NORTH-HOLLAND

Scaled Toda-like Flows

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ABSTRACT

This paper discusses the class of isospectral flows $\dot{X} = [X, A \circ X]$, where $\circ$ denotes the Hadamard product and $[\cdot, \cdot]$ is the Lie bracket. The presence of A allows arbitrary and independent scaling for each element in the matrix X. The time-1 mapping of the scaled Toda-like flow still enjoys a QR-like iteration. The scaled structure includes the classical Toda flow, Brockett's double bracket flow, and other interesting flows as special cases. Convergence proof is thus unified and simplified. The effect of scaling on a variety of applications is demonstrated by examples.

1. INTRODUCTION

For simplicity, we will confine our discussion in this paper to the real case only. It is convenient to introduce two special subsets in $R^{n\times n}$:

$$\begin{aligned} \mathcal{S}(n) &:= \{X \in R^{n\times n} \mid X^T = X\}, \\ \mathcal{O} &:= \{Q \in R^{n\times n} \mid Q^T Q = I\}. \end{aligned}$$

Recent research has revealed a number of remarkable connections between smooth flows and discrete numerical algorithms [2, 11, 9, 10, 15, 16]. Among these, a by now classic result is the relationship between the Toda lattice and the

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QR algorithm. That is, the time-1 mapping $\{X(k)\}$ of the solution $X(t)$ to the initial value problem

$$\begin{aligned} \dot{X} &= [X, \Pi_0(X)], \\ X(0) &= X_0 \end{aligned} \tag{1}$$

corresponds exactly to the sequence obtained by applying the QR algorithm to the matrix $e^{X(0)}$ [11, 15, 5]. In (1) $\Pi_0(X) := X^- - X^{-T}$, where X^- denotes the strictly lower triangular matrix of X.

The Toda flow (1) later was generalized to the class [8]

$$\begin{aligned} \dot{X} &= [X, \mathcal{P}_{\mathcal{L}}(X)], \\ X(0) &= X_0, \end{aligned} \tag{2}$$

where $\mathcal{P}_{\mathcal{L}}(X)$ denotes the projection of X onto a certain specified *linear subspace* $\mathcal{L}$ of $R^{n\times n}$. On specifying different $\mathcal{L}$, (2) gives rise to different types of matrix factorizations, many of which are in abstract forms. For example, the following theorem, which includes the well-known Schur decomposition theorem as a special case, has been proved in [8] by using (2).

THEOREM 1.1. *Given a symmetric matrix $A \in R^{n\times n}$, there exists a real and orthogonal matrix Q such that the symmetric matrix $T = Q^T AQ$ has zero entries in any prescribed positions of T except possibly along the diagonal.*

Another interesting isospectral flow is the so-called Brockett's double bracket flow [3, 4]

$$\begin{aligned} \dot{X} &= [X, [X, D]], \\ X(0) &= X_0, \end{aligned} \tag{3}$$

where X and D are matrices in $\mathcal{S}(n)$ and D is fixed. The flow originally arises as a gradient flow. Remarkably, it is noticed in [2] that if X is tridiagonal and

$$D = \mathrm{diag}\{n, \ldots, 2, 1\}, \tag{4}$$

then (3) coincides precisely with (1). A gradient flow hence becomes Hamiltonian [1].

Equation (3) is a special case of a more general projected gradient flows [9]:

$$\begin{aligned} \dot{X} &= [X, [X, \mathcal{P}_{\mathcal{A}}(X)]], \\ X(0) &= X_0, \end{aligned} \tag{5}$$

where $\mathcal{P}_{\mathcal{A}}(X)$ denotes the projection of $X \in \mathcal{S}(n)$ onto an *affine subspace* $\mathcal{A}$ of $\mathcal{S}(n)$. The vector field in (5) represents the projection of the negative gradient of the objective function

$$F(X) := \tfrac{1}{2}\|X - \mathcal{P}_{\mathcal{A}}(X)\|^2 \tag{6}$$

onto the isospectral feasible set

$$\mathcal{M}(X_0) := \{Q^T X_0 Q \mid Q \in \mathcal{O}(n)\}. \tag{7}$$

The object is to minimize the distance between the sets $\mathcal{M}(X_0)$ and $\mathcal{A}$. Taking $\mathcal{A} = \{D\}$, we have (3). Thus the Brockett double bracket flow gives the least squares approximation of D subject to the spectral constraint. Such a solution, which itself has many interesting applications, can be characterized in terms of the spectral decomposition [4, 9].

THEOREM 1.2. *Suppose both D and X_0 are in $\mathcal{S}(n)$ and have distinct eigenvalues. Let the eigenvalues of D and X_0 be ordered as $\mu_1 < \cdots < \mu_n$ and $\lambda_1 < \cdots < \lambda_n$, respectively. Then the unique asymptotically stable equilibrium point of* (3) *is given by*

$$\widehat{X} = \lambda_1 q_1 q_1^T + \cdots + \lambda_n q_n q_n^T, \tag{8}$$

where $q_1, \ldots, q_n$ are the normalized eigenvectors of D corresponding respectively to $\mu_1, \ldots, \mu_n$. In particular, if D is a diagonal matrix with distinct eigenvalues, then $\widehat{X}$ must be a diagonal matrix whose elements are ordered like those in D.

One common characteristic of all the flows discussed above is that they are always described by the so-called Lax pair

$$\dot{X} = [X, k(X)], \tag{9}$$

where $k(X)$ is matrix-valued function of X. Of particular interest is the case when $X \in \mathcal{S}(n)$ and $k(X)$ is skew-symmetric. In this paper, we propose another Toda-like flow by taking $k(X) = A \circ X$, where A is a constant matrix and $\circ$ represents the Hadamard product. In the context that X is being scaled componentwise by A, we call the flow associated with the differential equation

$$\begin{aligned} \dot{X} &= [X, A \circ X], \\ X(0) &= X_0 \end{aligned} \tag{10}$$

a *scaled Toda-like flow*.

We shall show that different choices of the scaling matrix A result in (1), (2), and (3) as special cases. At least in theory, the time-1 mapping of the scaled Toda-like flow enjoys a QR-like iteration. For symmetric cases, we provide a simple proof on the global convergence of the scaled Toda-like flow. Finally the effect of scaling is discussed.

2. QR-LIKE ITERATION

In this section we explain why the flow $X(t)$ of (10) evaluated at integer times still enjoys a QR-like iteration. The notion of the Q and R matrices in the QR decomposition will be replaced by the L and R matrices defined in the sequel. We shall state the results without proofs, since they are very similar to those already done in [8], only keeping in mind that the matrix A allows arbitrary scaling.

Given any square matrix $A = [a_{ij}]$, let $\widetilde{A} = [\widetilde{a}_{ij}]$ denote the "complementary" matrix where $\widetilde{a}_{ij} := 1 - a_{ij}$. Associated with (10) are the two differential systems

$$\begin{aligned} \dot{L} &= L(A \circ X), \\ L(0) &= I \end{aligned} \tag{11}$$

and

$$\begin{aligned} \dot{R} &= (\widetilde{A} \circ X)R, \\ R(0) &= I. \end{aligned} \tag{12}$$

Here we adopt the notation L and R only as a reminder of how the multiplication is involved in (11) and (12), respectively. Let $X(t)$, $L(t)$, and $R(t)$ represent the solution to the initial value problems (10), (11), and (12), respectively, over an interval $[0, T]$ for some $T > 0$. Then we have

THEOREM 2.1.

$$X(t) = L(t)^{-1}X_0L(t) = R(t)X_0R(t)^{-1}. \tag{13}$$

THEOREM 2.2.

$$e^{X_0t} = L(t)R(t). \tag{14}$$

THEOREM 2.3.

$$e^{X(t)t} = R(t)L(t). \tag{15}$$

Because of (13), we may rewrite (11) as

$$\begin{aligned} \dot{L} &= L(A \circ L^{-1}X_0L) \\ L(0) &= I. \end{aligned} \tag{16}$$

So the differential system becomes autonomous. In a similar way we may rewrite (12). To emphasize the dependence on the initial matrix X_0, we now denote the solutions of (10) and the associated (11) and (12) by $X(t; X_0)$, $L(t; X_0)$, and $R(t; X_0)$, respectively. By setting $t = 1$ in (14) and (15), it becomes clear that for positive integer k in the domain of existence we have

$$e^{X(k;X_0)} = e^{X(0;X(k;X_0))} = L(1; X(k; X_0))R(1; X(k; X_0)), \tag{17}$$

$$e^{X(k+1;X_0)} = e^{X(1;X(k;X_0))} = R(1; X(k; X_0))L(1; X(k; X_0)). \tag{18}$$

That is, if LR is an abstract LR decomposition of $e^{X(k)}$, then RL is one for $e^{X(k+1)}$. Such a property as in (17) and (18) is referred to a *QR-like iteration.*

3. CONVERGENCE

Henceforth we shall consider only flows in $\mathcal{S}(n)$. In order that $X(t) = [x_{ij}(t)] \in \mathcal{S}(n)$ for all t, the scaling matrix A in (10) is necessarily skew-symmetric. In this case, it follows from (11) that $L(t)$ is orthogonal.

We now prove a very useful convergence property for the scaled Toda-like flow. Our major result is as follows.

THEOREM 3.1. *Suppose the strictly lower triangular part of $A = [a_{ij}]$ is nonnegative. Then*

$$\lim_{t \longrightarrow \infty} A \circ X(t) = 0. \tag{19}$$

More precisely, whenever $a_{ij} > 0$, the corresponding entry $x_{ij}(t)$ (and $x_{ji}(t)$) converges to 0 as t goes to infinity.

PROOF. Consider the partial sums $\{\sigma_1, \ldots, \sigma_n\}$ of the diagonal entries of X, i.e.,

$$\sigma_k := \sum_{i=1}^{k} x_{ii}. \tag{20}$$

Since $L(t)$ is orthogonal, we have from (13) that $\|X(t)\|_F = \|X_0\|_F$, where $\|\cdot\|_F$ denotes the Frobenius matrix norm, and hence $\sigma_k(t)$ is bounded for all t.

It is not difficult to see from the equation (10) that

$$\dot{\sigma}_n = 0 \tag{21}$$

and that

$$\dot{\sigma}_k = 2 \sum_{i=k+1}^{n} \sum_{j=1}^{k} a_{ij} x_{ij}^2 \tag{22}$$

for $1 \leq k < n$. Since $a_{ij} \geq 0$ for all $i > j$, (22) implies that each $\sigma_k(t)$ is a nondecreasing function in t. It follows that both $\lim_{t\to\infty} \sigma_k(t)$ and $\lim_{t\to\infty} \sigma_k(t)$ exist. Using (22), we find

$$\int_{-\infty}^{\infty} \sum_{i=k+1}^{n} \sum_{j=1}^{k} a_{ij} x_{ij}^2(t)\, dt$$

is integrable. In particular, so long as $a_{ij} > 0$, we find that each $x_{ij}(t)$ is L^2 integrable over $(-\infty, \infty)$. Together with the fact that (x_{ij}^2) is uniformly bounded, it follows that $\lim_{t\to\infty} x_{ij}(t) = 0$ (see [8]). ■

In the next section we shall see how different choices of A lead to a variety of interesting flows, including (1), (2), and (3). Thus we think the above theorem, unifying the proof of convergence, is of interest in its own right.

4. CHOICES OF A

We now demonstrate how different choices of A result in some classical flows. More exotic applications will be discussed in the next section.

EXAMPLE 1. Choose $A = [a_{ij}]$ such that

$$a_{ij} := \begin{cases} 1 & \text{if } \ j = 1 \text{ and } i > j, \\ -1 & \text{if } \ i = 1 \text{ and } j > i, \\ 0 & \text{otherwise.} \end{cases} \tag{23}$$

Let the columns of $L(t)$ be denoted as $L(t) = [l_1(t), \ldots, l_n(t)]$. The first column of $L(t)$ is of particular interest. From (11), we have

$$\frac{dl_1}{dt} = \sum_{i=2}^{n} x_{i1} l_i. \tag{24}$$

On the other hand, from (13), we have

$$\sum_{i=1}^{n} x_{i1} l_i = X_0 l_1. \tag{25}$$

From these, we find that

$$\frac{dl_1}{dt} = X_0 l_1 - \left(l_1^T X_0 l_1\right) l_1, \tag{26}$$

since $x_{11} = l_1^T X_0 l_1$. It is easy to see that the right hand side of (26) is precisely the projected gradient for the problem

$$\text{maximize} \qquad F(x) := x^T X_0 x \tag{27}$$

$$\text{subject to} \qquad x^T x = 1, \tag{28}$$

and hence the flow $l_1(t)$ converges to the eigenvector associated with the most dominant eigenvalue. Indeed, the exact solution of (26) is given by

$$l_1(t) = \frac{e^{X_0 t} l_1(0)}{\|e^{X_0 t} l_1(0)\|} \tag{29}$$

which is related to the Toda flow [11,13] and has been studied as the continuous power method [7]. From (13) and Theorem 3.1, it is obvious that $x_{11}(t)$ converges to the most dominant eigenvalue of X_0.

EXAMPLE 2. Choose $A = [a_{ij}]$ such that

$$a_{ij} := \begin{cases} 1 & \text{if} \quad i > j, \\ -1 & \text{if} \quad j > 1, \\ 0 & \text{otherwise} \end{cases} \tag{30}$$

Obviously the resulting (10) is the classical Toda lattice equation [see (1)]. The convergence of the classical Toda lattice and hence of the QR algorithm to a diagonal matrix follows from Theorem 3.1 [11, 15] immediately.

EXAMPLE 3. Let Δ be an arbitrary subset of ordered integer pairs $\{(i, j) \mid 1 \le j < i \le n\}$. Choose $A = [a_{ij}]$ such that

$$a_{ij} := \begin{cases} 1 & \text{if} \quad (i, j) \in \Delta, \\ -1 & \text{if} \quad (j, i) \in \Delta, \\ 0 & \text{otherwise} \end{cases} \tag{31}$$

Theorem 3.1 implies that $x_{ij}(t)$ of the corresponding (10) converges to zero whenever $(i, j) \in \Delta$ [see (2)]. This re-proves Theorem 1.1.

In all the examples above, the values ± 1 can be replaced by arbitrary numbers (except that $a_{ij} \ge 0$ for $i > j$ and A skew-symmetric) and by Theorem 3.1 we shall have similar convergence results. The following is one particular example.

EXAMPLE 4. Let $D = \operatorname{diag}\{d_1, \ldots, d_n\}$ be an arbitrary diagonal matrix with $d_i \geq d_j$ if $i \leq j$. Choose $A = [a_{ij}]$ such that

$$a_{ij} := d_i - d_j. \tag{32}$$

Then (10) becomes a Brockett double bracket equation [see (3) and (4)]. Theorem 3.1 can now be used to show that the Brocket flow (3) and (4) converges to one of $n!$ possible diagonal matrices (see Theorem 1.2), but it says nothing about which one is the stable equilibrium point.

5. EFFECT OF SCALING

In addition to generating different flows, the scaling introduced by the matrix A has several other interesting effects from computational point of view. To illustrate the idea, we shall assume that the initial value X_0 is generic, i.e., X_0 is not an equilibrium point of (10); such points, being on algebraic curves, form a nowhere dense set of measure zero.

The most obvious effect can be seen by comparing the "uniformly" scaled Toda flow where $a_{ij} = \pm c$, $c > 1$, with the classical Toda flow where $a_{ij} = \pm 1$ [see (30)]. The differential system being autonomous, it is clear that

$$X_{c-\text{scaledToda}}(t; X_0) = X_{\text{Toda}}(ct; X_0).$$

That is, the scaled Toda flow is expected to reach convergence c times faster than the classical Toda flow.

A more subtle comparison is to consider a *partial ordering* $\succeq$ on skew-symmetric matrices defined by

$$A \succeq 0 \qquad \text{if} \quad a_{ij} \geq 0 \quad \text{for all } i > j, \tag{33}$$

$$A \succeq B \qquad \text{if } A - B \succeq 0. \tag{34}$$

Given the same X, it can be seen from (22) that if $A \succeq B$, then the σ_k corresponding to A "grows" infinitesimally faster then that corresponding to B. Thus, for example, to Brockett flow $X_{\text{Brockett}}(t; X_0)$ [see (32) with D defined by (4)] grows faster in the sense of majorization [12, p. 166] than the classical Toda flow $X_{\text{Toda}}(t; X_0)$ [see (30)], at least for sufficiently small $t > 0$. Figure 1 illustrates this majorization property of

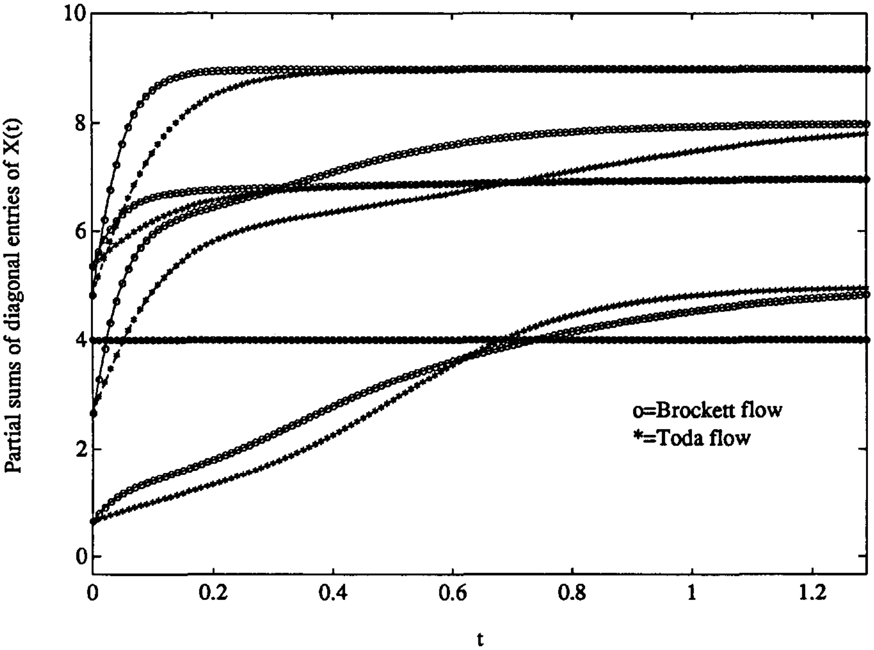

FIG. 1. Majorization of Brockett flow versus Toda flow.

Brockett flow versus Toda flow for the matrix

$$X_0 = \begin{bmatrix} 0.6489 & 0.3286 & -0.1870 & 0.4121 & -1.3056 \\ 0.3286 & 2.0112 & -0.4956 & 3.4960 & 0.4198 \\ -0.1870 & -0.4956 & 2.1534 & -0.1380 & -1.8459 \\ 0.4121 & 3.4960 & -0.1380 & 0.5415 & -0.5440 \\ -1.3056 & 0.4198 & -1.8459 & -0.5440 & -1.3550 \end{bmatrix}.$$

We note, as is demonstrated in Figure 1, that at some latter stage of integration it is possible that

$$\sigma_{i,\,\text{Toda}}(t) \geq \sigma_{i,\,\text{Brockett}}(t) \qquad \text{for some } i.$$

The choice of A in the form (32) is of particular interest. Apparently what is important in the diagonal matrix D is not the values of d_i, $i = 1, \ldots, n$, but rather the relative spacing of these elements. Diagonal matrices with elements either $\{d_1, \ldots, d_n\}$ or $\{d_1 + c, \ldots, d_n + c\}$ generate the same flow. We note then that the choice

$$D = \text{diag}\{1, 0, \dots, 0\} \tag{35}$$

gives rise to the matrix (23) which leads to the continuous power method. The choice

$$D = \text{diag}\{2, 1, 0, \dots, 0\}, \tag{36}$$

on the other hand, will cause the corresponding flow $X(t)$ to converge, according to Theorem 3.1, to a limit point of the form

$$x(\infty) = \begin{bmatrix} \times & 0 & 0 & \cdots & 0 \\ 0 & \times & 0 & \cdots & 0 \\ 0 & 0 & \times & \cdots & \times \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & \times & \cdots & \times \end{bmatrix},$$

where $\times$ indicates some nonzero values. Furthermore, since $X(\infty)$ is the least squares approximation to D, the sorting property guarantees that $x_{11}(\infty)$ and $x_{22}(\infty)$ are the two largest eigenvalues of X_0. This is a continuous version of the so-called simultaneous iteration [14, Chapter 14].

Motivated by the above observation, we find another application of the Brockett flow, which is aimed at *aggregating* eigenvalues into blocks. For example, the limit point $X(\infty)$ of the flow corresponding to the choice

$$D = \text{diag}\{\underbrace{3, \dots, 3}_{n_1 \text{ many}}, \underbrace{2, \dots, 2}_{n_2 \text{ many}}, \underbrace{1, \dots, 1}_{n_3 \text{ many}}\} \tag{37}$$

will be a block diagonal matrix with three blocks. The eigenvalues of the (1, 1) block of $X(\infty)$ are the n_1 most dominant eigenvalues of X_0; the eigenvalues of the (3, 3) block are the n_3 least dominant eigenvalues of X_0; and the (2, 2) block contains the remaining eigenvalues. In this way the eigenvalues of X_0 are aggregated into three groups according to their ordering. In the special case when $n_2 = 1$, we are able to single out the $(n_1 + 1)$th largest eigenvalue of X_0 by solving the differential equation. We think this feature is very interesting and useful.

Of course, the choice of values 0, 1, 2, or 3 for diagonal matrices D in (35), (36), or (37) is for the purpose of demonstration only. One may certainly choose different values and consider the possible speedup in convergence as we have done earlier.

Given any diagonal matrix $D = \text{diag}\{d_1, \dots, d_n\}$, let $\Omega(D)$ denote the polytope in R^n whose vertices are exactly the columns of D. Given $X_0 \in S(n)$, let its eigenvalues be written into the diagonal matrix $\Lambda = \text{diag}\{\lambda_1, \dots, \lambda_n\}$. Consider

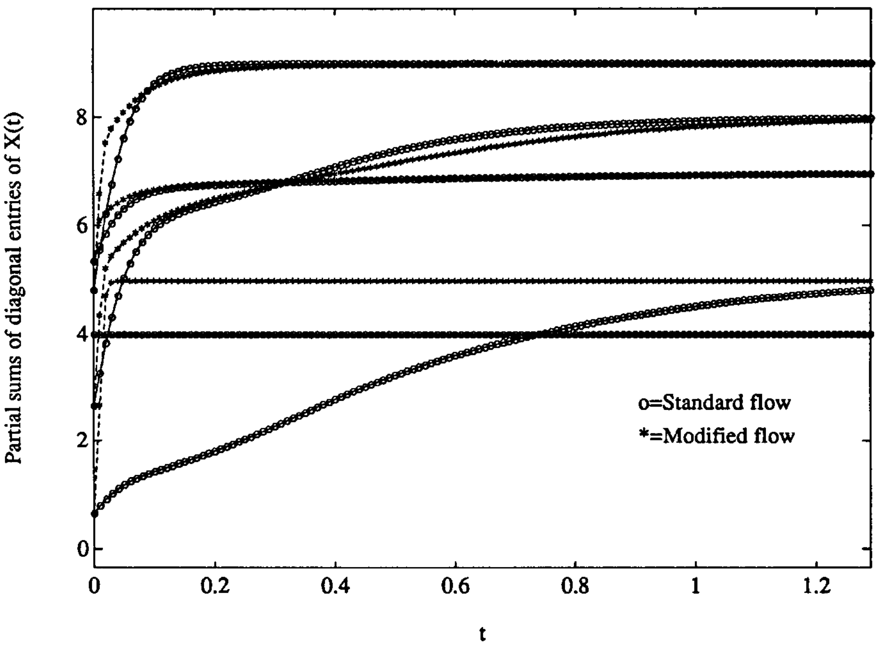

FIG. 2. Majorization of standard Brockett flow versus modified Brockett flow.

the two polytopes $\Omega(D)$ and $\Omega(\Lambda)$. Our theory suggests that the least squares approximation to D subject to the spectral constraint $\lambda_1, \ldots, \lambda_n$ is the diagonal matrix Λ such that the polytope $\Omega(\Lambda)$ is as similar to $\Omega(D)$ as possible in the sense of Theorem 1.2. This feature should find applications in geometric design. Suppose we make one or more vertices of D more distinguishable than other vertices; then the corresponding Brockett flow (3) should show up the corresponding eigenvalues earlier than other eigenvalues. This is like rattling a long and narrow polytope $\Omega(\Lambda)$ inside a long and narrow polytope $\Omega(D)$. It is expected that the longer edges of $\Omega(\Lambda)$ will align with those of $\Omega(D)$ first while the shorter edges of $\Omega(\Lambda)$ are yet to be settled. Our numerical experiment seems to confirm this intuition. In Figure 2, we compare the standard Brockett flow where D is defined by (4) with the modified Brockett flow where

$$D = \operatorname{diag}\{10n,\ n-1, \ldots, 2,\ 1\}. \tag{38}$$

Clearly, $\sigma_{1,\,\mathrm{Modified}}(t)$ converges significantly faster than $\sigma_{1,\,\mathrm{Standard}}(t)$, while the rest are converging at almost the same rate.

6. CONCLUSION

The structure of Toda lattice has been modified to allow scaling in the second component of the Lax pair. A number of interesting facts concerning the scaled Toda-like flow (10) have been studied in this paper.

With specially selected scaling matrix A, the scaled Toda-like flow includes as special cases several well-known flows that are related to important numerical linear algebra algorithms. We have shown that the time-1 mapping of the scaled Toda-like flow still enjoy a QR-like iteration except that the corresponding QR-like decomposition now becomes metaphysical. We restricted to symmetric matrices, a unified proof of global convergence is given in Theorem 3.1. The effect of scaling is demonstrated through numerical examples. It seems that by increasing the scaling factor one might cut short the interval of integration for reaching the equilibrium. Of particular interest is that by maneuvering the diagonal matrix D one can locate intermediate eigenvalues of matrix X_0 according to their ordering.

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