An Arnoldi method with structured starting vectors for the delay eigenvalue problem

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Abstract: The method called *Arnoldi* is currently a very popular method to solve large-scale eigenvalue problems. The general purpose of this paper is to generalize Arnoldi to the characteristic equation of a *time-delay system*, here called a *delay eigenvalue problem*. The presented generalization is mathematically equivalent to Arnoldi applied to the problem corresponding to a Taylor approximation of the exponential. Even though the derivation of the result is with a Taylor approximation, the constructed method can be implemented in such a way that it is independent of the Taylor truncation paramater N. This is achieved by exploiting properties of vectors with a special structure, the vectorization of a rank one matrix plus the vectorization of a matrix which right-most columns are zero. It turns out that this set of vectors is closed under the matrix vector product as well as orthogonalization. Moreover, both operations can be efficiently computed. Since Arnoldi only consists of these operations, if Arnoldi is started with the special vector structure, the method can be efficiently executed. The presented numerical experiments indicate that the method is very efficient in comparison to methods in the literature.

Keywords: Arnoldi, time-delay systems, nonlinear eigenvalue problems, characteristic roots, companion linearization, polynomial eigenvalue problems, stability

1. INTRODUCTION

The following problem will be referred to as the *delay eigenvalue problem* (DEP): given matrices $A, B \in \mathbb{R}^{n\times n}$ and delay $\tau > 0$, find $s \in \mathbb{C}$ and $v \in \mathbb{C}^n \backslash \{0\}$ such that

$$sv = (A + Be^{-\tau s})v. \tag{1}$$

The DEP is an important problem since the solutions s are the characteristic roots of the delay-differential equation (DDE),

$$\dot{x}(t) = Ax(t) + Bx(t-\tau). \tag{2}$$

The characteristic roots, which are sometimes called eigenvalues, are most importantly relevant when studying the stability of (2) but they are also used to characterize other properties such as exponential decay rate, oscillation, controllability and observability. See Michiels and Niculescu (2007) for recent results related to the stability of (2) and generalizations expressed in terms of the eigenvalues.

The DEP (1) reduces to a standard eigenvalue problem if $\tau = 0$ or $B = 0$. The method called Arnoldi is the most widely used method for large scale standard eigenvalue problems. It is implemented in the Fortran software package ARPACK (see, e.g., Lehoucq et al. (1998)) which is the underlying software in the commonly used matlab function `eigs`. The general goal of this paper is to generalize Arnoldi to the DEP (1) in such a way that the appealing properties for the standard eigenvalue problem are preserved.

Arnoldi is truly efficient only if we can compute the corresponding matrix vector efficiently. The first important result of our study (presented in Section 3.1) is that for vectors with a special structure, the matrix vector operation corresponding to a truncated Taylor approximation of (1) can be computed efficiently. More importantly, the representation is such that it can be implemented without introducing any Taylor series truncation error. The efficient representation of the matrix vector product and a corresponding orthogonalization scheme allows us to construct an efficient method mathematically equivalent to the Arnoldi method.

The currently most common approach to solve the DEP is a two-stage approach, where the first step consists of estimating many eigenvalues (predictor) and then use a local correction scheme to gain high precision (correction). The two-stage predictor-corrector approach is used in the software package DDE-BIFTOOL (Engelborghs et al. (2001, 2002)) but also in other context, e.g., Gumussoy and Michiels (2009).

The estimation step normally consists of approximating the eigenvalues of (1) by solving an eigenvalue problem of larger dimension. The approximation in DDE-BIFTOOL is based on a linear multi-step scheme and with (psuedo) spectral methods in other works Breda et al. (2004, 2005, 2006). The associated large eigenvalue problem is solved with the Matlab command `eig` or `eigs` in most implementations.

Unlike the classical two-stage predictor-corrector approach, the method presented in this paper is a direct generalization of Arnoldi. An advantage of this is that several eigenvalues can be found and made more accurate by simply iterating further. Moreover, the predictor step in the two-stage approach typically involves some form of heuristics. This is not necessary for the presented Arnoldi approach.

The DEP belongs to a class of problems called nonlinear eigenvalue problems. There are several general purpose method for nonlinear eigenvalue problems; see Ruhe (1973); Mehrmann and Voss (2004). There is for instance the nonlinear Arnoldi method (Voss (2004)), some Newton-type methods (Schreiber (2008); Neumaier (1985)), a nonlinear version of Jacobi-Davidson (Betcke and Voss (2004)). In comparison to these methods, the presented method is expected to be more reliable since it inherits most properties of Arnoldi, e.g., simultaneous convergence to several eigenvalues and robustness.

The block Newton method was recently generalized to nonlinear eigenvalue problems (Kressner (2009)) and has been applied to the delay eigenvalue problem. The differences between block Newton and Arnoldi for standard eigenvalue problems seem to hold here as well. Arnoldi is often more efficient for very large systems since only the right-hand side and not the matrix of the linear system changes in each iteration. A LU-decomposition can be computed before the iteration starts and the linear system can be solved very efficiently. Moreover, in Arnoldi, it is not necessary to fix the number of vectors before the iteration starts.

There are other approaches for the DEP, e.g., the method QPMR (Vyhlídal and Zítek (2009)) which is based on the coefficients of characteristic equation and hence likely not very suitable for very large and sparse problems which is the context of the presented approach. See (Jarlebring, 2008, Chapter 2) for more methods.

Finally, we note that Arnoldi has been generalized in different contexts, e.g., to the quadratic eigenvalue problem in Bai and Su (2005); Meerbergen (2008).

2. ARNOLDI

Consider the space generated by the linear combination of a power sequence associated with matrix $A \in \mathbb{R}^{n\times n}$ and vector $b \in \mathbb{R}^n$,

$$\mathcal{K}_k(A, b) := \text{span}\{b, Ab, \ldots, A^{k-1}b\}.$$

This subspace is called a *Krylov subspace* and is fundamental for the understanding, analysis and presentation of the method called Arnoldi; first presented in Arnoldi (1951). Let $\{v_i\}_{i=1}^k$ be an orthogonal basis of $\mathcal{K}_k(A, b)$ and let the matrix V be the composition of vectors, $V = (v_1, \ldots, v_k)$. The eigenvalues of V^HAV are called *Ritz values*. They are the approximations to eigenvalues of A obtained from a Galerkin projection of $Ax = sx$ on the Krylov space.

Arnoldi is (in exact arithmetic) a method to construct an orthogonal basis of the Krylov subspace $\mathcal{K}_k(A, b)$. Roughly speaking, Arnoldi consists of expanding the matrix V containing the basis by the Av_k (or $A^{-1}v_k$) orthogonalized to V. The orthogonal component of Av_k is (in exact arithmetic) $x = (I-VV^H)Av_k$. The vector x is normalized and added to the vectors V. Note that in this fashion the projected matrix V^HAV is an upper Hessenberg matrix that consists of the Gram-Schmidt coefficients from the orthogonalization procedure. In some cases, it is preferred to explicitly compute V^HAV, which requires k matrix vector products and $k(k+1)^2/2$ vector innerproducts.

It is known from the theory of Krylov subspaces that the Ritz values first converge to the well-separated extreme eigenvalues of A. In our case, and many cases in the literature,the eigenvalues of interest are not the extreme well-separated eigenvalues. They often are close to a target point in the complex plane. Suppose the target is the origin. To this end, we consider the Krylov subspace associated with A^{-1}. Note that s^{-1} is an eigenvalue of A^{-1}. Let V be an orthogonal basis of $\mathcal{K}_k(A^{-1}, b)$, then the eigenvalues of $V^HA^{-1}V$ will first approximate the eigenvalues corresponding to the extreme well-separated eigenvalues of the inverted spectrum. These eigenvalues typically correspond to the eigenvalues of A close to the origin.

Also, note that the convergence and numerical stability of Arnoldi heavily depends on the the type of orthogonalization used. We will use iterative reorthogonalization as in ARPACK (Lehoucq et al. (1998)).

3. TDS ARNOLDI

If we approximate the exponential in (1) with a polynomial or rational function, the DEP turns into the problem of finding the characteristic roots of a matrix polynomial, often called a *polynomial eigenvalue problem* (PEP). PEPs are commonly solved by rewriting the problem into a generalized eigenvalue problem (GEP). If the GEP is solved with a general purpose eigenvalue solver, the approach is similar to the predictor step in a classical two-stage approach and has the drawback that the corresponding GEP may be very large and we introduce an approximation error.

In this section we will see that if we truncate the Taylor expansion, do a clever linearization and use a clever starting vector we do not have any approximation error.

We will make some assumptions in order to simplify the presentation. Without loss of generality (but possibly numerical stability) it is assumed that $\tau = 1$. With minor loss of generality we assume that $A + B$ is invertible. As usual with Arnoldi, we suppose we are looking for eigenvalues close to some target. Because the set of solutions can always be shifted, we can set the target equal to the origin without loosing generality.

Let $a_0 = 1, a_1 = -1, a_2 = 1/2, a_3 = -1/6\ldots$, be the Taylor coefficients for e^{-s}, i.e.,

$$e^{-s} \approx a_0 + a_1 s + \cdots + a_N s^N. \tag{3}$$

If we replace the exponential with the truncated Taylor series, the polynomial eigenvalue problem approximating the DEP (1) turns into

$$(A+a_0B+(a_1B-I)s+a_2Bs^2+a_3Bs^3+\cdots+a_NBs^N)x = 0.$$

The most common approach to solve PEPs is to rewrite the problem into a generalized eigenvalue problem. This

operation is called companion linearization and there are many ways to do such an operation (see e.g. Mackey et al. (2006)). Even though we have carried out experiments for several linearizations, we will only present the one where we observed the best numerical and theoretical properties. Consider the companion matrix $A_N \in \mathbb{C}^{Nn\times Nn}$, where

$$s^{-1}\begin{pmatrix} x \\ -\frac{1}{2}sx \\ \vdots \\ (-1)^N \frac{s^{N-1}}{N!}x \end{pmatrix} = A_N \begin{pmatrix} x \\ -\frac{1}{2}sx \\ \vdots \\ (-1)^N \frac{s^{N-1}}{N!}x \end{pmatrix}, \quad (4)$$

and

$$A_N = \begin{pmatrix} (A+B)^{-1}(I+B) & (A+B)^{-1}B & \cdots & (A+B)^{-1}B \\ -\frac{1}{2}I & & & \\ & \ddots & & \\ & & & -\frac{1}{N}I \end{pmatrix}. \quad (5)$$

In the subsections that follow we will need a special representation of the matrix vector product. We denote column i of matrix Y by y_i and the operation of stacking the columns of a matrix into a vector by $\text{vec}(Y) := (y_1^T, \ldots, y_N^T)^T$.

Lemma 1. Let A_N be the companion matrix (5). For any $Y \in \mathbb{C}^{n\times N}$,

$$A_N \text{vec}(Y) = \text{vec}(\hat{x}, YD_{N,N-1})$$

where

$$\hat{x} = (A+B)^{-1}\left(y_1 + B\sum_{i=1}^{N} y_i\right), \quad (6)$$

and

$$D_{N,N-1} = \begin{pmatrix} -\frac{1}{2} & & \\ & \ddots & \\ & & -\frac{1}{N} \\ 0 & 0 & 0 \end{pmatrix} \in \mathbb{R}^{N\times(N-1)}.$$

Proof. The general idea of the proof is to express A_N in terms of Kronecker products and apply vectorization rules. Note that,

$$A_N = \begin{pmatrix} e_1^T \otimes (A+B)^{-1} + e^T \otimes (A+B)^{-1}B \\ D_{N,N-1}^T \otimes I \end{pmatrix},$$

where $e^T = (1, \ldots, 1)$ and e_1 is the first unit vector. Moreover,

$$A_N \text{vec}(Y) = \begin{pmatrix} \left(e_1^T \otimes (A+B)^{-1} + e^T \otimes (A+B)^{-1}B\right)\text{vec}(Y) \\ (D_{N,N-1}^T \otimes I)\text{vec}(Y) \end{pmatrix} \quad (7)$$

The rest of the proof consists of applying the vectorization rule $(C^T \otimes A)\text{vec}(Y) = \text{vec}(AYC)$. The first block row in (7) reduces to,

$$\text{vec}\left((A+B)^{-1}Ye_1 + (A+B)^{-1}BYe\right) = (A+B)^{-1}y_1 + (A+B)^{-1}B\sum_{i=1}^{N} y_i = \hat{x},$$

proving (6). Similarly, by again applying the vectorization rule, we find that the second block row in (7) is $\text{vec}(YD_{N,N-1})$. The proof is complete.

Remark 2. (Generalizations). Lemma 1 is somewhat fundamental for this paper. In fact, it is not difficult to show a generalization of Lemma 1 for systems with multiple delays. The rest of the results of the paper, including the proposed methods can also be generalized. If we have multiple delays, the top right block-element of A_N is not constant with respect to N. We observed numerical stability problems when the top right block-element of A_N is unbounded with respect to N, and will in this work only focus on single delays.

The similar reasoning for neutral systems and systems with distributed delays is also left for topics of future research.

3.1 Version 1: Hessenberg version

Ideally, we would like N to be very large since that implies that the approximation error introduced by the truncation of the Taylor series (3) is small. It is already mentioned that this causes computational difficulties in a classical approach since A_N becomes large. We will now present an approach which resolves this in a perfect sense. If we start the Arnoldi process with a special type of vector, Arnoldi applied to A_N can be carried out efficiently in a way which is independent of N, i.e., in a way such that there is no truncation error.

Suppose we start the iteration with a structured vector $x_0 = \text{vec}(y, 0, \ldots, 0) \in \mathbb{R}^{nN}$ and $y \in \mathbb{R}^n$. From Lemma 1, we see that the operation A_N shifts and scales the vector y and a new vector $\hat{x}$ is added to the left of the vectorized matrix. The operation can be formalized and generalized in the following sense.

Theorem 3. Let A_N be the companion matrix (5). Suppose

$$Y = (\hat{Y}, 0, \ldots, 0) \in \mathbb{C}^{n\times N}$$

and $\hat{Y} \in \mathbb{C}^{n\times k}$, $k < N$. Then,

$$A_N \text{vec}(Y) = \text{vec}(\hat{x}, \hat{Y}D_{k,k}, 0, \ldots, 0),$$

where

$$\hat{x} = (A+B)^{-1}\left(y_1 + B\sum_{i=1}^{k} y_i\right),$$

and

$$D_{k,k} = \begin{pmatrix} -\frac{1}{2} & & \\ & \ddots & \\ & & -\frac{1}{k+1} \end{pmatrix} \in \mathbb{R}^{k\times k}.$$

It is important to note that the number of floating point operations to compute $A_N\text{vec}(Y, 0, \ldots, 0)$ is independent of the number of zero elements. Hence, roughly speaking we have an infinite number of zeros and no approximation error.

Note 1. (Orthogonalization). Let $Y_1, \ldots, Y_N$ be the matrix version of the vectors after N Arnoldi iterations. Note that the tailing zeros of the new vector $A_N \text{vec}(Y_N)$ are preserved even if we orthogonalize it against $Y_1, \ldots, Y_N$.

We have shown that the representation $Y = (\hat{Y}, 0, \ldots, 0)$ is almost closed under A_N since the structure of the vector is only changed by expanding the number of first non-zero block. It is also closed under orthogonalization. Since these are the only operations necessary for Arnoldi, we conclude that the representation is suitable.

Note 2. (Comparison with standard Arnoldi). In principle one could apply the standard Arnoldi directly to the companion matrix (5). This would be mathematically equivalent to our approach. The presented representation has several advantages.

- One matrix vector product of TDS Arnoldi is more efficient than for standard Arnoldi since the non-zero elements of (5) are not explicitly stored.
- The orthogonalization is more efficient for the TDS Arnoldi since in the beginning, the vectors are smaller than for the standard Arnoldi.
- In the standard Arnoldi we would have to choose N before we start the iteration. In our presented approach N does not have to be chosen a priori. One can inspect the eigenvalues during the iteration and stop once sufficient accuracy is observed.

3.2 Version 2: Projection version

In the previous subsection we considered vectors of the form $x = \text{vec}(Y, 0, \ldots, 0)$. We see from (4) that the eigenvector is not of this form. Since the method is expected to converge to an eigenvector of that form, a form where such an eigenvector can be accurately and compactly represented seems advantegous. Hence, we will now consider the case that $x = \text{vec}(uv^*)$ where v is possibly very long vector. This representation allows a compact but accurate representation of an eigenvector.

In the following we use subscript to denote an element of a vector, e.g., $v_i \in \mathbb{C}$ is the ith element of $v \in \mathbb{C}^n$.

Theorem 4. (Rank one). Let A_N be the companion matrix (5) and $u \in \mathbb{C}^n$, $v \in \mathbb{C}^N$. Then,

$$A_N \text{vec}(uv^*) = \text{vec}((\hat{x}, 0, \ldots, 0) + u\hat{v}^*)$$

where $\hat{v}^* = (0, v^* D_{N,N-1})$ and

$$\hat{x} = (A + B)^{-1}(uv_1^* + Bu(\sum_{i=1}^{N} v_i^*)).$$

Note 3. (Rank one is not almost closed). We saw in the previous section that the set of vectors of the form $\text{vec}(\hat{Y}, 0, \ldots, 0)$ were almost closed under operation of A_N. The rank-one vectors are not closed in the same sense since the result of the application of A_N to a rank-one vectors is a different vector of rank one plus a term $(\hat{x}, 0, \ldots, 0)$. However, $(\hat{x}, 0, \ldots, 0)$ is of the form $Y = (\hat{Y}, 0, \ldots, 0)$. We can combine the results Theorem 3, Theorem 4 to again find a set which contains rank one matrices and is almost closed as in Theorem 3.

Corollary 5. (Combined). Let A_N be the companion matrix (5) and $u \in \mathbb{C}^n$, $v \in \mathbb{C}^N$ as in Theorem 3 and $Y \in \mathbb{C}^{n \times N}$, $\hat{Y} \in \mathbb{C}^{n \times k}$ as in Theorem 4. Then

$$A_N \text{vec}(Y + uv^*) = \text{vec}(\tilde{Y} + u\hat{v}^*),$$

where $\hat{v}^* = (0, v^* D_N)$,

$$\hat{x} = (A + B)^{-1}\left(uv_1^* + Bu(\sum_{i=1}^{N} v_i^*) + y_1 + B\sum_{i=1}^{k} y_i\right),$$

and

$$\tilde{Y} = (\hat{x}, \hat{Y} D_{k,k}, 0, \ldots, 0).$$

Note 4. (Number of flops). It is important to note that Corollary 5 describes a method to compute the result of A_N applied to a vector $\text{vec}(Y + uv^*)$ efficiently. In rough terms the computational effort is as follows. The dominating part is the computation of $\hat{x}$. In order to compute $\hat{x}$ we need to solve one linear system (which remains the same througout the iteration) of dimension n, sum N scalars and sum k vectors of dimension n. Since the vector operations and not the sum of scalars is the dominating part for large n, we can choose N very large without any considerable extra computational effort.

Note 5. (Orthogonalization and projection). The standard orthogonalization procedure does not seem suitable for the rank one structure, since it would involve orthogonalizing vectors of size nN. Note that in exact arithmetic, Arnoldi is independent of the type of orthogonalization. We can hence use a different orthogonalization without and still have a method mathematically equivalent to Arnoldi. For the rank-one structure we propose an orthogonalization scheme, where we only orthogonilize the first n elements of the vectors in each vector. This approach has been taken in several other works, e.g., Bai and Su (2005).

For this type of orthogonalization it is also more suitable to project the nonlinear problem instead of the large Taylor approximation. Let $V \in \mathbb{R}^{n \times k}$ be the first n parts of the result of Arnoldi, i.e., $V^*V = I$. The projected nonlinear problem is now

$$(-sI + V^*AV + V^*BVe^{-\tau s})w = 0. \tag{8}$$

At this point we are no longer mathematically equivalent to Arnoldi. However, V will typically contain very accurate approximation of the eigenvectors. This implies that the projected problem also contains a very accurate solution. One of the solutions of the projected problem is hence very similar to Arnoldi in exact arithmetic.

Also note that (8) is a small delay eigenvalue problem solvable with any method for small delay eigenvalue problems. We solve the small projected problem with a spectral discretization of the infinitesimal generator Breda et al. (2006).

3.3 Remarks about infinite dimensionality

In a sense it is not extremely surprising that we can apply Arnoldi without approximation error, since a DDE can be represented as a linear infinite dimensional system (see, e.g. Curtain and Zwart (1995); Hale and Verduyn Lunel (1993)) and Arnoldi can be applied to infinite dimensional systems (see, e.g., Chatelin (1983)).

It is however a bit surprising that the infinite-dimensional vectors can be represented in such a way that the action of the infinite dimensional operator can be computed with standard (finite-dimensional) linear algebra operations.

4. NUMERICAL EXAMPLES

4.1 Example: Arnoldi version 1

We use the example in Verheyden et al. (2008), where

$$A = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -10 & -4 \\ 0 & 0 & 4 & -10 \end{pmatrix}, \; B = \begin{pmatrix} 3 & 3 & 3 & 3 \\ 0 & -1.5 & 0 & 0 \\ 0 & 0 & 3 & -5 \\ 0 & 5 & 5 & 5 \end{pmatrix}.$$

The convergence history of the Ritz values are shown in Figure 2. After 100 iterations we find 21 eigenvalues to an accuracy 10^{-10} (shown in Figure 1). Note that the higher eigenvalues are large in magnitude and badly conditioned, which is likely the reason why not full accuracy is achieved.

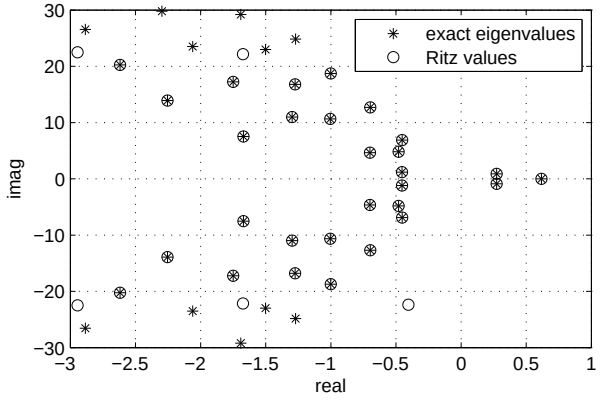

Fig. 1. Ritz values of Example 1

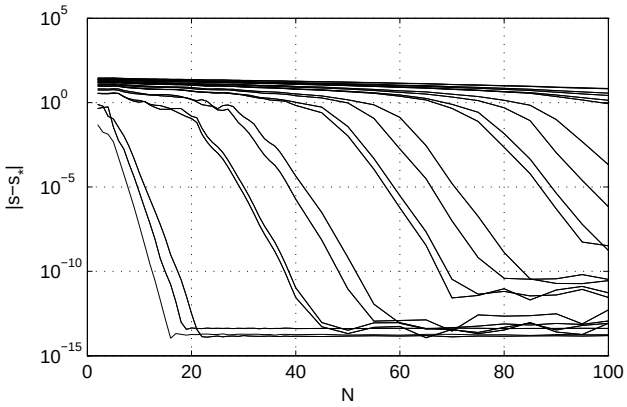

Fig. 2. Convergence for Example 1

4.2 Example: Arnoldi version 2

The second example is a large scale problem inspired by the discretization of a boundary controlled heat equation in Berrone and Mannucci (2004).

The discretized problem is

$$\dot{x}(t) = Ax(t) + Bx(t-\tau),$$

where $A \in \mathbb{R}^{n\times n}$ is the discretized two-dimensional Laplacian with zero boundary conditions and B is a matrix of rank $\sqrt{n}-2$ corresponding to a feedback on one edge.

We illustrate the usefulness of the possibility to start with a vector corresponding to a large rank one matrix. This is done by starting the iteration with a quite accurate approximation.

We see the error history in Figure 3 for $n = 3600$. The computation time for $N = 40$ is 18 seconds on a Intel 2.66 GHz computer with 3 Gb of memory. Note that DDE-BIFTOOL is not suitable for problems of this size. It returns out of memory error due to the very large companion matrices which have to be explicitly constructed.

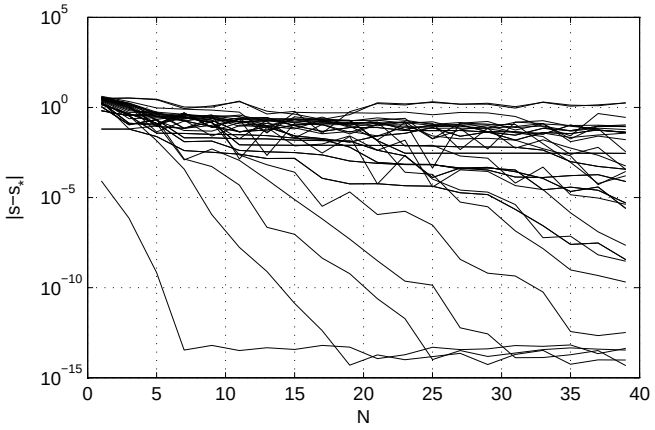

Fig. 3. Convergence for Example 2

5. CONCLUSIONS AND OUTLOOK

The result of this paper is a construction of an Arnoldi method for the delay eigenvalue problem. We have considered structured sets of starting vectors. It turns out that for these structured vectors, the matrix vector product corresponding to the companion linearization Taylor approximation of the delay eigenvalue problem can be computed efficiently and (more importanly) without any truncation error.

The presented method is mathematically equivalent to Arnoldi and we have shown by examples that these properties makes the method very competitive in comparison to current state of the art methods. It is competitive in terms of computation time and reliability.

Finally, we wish to point out some issues not addressed in this paper. The computational effort of the presented Arnoldi method grows with the number of iterations. For standard Arnoldi this is resolved by (so called) implicit or explicit restarting and deflation. In this paper we assumed that the shift is zero. This is not really a restriction if the shift remains constant. However, in standard Arnoldi the shift is sometimes updated to gain convergence speed. We also note that for standard eigenvalue problem, if the shift is updated in each step of Arnoldi there is a strong connection with block Newton methods which have been developed (in Kressner (2009)) for the delay eigenvalue problem. This interesting relation is not addressed here. Even though some of these techniques and results about restart, deflation, shift updates, stopping criteria and relations with block Newton seem to carry over naturally to TDS Arnoldi, we leave these topic as possible future research.

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