International Symposium on Nonlinear Theory and its Applications
Xi'an, PRC, October 7–11, 2002

Proposal of a New Discretization Method for Oja's Equation

Yutaka KUWAJIMA and Takaomi SHIGEHARA

Department of Information and Computer Sciences
Faculty of Engineering
Saitama University
Shimo-Okubo 255, Saitama, Saitama 338-8570, Japan
Phone:+81-48-858-9035, Fax:+81-48-858-3716
Email: kuwa@me.ics.saitama-u.ac.jp

Abstract

Based on the bilinearization method, we propose a new difference scheme for Oja's learning equation in neural network. It is shown that the proposed scheme is efficient even when the autocorrelation matrix has the nearly degenerate eigenvalues. Some fundamental aspects of the proposed difference scheme are also discussed.

1. Introduction

A close relation between algorithms and nonlinear dynamical systems has been recently attracted much attention in the field of numerical computation. For example, the time evolution for the unit time interval of the finite non-periodic Toda lattice [1] is equivalent to the one-step of the QR algorithm for computing all the eigenvalues of a tridiagonal symmetric matrix [2].

Another promising candidate is Oja's learning equation in neural network [3], which is exactly the object we will discuss in this paper. Oja's learning equation is a nonlinear differential equation for $\vec{x}(t) \in \mathbf{R}^n$, defined by

$$\frac{d\vec{x}(t)}{dt} = A\vec{x}(t) - \vec{x}(t)\vec{x}^T(t)A\vec{x}(t) \tag{1}$$

with the autocorrelation matrix A, which is an n-by-n positive definite real symmetric matrix in general. The equation (1) is known to be described as the gradient flow of Rayleigh quotient of A on the unit sphere, the maximum on which is attained at a normalized eigenvector associated with the largest eigenvalue of A. Forward Euler method after a suitable linearization of the equation gives rise to the power method with shift on the unit sphere for calculating the eigenvector associated with the largest eigenvalue of A [4]. However, the convergence rate of the algorithm on the unit sphere is not necessarily high. To settle this problem, we propose in this paper a new difference scheme for (1) which is applicable even to the outside of the unit sphere. It will be shown that the proposed difference equation is more efficient than the power method with shift in case that the matrix A has close eigenvalues. Even for generic matrices, the convergence rate of the proposed difference equation with a suitable discretization stepsize is the same as in the power method with shift. We also prove in this paper that the proposed difference equation satisfies some fundamental conditions which are required in numerical scheme.

The paper is organized as follows. In section 2, using the so-called bilinearization method, we introduce a new difference equation for (1). Some theorems which reveal fundamental aspects of the proposed difference scheme are also presented. In section 3, we show numerical results for the proposed difference equation, and the merit compared to the power method with shift is discussed. Summary and conclusion are given in section 4. The proofs for the theorems in section 2 are given in appendix.

2. New Difference Scheme for Oja's Equation

In deriving a difference scheme for a nonlinear differential equation, it is required to keep not only local properties but also global properties of the original equation. One promising technique for this purpose is the bilinearization method, which has been originally developed in the soliton theory [5, 6]. Applying the bilinearization method to Oja's equation (1), we have the difference equation

$$\begin{aligned} \vec{x}(t+\delta) &= \vec{x}(t) \\ &+ \delta\left(A\vec{x}(t) - \frac{\vec{x}^T(t)A(I+\delta A)\vec{x}(t)}{1+\delta\vec{x}^T(t)A\vec{x}(t)}\vec{x}(t)\right), \end{aligned} \tag{2}$$

where δ is discretization stepsize. It is easy to see that the difference equation (2) reproduces (1) in the limit of $\delta \longrightarrow 0$.

Note that the bilinearization method does not give rise to a unique difference scheme for a given differential equation in general. In this paper, however, after a fine examination of the method theoretically as well as experimentally, we have found the difference scheme (2) is most desirable.

Concerning the difference equation (2), the following theorems hold. The proofs are given in appendix in this paper. The theorems assert that the fixed points and their stability of the difference equation (2) are exactly the same as in Oja's equation (1).

Theorem 1 *Let A be an n-by-n positive definite real symmetric matrix. Then, $\vec{x} \in \mathbf{R}^n$ is a fixed point of (2) if and only if $\vec{x} = \vec{0}$ or $\vec{x}$ is a normalized eigenvector of A.*

Theorem 2 *Let A be an n-by-n positive definite real symmetric matrix with the eigenvalues $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n > 0$. Let $\vec{x} \in \mathbf{R}^n$ be a fixed point of (2). If $\delta > 0$, then $\vec{x}$ is stable if and only if $0 < \delta < 2/(\lambda_1 - \lambda_n)$ and $\vec{x}$ is a normalized eigenvector associated with the largest eigenvalue λ_1. If $\delta < 0$, then $\vec{x}$ is stable if and only if $-\frac{2}{\lambda_1} < \delta < 0$ and $\vec{x} = \vec{0}$.*

The following corollary immediately follows from Theorem 2.

Corollary 1 *The maximal discretization stepsize in (2) which ensures the convergence is twice as that in forward Euler method.*

3. Numerical Experiments

In this section, we examine the convergence rate of the iteration scheme (2) numerically and compare it to the convergence rate of the power method with shift

$$\vec{x}(t+\delta) = \frac{(A + \frac{1}{\delta}I)\vec{x}(t)}{||(A + \frac{1}{\delta}I)\vec{x}(t)||_2}. \tag{3}$$

It is known that for any arbitrary non-zero initial vector, the vector sequence on the unit sphere generated by (3) is converged (to a normalized eigenvector associated with the largest eigenvalue λ_1) if and only if

$$\delta > 0 \quad \text{or} \quad \delta < -\frac{2}{\lambda_1 + \lambda_n}, \tag{4}$$

where $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n > 0$ are the eigenvalues of A. In particular, the optimal δ which causes the fastest convergence is given by

$$\delta_{opt} = -\frac{2}{\lambda_2 + \lambda_n}. \tag{5}$$

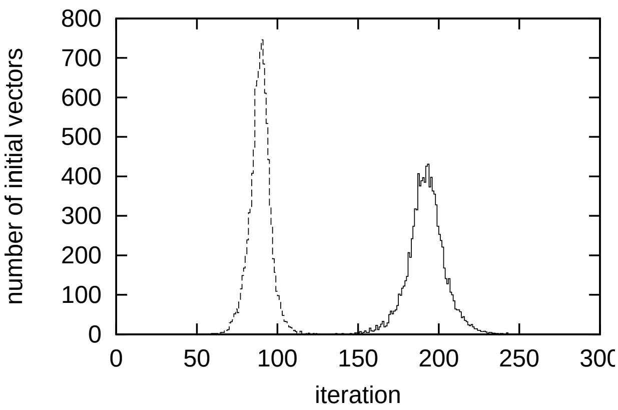

Figure 1: Occurrence frequency of the initial vectors, for which the number of iterations indicated on the horizontal axis is required to get the convergence. $A = A_1$ and $\delta = 0.5$ are taken. Broken (solid) curve is the result for the proposed difference scheme (the power method with shift).

We consider the three typical cases; $A = A_i$ $(i = 1, 2, 3)$, where

$$\begin{aligned} A_1 &= \text{diag}(2.0, 1.5, 1.0, 0.5), & (6)\\ A_2 &= \text{diag}(2.0, 1.0, 0.5, 0.2), & (7)\\ A_3 &= \text{diag}(2.0, 1.9, 1.8, 1.7). & (8) \end{aligned}$$

A_1 has the equally spaced eigenvalues on the positive real axis below the maximum eigenvalue. A_2 corresponds to the case that the maximum eigenvalue is far larger than the other eigenvalues, where even a simple power method works well. On the other hand, A_3 corresponds to the case that all the eigenvalues are nearly degenerate, where the power method does not work well.

Throughout figures 1–4 below, the criterion for the convergence is taken as

$$\frac{||\vec{x}(t+\delta) - \vec{x}(t)||_2}{||\vec{x}(t)||_2} < 10^{-12}. \tag{9}$$

To minimize the dependence on the initial vectors, we consider the average number of iterations to obtain the convergence at the level of accuracy given in (9). We take 10000 random initial vectors uniformly distributed on $\mathbf{R}^4$. Figure 1 shows a typical pattern of the occurrence frequency of the initial vectors, for which the number of iterations indicated on the horizontal axis is required to get the convergence. We take $A = A_1$ and $\delta = 0.5$ in figure 1. Both for the proposed method and the power method with shift, the histogram has a Gaussian-like shape, which justifies regarding the average number of iterations to get the convergence as a reliable numerical measure for the convergence rate.

Figures 2–4 show the dependence of the average iteration number to get the convergence on the discretization stepsize δ in case of $A = A_1, A_2, A_3$, respectively. We recognize from figure 4 that the iteration scheme (2) is efficient for the almost degenerate case, in which the power method with shift does not work well. The range of discretization stepsize δ which ensures fast convergence is wide and thus the iteration scheme (2) is expected to be robust in this case. Even for $A = A_1, A_2$, the average number of iterations with an optimal discretization stepsize δ is almost the same both for the proposed difference equation (2) and the power method with shift (3), although the optimal region is somewhat narrow in (2).

Note that the most expensive part in numerical computation at each iteration step is a matrix-vector product both for (2) and (3), and thus the number of iterations to obtain the convergence directly reflects the execution time. This means that the proposed iteration scheme (2) is indeed efficient especially for the nearly degenerate case, and (2) and (3) are expected to be complementary to each other.

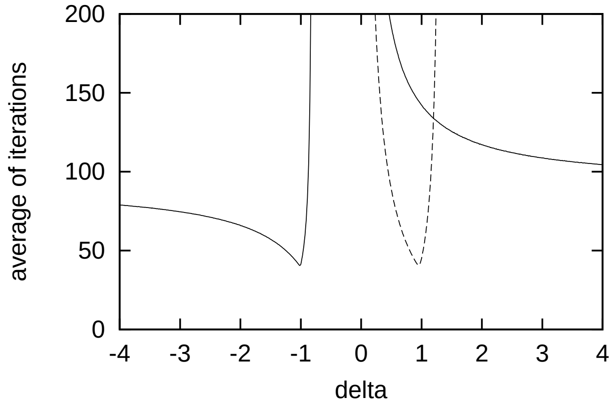

Figure 2: Dependence of the average number of iterations to get the convergence on the discretization stepsize δ with $A = A_1 = \mathrm{diag}(2.0, 1.5, 1.0, 0.5)$. Broken (solid) curve is the result for the proposed difference scheme (the power method with shift).

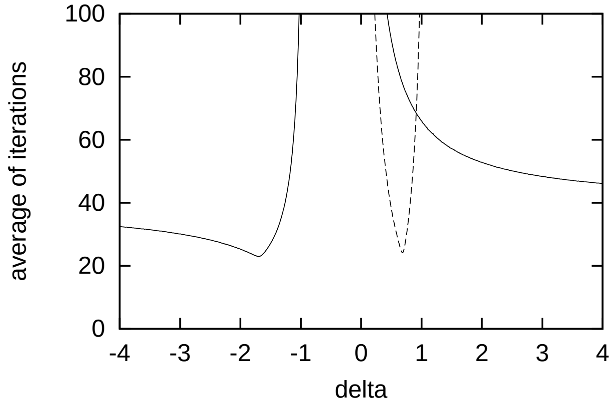

Figure 3: The same as in figure 2 except that $A = A_2 = \mathrm{diag}(2.0, 1.0, 0.5, 0.2)$.

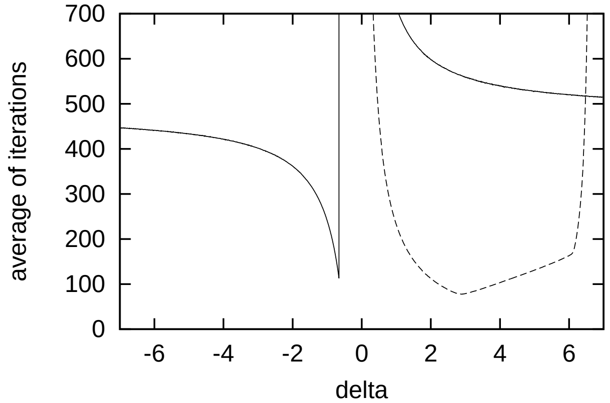

Figure 4: The same as in figure 2 except that $A = A_3 = \mathrm{diag}(2.0, 1.9, 1.8, 1.7)$.

4. Summary

Based on the bilinearization method originally developed in the soliton theory, we propose a new difference scheme for Oja's learning equation in neural network. The proposed difference scheme is efficient even in the case of the nearly degenerate eigenvalues. Thus the proposed scheme and the power method with shift are complementary to each other. Some local properties of the equilibrium of the proposed difference scheme have been also clarified.

5. Appendix

In this appendix, proofs of the theorems in section 2 are given.

Proof of Theorem 1. Obviously, $\vec{x} = \vec{0}$ and the normalized eigenvectors of A are the fixed points of (2). Let $\vec{x} \neq \vec{0}$ be a fixed point of (2). It is easy to see that $\vec{x}$ is an eigenvector of A. Let λ be the eigenvalue associated with the eigenvector $\vec{x}$. Then, since

$$\lambda = \frac{\vec{x}^T A(I + \delta A)\vec{x}}{1 + \delta \vec{x}^T A \vec{x}} = \frac{\lambda ||\vec{x}||_2^2 + \delta\lambda^2 ||\vec{x}||_2^2}{1 + \delta\lambda ||\vec{x}||_2^2}, \tag{10}$$

$\vec{x}$ is normalized. □

We need the following lemma to prove theorem 2.

Lemma 1 *Let $\vec{f}: \mathbf{R}^n \to \mathbf{R}^n$ be a C^1-mapping. Let $\vec{x}$ be a fixed point of $\vec{f}$; $\vec{f}(\vec{x}) = \vec{x}$. Then,*

1. *if $\rho(J_{\vec{f}}(\vec{x})) < 1$, $\vec{x}$ is stable,*
2. *if $\rho(J_{\vec{f}}(\vec{x})) > 1$, $\vec{x}$ is not stable,*

where

$$J_{\vec{f}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix} \tag{11}$$

is the Jacobian matrix of $\vec{f}$ and $\rho(\cdot)$ is the spectral radius.

Proof of theorem 2. Since A is real symmetric, there exists an n-by-n orthogonal matrix P such that

$$P^T A P = \Lambda \equiv \mathrm{diag}(\lambda_1, \lambda_2, \cdots, \lambda_n). \tag{12}$$

By the coordinate transformation $\vec{r}(t) = P^T \vec{x}(t)$, the difference equation (2) is reduced to

$$\begin{aligned} \vec{r}(t+\delta) &= \vec{r}(t) \\ &+ \delta \left(\Lambda \vec{r}(t) - \frac{\vec{r}^T(t)\Lambda(I+\delta\Lambda)\vec{r}(t)}{1+\delta\vec{r}^T(t)\Lambda\vec{r}(t)} \vec{r}(t) \right). \end{aligned} \tag{13}$$

By theorem 1, the fixed point of (13) is $\vec{r} = \vec{0}$ or $\vec{r} = \pm\vec{e}_i$, where $\vec{e}_i$ is the i-th column of the n-by-n identity matrix. Eq. (13) is written as

$$\vec{r}(t+\delta) = \vec{f}(\vec{r}(t)) \tag{14}$$

with a C^1-function

$$\vec{f}(\vec{r}) = \frac{1 - \delta^2 \vec{r}^T \Lambda^2 \vec{r}}{1 + \delta \vec{r}^T \Lambda \vec{r}} \vec{r} + \delta \Lambda \vec{r}. \tag{15}$$

Lemma 1 shows that, since

$$\rho(J_{\vec{f}}(\vec{0})) = \max_{1 \le j \le n} \{|1 + \delta\lambda_j|\}, \tag{16}$$

the origin $\vec{x} = \vec{0}$ is stable if and only if $-\frac{2}{\lambda_1} < \delta < 0$ holds. It is not difficult to see that

$$\begin{aligned} \rho(J_{\vec{f}}(\pm\vec{e}_i)) = \; & \max\{|1+\delta(\lambda_1-\lambda_i)|, \cdots, \\ & |1+\delta(\lambda_{i-1}-\lambda_i)|, \left|\frac{1-\delta\lambda_i}{1+\delta\lambda_i}\right|, \\ & |1+\delta(\lambda_{i+1}-\lambda_i)|, \cdots, |1+\delta(\lambda_n-\lambda_i)|\} \end{aligned} \tag{17}$$

$(i = 1, 2, 3, \cdots, n)$. For $i = 2, 3, \cdots, n$, $\rho(J_{\vec{f}}(\pm\vec{e}_i)) > 1$ holds if $\delta \neq 0$. Thus $\pm\vec{e}_2, \cdots, \pm\vec{e}_n$ are unstable from Lemma 1, irrespective to the sign of δ. On the other hand, $\rho(J_{\vec{f}}(\pm\vec{e}_1)) < 1$ holds if and only if $0 < \delta < 2/(\lambda_1 - \lambda_n)$. From Lemma 1, this gives the necessary and sufficient condition for the fixed point $\pm\vec{e}_1$ to be stable. □

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