Vol.2011-MPS-84 No.4
2011/7/18

An Improved Shift Strategy for the Modified Discrete Lotka-Volterra with Shift Algorithm

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We propose a new mathematical shift strategy for the modified discrete Lotka-Volterra with shift (mdLVs) algorithm. The mdLVs algorithm computes the singular values of bidiagonal matrices. It is known that the convergence of the mdLVs algorithm is accelerated when the shift is close to and less than the square of the smallest singular value of the input matrix. In the original mdLVs algorithm, the Johnson bound is adopted. Our improved mdLVs algorithm combines the Gerschgorin-type bound, the Kato-Temple bound, the Laguerre shift, and the generalized Newton shift. For different combinations, we discuss the computational time and number of iterations.

1. Introduction

Singular value decomposition (SVD) is one of the most important matrix operations in numerical algebra, and it plays an important role in fields such as data search systems[5] and image processing[13].

Several SVD algorithms are composed by computing singular values and singular vectors. The modified discrete Lotka-Volterra with shift (mdLVs) algorithm[3),4),14),15] computes singular values; its speed and relative accuracy are excellent.

The mdLVs iteration involves the computation of shifts. It is known that the convergence of the mdLVs algorithm is accelerated when the shift is close to and less than the square of the smallest singular value of the input matrix. The Integrable-SVD[3),14)–16], for which a library has been developed[2], includes the original mdLVs algorithm. It uses the Johnson bound[6] as shift strategy. This bound can compute a sharper bound among various shift strategies. However, since $2M-1$ square roots must be found, the Johnson bound has a large computational time. Here, M is the dimension size of the input matrix. Therefore, a fast and mathematically rigorous shift strategy is needed.

In this paper, we improve the shift strategy for the mdLVs algorithm. First, we compute a lower bound of the smallest singular value from the Gerschgorin theorem[1]. Let us call this bound the Gerschgorin-type bound. Since this is always weaker than the Johnson bound after enough number of iterations, we then consider the Kato-Temple bound[7]. We compare the two bounds to determine a shift for the mdLVs algorithm. In some cases, the Laguerre shift[11] or the generalized Newton shift[9),10] instead of the Gerschgorin-type bound is adopted. The improved shift can be computed with M square-root operations.

In Section 2, we explain the mdLVs algorithm. In Section 3, we introduce the Johnson bound. In Section 4, we describe the improved shift strategy for the mdLVs algorithm. In Section 5, we present numerical experiments and confirm that the mdLVs algorithm with the new strategy is faster than the original algorithm.

2. Modified discrete Lotka-Volterra with shift algorithm

In Section 2.1, we give a summary of the singular value computation based on the discrete Lotka-Volterra (dLV) system. In Section 2.2, we outline the mdLVs algorithm. In Section 2.3, we briefly describe the implementation of the mdLVs algorithm.

2.1 Singular value computation based on the discrete Lotka-Volterra system

In mathematical biology, the Lotka-Volterra (LV) system is known as a fundamental prey-predator model. In some cases, the LV system is a completely integrable dynamical system with explicit solutions and sufficiently many conservation laws. A time discretization

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

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of the LV system is known (cf. 3)). This system also has an explicit solution and many conservation laws. Therefore, it is called the integrable dLV system. Here, k ($k = 1, 2, \cdots, 2M-1$) indicates the kth species, the discrete time n ($n = 0, 1, 2, \cdots$) corresponds to the iteration number of the algorithm, $u_k^{(n)}$ is the value of u_k at n, and the arbitrary nonzero number $\delta^{(n)}$ is a discrete step-size. Let the initial value $u_k^{(0)}$ be positive. In the case where $\delta^{(n)} > 0$, any subtraction and division by zero do not occur in Eq.(1) and $u_k^{(n)}$ is always positive. Consequently, cancellation and numerical instability do not occur. Note that we do not need to treat negative numbers in singular value computations.

The boundary condition and the initial condition are given by

$$u_0^{(n)} \equiv 0, \quad u_{2M}^{(n)} \equiv 0, \tag{2}$$

$$u_k^{(0)} = \frac{(b_k)^2}{1+\delta^{(0)} u_{k-1}^{(0)}}. \tag{3}$$

respectively. Here, b_{2i-1} (> 0) and b_{2i} (> 0) (i: $1 \le i \le M$) are the diagonal and upper-subdiagonal elements, respectively, of the $M \times M$ bidiagonal matrix B. When $n \to \infty$, $u_{2i-1}^{(n)}$ and $u_{2i}^{(n)}$ converge to the square of the ith singular value σ_i and 0, respectively. Thus the dLV system gives rise to a stable scheme for computing the singular values[3)].

2.2 Improved speed via a shifted discrete Lotka-Volterra scheme

The mdLVs algorithm, the integrable dLV system with a shift, can compute the singular values more quickly. The mdLVs algorithm is as follows[4)].

Let us introduce new elements $w_k^{(n)}$ and $v_k^{(n)}$ by

$$w_k^{(n)} = u_k^{(n)}(1+\delta^{(n)} u_{k-1}^{(n)}), \tag{4}$$

$$v_k^{(n)} = u_k^{(n)}(1+\delta^{(n)} u_{k+1}^{(n)}). \tag{5}$$

By Eq.(3), the initial $w_k^{(0)}$ is just b_k^2. The shifted integrable dLV system is defined by adding to Eq.(1) a shift Θ at the nth iteration defined as $0 \le \Theta < \sigma_{min}^2$ where σ_{min} is the smallest singular value of B. This gives

$$\begin{aligned} w_{2i-1}^{(n+1)} &= v_{2i-1}^{(n)} + v_{2i-2}^{(n)} - w_{2i-2}^{(n+1)} - \Theta, \\ w_{2i}^{(n+1)} &= v_{2i-1}^{(n)} v_{2i}^{(n)} / w_{2i-1}^{(n+1)}. \end{aligned} \tag{6}$$

In general, the convergence is accelerated by increasing Θ. However, since the positivity of $u_k^{(n)}$ may be destroyed by a larger Θ at the nth iteration, this causes a numerical instability. It is proved in[4)] that $u_k^{(n)} > 0$ if and only if $0 \le \Theta < \sigma_{min}^2$. Hence, we can determine the shift Θ for estimating σ_{min}.

2.3 Algorithm for singular value computation based on the Lotka-Volterra system

Each iteration in the mdLVs algorithm is as follows.

(1) Calculate $u_k^{(n)}$ from $w_k^{(n)}$ via Eq.(4).
(2) Calculate $v_k^{(n)}$ from $u_k^{(n)}$ via Eq.(5).
(3) Calculate the shift Θ at the nth iteration.
(4) Check Θ and calculate $w_k^{(n+1)}$ accordingly.
  - If Θ is valid, calculate $w_k^{(n+1)}$ from $v_k^{(n)}$ via Eq.(6).
  - Otherwise, $w_k^{(n+1)} = v_k^{(n)}$.

(5) If $w_{2i}^{(n+1)}$ is much smaller than $w_{2i-1}^{(n+1)}$, perform SPLIT or a deflation of the dimension as described in[12)].

SPLIT, which divides the matrix into two parts, and the deflation are defined.

The arrays of the algorithm are calculated as follows. In Step 1), the array $U = (u_1^{(n)}, u_2^{(n)}, \cdots, u_{2M-1}^{(n)})$ is calculated from the array $W = (w_1^{(n)}, w_2^{(n)}, \cdots, w_{2M-1}^{(n)})$. Since we do not keep the data for each n, each array is a one-dimensional array corresponding to the subscript. In Step 2), the array $V = (v_1^{(n)}, v_2^{(n)}, \cdots, v_{2M-1}^{(n)})$ is calculated from U. In Step 3), the shift Θ at the nth iteration is calculated from V. Using the valid Θ, we overwrite W with V in Step 4).

3. Johnson bound

The theorem for the Johnson bound is a corollary of the Gerschgorin circle theorem for $\dfrac{(B^\top + B)}{2}$. Since the singular values in B are equal to those in $B^\top$, the Johnson bound for the smallest singular value of an upper bidiagonal matrix B is given as the following inequality:

$$\sigma_{min} \ge \min_{1 \le i \le M} \left[b_{2i-1} - \frac{1}{2}(b_{2i} + b_{2i-2}) \right], \tag{7}$$

where $b_0 = b_{2M} = 0$.

In the mdLVs algorithm, b_k becomes $\sqrt{v_k^{(n)}}$ at the nth iteration, and the shift Θ is defined as $0 \le \Theta < \sigma_{min}^2$. Therefore, the Johnson shift Θ_J is computed using the Johnson bound as follows:

$$\Theta_J = \left(\frac{1}{2}\left(\min_{1\le i\le M}\left[2\sqrt{v_{2i-1}^{(n)}} - \left(\sqrt{v_{2i}^{(n)}} + \sqrt{v_{2i-2}^{(n)}}\right)\right]\right)\right)^2. \quad (8)$$

Since B is a positive definite matrix, we adopt a zero shift when the bound is less than zero.

The number of square-root operations is $2M-1$, since $\sqrt{v_{2i}^{(n)}}$ can be reused in the $(i+1)$th computation.

4. Improved shift strategy

The Johnson bound, which is used in the original mdLVs algorithm, needs $2M-1$ square-root operations. When numerical algorithms are computed using microprocessors, square-root operations take longer than addition and multiplication operations. Therefore, a new high-accuracy shift with fewer square-root operations is needed. Consequently, we improve the shift strategy for the computation of the singular values. The improved strategy consists of the Gerschgorin-type bound, the Kato-Temple bound, the Laguerre shift, and the generalized Newton shift.

In Section 4.1, we describe Gerschgorin's theorem for the smallest eigenvalue. In Section 4.2, we explain the Kato-Temple inequality and the Kato-Temple bound. In Section 4.3, we discuss the Laguerre shift, and in Section 4.4, we introduce the generalized Newton shift. In Section 4.5, we discuss the improved shift strategy and its implementation in the mdLVs algorithm.

4.1 Gerschgorin-type bound

Let A be an $M \times M$ complex matrix.

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & & & \\ a_{2,1} & a_{2,2} & a_{2,3} & & \\ & \ddots & \ddots & \ddots & \\ & & a_{M-1,M-2} & a_{M-1,M-1} & a_{M-1,M} \\ & & & a_{M,M-1} & a_{M,M} \end{pmatrix}. \quad (9)$$

For $i = 1, \cdots, M$, the Gerschgorin disk D_i is defined as

$$D_i = \left\{ z : |z - a_{i,i}| \le \sum_{j=1, j\ne i}^{M} |a_{i,j}| \right\}. \quad (10)$$

From the Gerschgorin theorem, the each eigenvalue of A exists in at least one of the disks D_i (i: $i = 1, \cdots, M$). Since the eigenvalues of the real symmetric tridiagonal matrix $BB^\top$ are equal to the square of the singular values of B, we can get the Gerschgorin-type bound for $(\sigma_{\min})^2$, the square of the smallest singular value of B, by applying the Gerschgorin theorem to $BB^\top$. Then, the Gerschgorin-type shift Θ_G is obtained using the Gerschgorin-type bound as the follows:

$$\Theta_G = \min_{1\le i\le M}[(b_{2i-1}^2 + b_{2i}^2) - (b_{2i-1}b_{2(i-1)} + b_{2(i+1)-1}b_{2i})], \quad (11)$$

where $b_0 = b_{2M} = 0$. Eq.(11) may give a negative value. However, since $BB^\top$ is a symmetric positive definite matrix, we use zero shift in such cases.

In the mdLVs algorithm, Eq.(11) can be written as

$$\Theta_G = \min_{1\le i\le M}\left[(v_{2i-1}^{(n)} + v_{2i}^{(n)}) - \left(\sqrt{v_{2i-1}^{(n)}v_{2(i-1)}^{(n)}} + \sqrt{v_{2(i+1)-1}^{(n)}v_{2i}^{(n)}}\right)\right], \quad (12)$$

where $v_0^{(n)} = v_{2M}^{(n)} = 0$. From symmetry of $BB^\top$, Eq.(12) requires only $M-1$ times of square-root operations.

4.2 Kato-Temple bound

Let A be a real symmetric matrix and x be a real vector. Let $\rho = x^\top Ax$ be its Rayleigh quotient with $x^\top x = 1$. For a given eigenvalue λ of A, we introduce the Kato-Temple inequality.

Let us assume that the open interval $(\underline{\lambda}, \bar{\lambda})$ includes an eigenvalue λ of A as well as the Rayleigh quotient ρ and that it does not include any other eigenvalues. Then, we have an inequality given by the following theorem:

$$\rho - \frac{\varepsilon^2}{\bar{\lambda} - \rho} \le \lambda \le \rho + \frac{\varepsilon^2}{\rho - \underline{\lambda}}, \quad (13)$$

where $\varepsilon^2 = \| Ax - \rho x \|_2^2$.

In the following discussion, we consider an application of the Kato-Temple inequality for the smallest eigenvalue $\lambda_{\min}$ of the symmetric positive definite tridiagonal matrix of the form $A = BB^\top$, except $M \le 2$. The eigenvalues λ_i of A satisfy $0 < \lambda_M < \lambda_{M-1} < \cdots < \lambda_1$. Let $A^{(i)}$ be a $i \times i$ submatrix of A such that $|A^{(i)}|$ is the ith principal minor determinant of A. Let $\{\lambda_j^{(i)}\}_{j=1,\ldots,i}$ be a set of eigenvalues of $A^{(i)}$. Note that $A = A^{(M)}$ and $\lambda_j = \lambda_j^{(M)}$. The separation theorem (interlacing property)[8] for eigenvalues of symmetric tridiagonal matrices is $\lambda_i^{(i)} < \lambda_{i-1}^{(i-1)} < \lambda_{i-1}^{(i)} < \lambda_{i-2}^{(i-1)} < \cdots < \lambda_1^{(i)}$ for $i = 1, \ldots, M$.

Define a sequence $\{t_i\}$ by $t_1 = b_1^2 + b_2^2$, $t_{i+1} = b_{2(i+1)-1}^2 + b_{2(i+1)}^2 - b_{2i-1}b_{2(i-1)}/t_i$ for $i = 1, 2, \ldots, M-2$, $t_M = b_{2M-1}^2 - b_{2M-1}b_{2(M-1)}/t_{M-1}$. Since $|A^{(i)}| = t_1 t_2 \cdots t_i > 0$, we see that $t_i > 0$. By definition, we have

$$\begin{aligned} b_{2M-1}^2 > t_M &= \frac{|A^{(M)}|}{|A^{(M-1)}|} \\ &= \frac{\lambda_1^{(M)} \cdots \lambda_M^{(M)}}{\lambda_1^{(M-1)} \cdots \lambda_{M-1}^{(M-1)}} \\ &= \frac{\lambda_1^{(M)}}{\lambda_1^{(M-1)}} \cdots \frac{\lambda_{M-1}^{(M)}}{\lambda_{M-1}^{(M-1)}} \lambda_M^{(M)} \\ &> \lambda_M^{(M)} = \lambda_M. \end{aligned} \tag{14}$$

Now we have a candidate for the Rayleigh quotient ρ such that $\lambda_M < \rho$. Let us choose the unit vector x for

$$x = (0, \ldots, 0, 1)^\top. \tag{15}$$

The Rayleigh quotient is then given by

$$\rho = x^\top A x = b_{2M-1}^2 \quad (> \lambda_M). \tag{16}$$

Finally, we consider how to choose the right endpoint $\bar{\lambda}$ of the open interval $(\underline{\lambda}, \bar{\lambda})$ including λ_m, and not including any other eigenvalues. The separation theorem says that a good bound of the smallest eigenvalue $\lambda_{m-1}^{(m-1)}$ of the submatrix

$$A^{(M-1)} = \begin{pmatrix} b_1^2 + b_2^2 & b_3 b_2 & & \\ b_3 b_2 & b_3^2 + b_4^2 & b_5 b_4 & \\ & \ddots & \ddots & \ddots \\ & & b_{2M-3}b_{2M-4} & b_{2M-3}^2 + b_{2M-2}^2 \end{pmatrix}. \tag{17}$$

may give $\bar{\lambda}$ such that the assumption $\lambda_M < \rho < \bar{\lambda}$ is satisfied. In this case, we obtain the Kato-Temple bound Θ_K of the smallest eigenvalue λ_M of A from the Kato-Temple inequality. The Kato-Temple bound Θ_K is given as follows:

$$\begin{aligned} \Theta_K &= \rho - \frac{\varepsilon^2}{\bar{\lambda} - \rho} \\ &= b_{2M-1}^2 - \frac{\| Ax - \rho x \|_2^2}{\bar{\lambda} - b_{2M-1}^2} \\ &= b_{2M-1}^2 - \frac{b_{2M-1}^2 b_{2(M-1)}^2}{\bar{\lambda} - b_{2M-1}^2} \\ &\le \lambda_M. \end{aligned} \tag{18}$$

The bound $\Theta^{(M-1)}$ of $\lambda_{M-1}^{(M-1)}$ should be computed using the original bound, for example, the Gerschgorin-type bound and the generalized Newton bound. We call such a bound an auxiliary bound. If the assumption $\Theta^{(M-1)} > b_{2M-1}^2\ (= \rho)$ is satisfied, we obtain the Kato-Temple bound by Eq.(18) where $\bar{\lambda} = \Theta^{(M-1)}$.

4.3 Laguerre shift

Let us set $J_1^{(-)} = \mathrm{trace}(BB^\top)^{-1}$ and $J_2^{(-)} = \mathrm{trace}((BB^\top)^2)^{-1}$. The Laguerre shift Θ_L is defined as follows[11] :

$$\Theta_L = \frac{1}{J_1^{(-)}} \cdot \frac{M}{1 + \sqrt{(M-1)\left(M \dfrac{J_2^{(-)}}{(J_1^{(-)})^2} - 1\right)}} > 0. \tag{19}$$

Theoretically, $\left(M \frac{J_2^{(-)}}{(J_1^{(-)})^2} - 1\right)$ is positive, however computationally, the value is occasionally negative.

When the iteration number n is small, the Gerschgorin-type bound may be non-positive. On the other hand, in almost cases, the Laguerre shift Θ_L becomes positive, since $\left(M \frac{J_2^{(-)}}{(J_1^{(-)})^2} - 1\right)$ is non-negative. However, computationally, if $a_{i,i} - (a_{i,i-1} + a_{i,i+1}) \le 0$ for some i (i: $(1-\kappa)M \le i \le M$), then the Laguerre shift is not so close to the smallest singular value when the iteration number is small. Here $\kappa \in (0, 1)$ is a constant. Therefore, if all the expressions $a_{i,i} - (a_{i,i-1} + a_{i,i+1})$ are positive for $(1-\kappa)M \le i \le M$, we calculate the Laguerre shift Θ_L instead of returning zero derived from the Gerschgorin theorem. Experimentally, $\kappa = 0.02$ is the best choice.

4.4 Generalized Newton shift

The generalized Newton bound of the smallest singular value σ_{min} of B is given as follows[8]:

$$\Theta_p^{(M)} = (\mathrm{trace}(B^\top B)^{-p})^{-\frac{1}{2p}} = \frac{1}{\left(\frac{1}{\sigma_1^{2p}} + \cdots + \frac{1}{\sigma_M^{2p}}\right)^{\frac{1}{2p}}} > 0, \quad (20)$$

where p is an arbitrary positive integer. These bounds have the properties listed in 9) 10).

$$\Theta_1^{(M)} < \Theta_2^{(M)} < \cdots < \sigma_M, \quad (21)$$

$$\lim_{p\to\infty} \Theta_p^{(M)} = \sigma_M. \quad (22)$$

Then, $(\Theta_p^{(M)})^2$ $(p = 1, 2, \ldots)$ can be used. Let us call $(\Theta_p^{(M)})^2$ the generalized Newton shift of order p.

The generalized Newton shift $(\Theta_p^{(M)})^2$ can be computed within $O(Mp^2)$ flops using a recurrence-relation formula. This proof for the computational cost should be discussed in another paper, on which T. Yamashita, K. Kimura, and Y. Nakamura are working.

4.5 New shift strategy and its implementation

In most microprocessors, a square-root operation takes longer time than addition and multiplication operations. Therefore, the number of square-root operations should be reduced.

The Johnson bound requires $2M - 1$ times of square-root operations. On the other hand, the Gerschgorin-type bound needs just $M - 1$ times of square-root operations. Consequently, the Gerschgorin-type bound is expected as a measure to improve the shift strategy with the Johnson bound. However, we have to consider the following possibilities. The Gerschgorin-type bound Θ_G may be smaller than the Johnson bound Θ_J. Especially, after enough number of iterations, since it holds

$$\Theta_J = \left(\sqrt{v_{2M-1}^{(n)}} - \frac{1}{2}\sqrt{v_{2(M-1)}^{(n)}}\right)^2, \quad (23)$$

$$\Theta_G = v_{2M-1}^{(n)} - \sqrt{v_{2M-1}^{(n)} v_{2(M-1)}^{(n)}}, \quad (24)$$

in the mdLVs algorithm, we have $\Theta_J > \Theta_G$.

Furthermore, the Gerschgorin-type bound may give a non-positive value. Then, we devise computation of shift as follows. If the Gerschgorin-type bound gives a positive value, we compute the Kato-Temple bound and adopt the square of larger bound between these two bounds as the shift. If the Gerschgorin-type bound gives a non-positive value, we compute the Laguerre shift or take shift zero according to the condition described in the Section 4.3. If the Laguerre shift numerically gives a complex number since $\left(M\frac{J_2^{(-)}}{(J_1^{(-)})^2} - 1\right)$ is occasionally negative, then we compute the generalized Newton shift.

Table 1 Computation time and iteration number in each shift

	computation time[sec.]	iteration number
SHIFT(J)	27.61	315021
SHIFT(G)	23.06	368773
SHIFT(GK)	23.09	362114
SHIFT(GKL)	20.78	206941

5. Numerical experiments

To confirm the performance of the improved shift strategy, the computational time and number of iterations for the mdLVs algorithm in [2] with four shift strategies. The shifts are as follows:

- SHIFT(J): Johnson bound
- SHIFT(G): Gerschgorin-type bound
- SHIFT(GK): SHIFT(G) and Kato-Temple bound
- SHIFT(GKL): SHIFT(GK), Laguerre and generalized Newton shifts.

We use a computer with an Intel(R) Xeon(R) X5570@2.93GHz CPU and 32GB of memory. Fedora 13 is installed on this computer. The input matrices B are bidiagonal and the diagonal and subdiagonal elements of B are set randomly in an interval $[0, 1]$. The dimension is 30000, We set $\kappa = 0.02$ and $\delta^{(n)} = 1$, respectively.

Table 1 gives the average computational time and number of iterations for 100 matrices.

SHIFT(G) and SHIFT(GK) require more iterations than SHIFT(J) does. This implies that Θ_J tends to be stronger than Θ_G and Θ_K. Thus, the Gerschgorin-type bound itself nor the combination of the Gerschgorin-type bound and the Kato-Temple bound lead to a suitable shift. In spite of much the number of iterations, the computational time of SHIFT(G) and SHIFT(GK) are shorter than that of SHIFT(J). This is because of the numbers of square-root operations in SHIFT(G) and SHIFT(GK) are smaller than that in SHIFT(J). A square-root operation requires relatively large computational time.

On the other hand, SHIFT(GKL) gives better results in both the computational time and the number of iterations than SHIFT(J). In SHIFT(GKL), when the Gerschgorin-type bound returns non-positive value, the Laguerre shift is computed under the condition.We suppose such result attained from utilization of the Laguerre shift. Therefore, we recommend SHIFT(GKL) as a shift strategy for the mdLVs algorithm.

6. Conclusions

In this paper, we have improved the shift strategy for the mdLVs algorithm with the Johnson bound. The improved strategy utilizes the Gerschgorin-type bound, the Kato-Temple bound, the Laguerre shift, and the generalized Newton shift. This improvement takes advantage of less times of square-root operations of the Gerschgorin-type bound than the Johnson bound. There are possibilities that the Gerschgorin-type bound gives a smaller value than the Johnson bound or a non-positive value. Then, we consider the Kato-Temple bound, the Laguerre shift, and the generalized Newton shift. To validate the performance of the improved strategy, we explored the computational time and the number of iterations. The result shows that the improved strategy is efficient.

In future work, we plan to study the relative errors of the computed singular values in the improved shift strategy.

Acknowledgments This work is partially supported by JSPS Grant-in-Aid for Scientific Research (A) Japan, No.20246027.

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