant i \geqslant 1$. In this case, the matrices $M(t)$ and $N(t)$ in particular can be represented as

$$M(t) = \Pi_0\left(X(t)\cdot X^T(t)\right) \tag{2.16}$$

and

$$N(t) = \Pi_0\left(X^T(t)\cdot X(t)\right), \tag{2.17}$$

respectively, where $\Pi_0(X)$ represents the skew-symmetric matrix defined by

$$\Pi_0(X) = X^- - (X^-)^T, \tag{2.18}$$

and X^- means the strictly lower triangular matrix of X. One should note that (2.16) and (2.17) are just for notational convenience, and should *not* be misled to think that $X^T \cdot X$ and $X \cdot X^T$ must be formed explicitly to define the system (2.2). Indeed, though the system (2.2) is now written as

$$\dot{X}(t) = X(t)\cdot\Pi_0(X^T(t)\cdot X(t)) - \Pi_0(X(t)\cdot X^T(t))\cdot X(t), \tag{2.19}$$

the resulting arithmetic is nothing more than

$$\dot{x}_{i,i} = x_{i,i}\left(x_{i,i+1}^2 - x_{i-1,i}^2\right) \qquad \text{for all} \qquad n \geqslant i \geqslant 1, \tag{2.20}$$

$$\dot{x}_{i,i+1} = x_{i,i+1}\left(x_{i+1,i+1}^2 - x_{i,i}^2\right) \qquad \text{for all} \quad n-1 \geqslant i \geqslant 1, \tag{2.21}$$

where we adopt the notation $x_{0,1} = x_{n,n+1} = 0$. Since this is an autonomous system, we see that the contraints (2.7) and (2.8) are sufficient conditions for (C1) and (C2) as well. Note that the system (2.19) is homogeneous and cubic. It is also worth noting that the Golub-Kahan SVD algorithm usually requires $20n$ flops and $2n$ square roots per step [8], whereas the function evaluation of (2.19) requires only $2n$ flops and $2n$ squares per step. In addition, the system (2.19) appears parallel in nature. An investigation of the possible advantages of implementing this system on parallel computers has just been initiated.

3. ASYMPTOTIC CONVERGENCE

In this section we want to explore the asymptotic behavior of the nontrivially coupled differential system (2.19). Our basic tool is the so-called Toda lattice [1–4]—a differential system of the form

$$\dot{Z}(t) = Z(t)\cdot\Pi_0(Z(t)) - \Pi_0(Z(t))\cdot Z(t). \tag{3.1}$$

To make this note complete, we review below some important properties of the Toda flow. Their proofs can be found in [1] and [3].

THEOREM 3.1. *The solution* $Z(t)$ *of* (3.1) *with initial value* $Z(0) = Z_0$ *can be written as*

$$Z(t) = Q^T(t) \cdot Z_0 \cdot Q(t), \tag{3.2}$$

where $Q(t)$ *solves the initial value problem*

$$\dot{Q}(t) = Q(t) \cdot \Pi_0(Z(t)), \qquad Q(0) = I. \tag{3.3}$$

THEOREM 3.2. *Let* $Z(t)$ *be an integral curve of* (3.1). *For* $k = 0, \pm 1, \pm 2, \ldots$, *suppose that the matrix* $\exp(Z(k))$ *has the QR decomposition*

$$\exp(Z(k)) = Q_k R_k. \tag{3.4}$$

Then

$$\exp(Z(k+1)) = R_k Q_k. \tag{3.5}$$

THEOREM 3.3. *Suppose the initial value* Z_0 *of* (3.1) *is upper Hessenberg and has a complete set of real eigenvalues. Then the solution* $Z(t)$ *of* (3.1) *converges to an upper triangular matrix with the eigenvalues of* Z_0 *appearing on the diagonal in a nondecreasing order as t goes to infinity. In this case, the corresponding* $Q(t)$ *of* (3.3) *also converges to a limit.*

Equipped with the knowledge of the Toda lattice, we now show the asymptotic convergence of the system (2.19). Let

$$Y(t) = X^T(t) \cdot X(t). \tag{3.6}$$

Then

$$\begin{aligned}
\dot{Y} &= \dot{X}^T \cdot X + X^T \cdot \dot{X} \\
&= \left\{ X \cdot \Pi_0(X^T \cdot X) - \Pi_0(X \cdot X^T) \cdot X \right\}^T \cdot X \\
&\quad + X^T \cdot \left\{ X \cdot \Pi_0(X^T \cdot X) - \Pi_0(X \cdot X^T) \cdot X \right\} \\
&= (X^T \cdot X) \cdot \Pi_0(X^T \cdot X) - \Pi_0(X^T \cdot X) \cdot (X^T \cdot X) \\
&= Y \cdot \Pi_0(Y) - \Pi_0(Y) \cdot Y.
\end{aligned} \tag{3.7}$$

In other words, $Y(t)$ satisfies the Toda lattice. We shall assume henceforth that $\Pi_0(Y) \not\equiv 0$, since otherwise $\dot{Y} \equiv 0$. Since $Y(t)$ is symmetric and hence has a complete set of real eigenvalues, by Theorem 3.3, $Y(t)$ converges to a diagonal matrix. Furthermore, from (2.6) and (2.17),

$$\dot{V}(t) = V(t) \cdot \Pi_0(Y(t)), \qquad V(0) = I. \tag{3.8}$$

So it also follows from Theorem 3.3 that $V(t)$ converges to a constant limit. Similar arguments can be applied to $U(t)$ as well. In conclusion, we observe from (3.6) that $X(t)$ converges to a matrix with mutually orthogonal columns. But $X(t)$ also maintains the bidiagonal form for all t. Therefore, $X(t)$ converges to a diagonal matrix.

We summarize our results in the following theorem.

THEOREM 3.4. *Let B be a real bidiagonal matrix such that not all $b_{i,i}b_{i,i+1}$ and $b_{i,i}b_{i-1,i}$ are zeros. Consider the initial value problem*

$$\dot{X}(t) = X(t) \cdot \Pi_0(X^T(t) \cdot X(t)) - \Pi_0(X(t) \cdot X^T(t)) \cdot X(t),$$
$$X(0) = B. \tag{3.9}$$

Then:

(1) *The solution $X(t)$ remains bidiagonal and can always be decomposed as*

$$X(t) = U(t) \cdot B \cdot V(t), \tag{3.10}$$

where both $U(t)$ and $V(t)$ are orthogonal matrices and are respectively solutions of the initial value problems

$$\dot{U}(t) = -\Pi_0(X(t) \cdot X^T(t)) \cdot U(t), \qquad U(0) = I, \tag{3.11}$$

$$\dot{V}(t) = V(t) \cdot \Pi_0(X^T(t) \cdot X(t)), \qquad V(0) = I. \tag{3.12}$$

(2) *As t goes to infinity, both $U(t)$ and $V(t)$ converge to certain constant matrices, say $U(t) \to U_*$ and $V(t) \to V_*$, and $X(t)$ converges to a diagonal matrix, say $X(t) \to \Sigma$. The decomposition*

$$B = U_*^T \Sigma V_*^T \tag{3.13}$$

is a singular value decomposition of B.

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