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PRECONDITIONED ITERATIVE METHODS FOR INDEFINITE SYMMETRIC TOEPLITZ SYSTEMS

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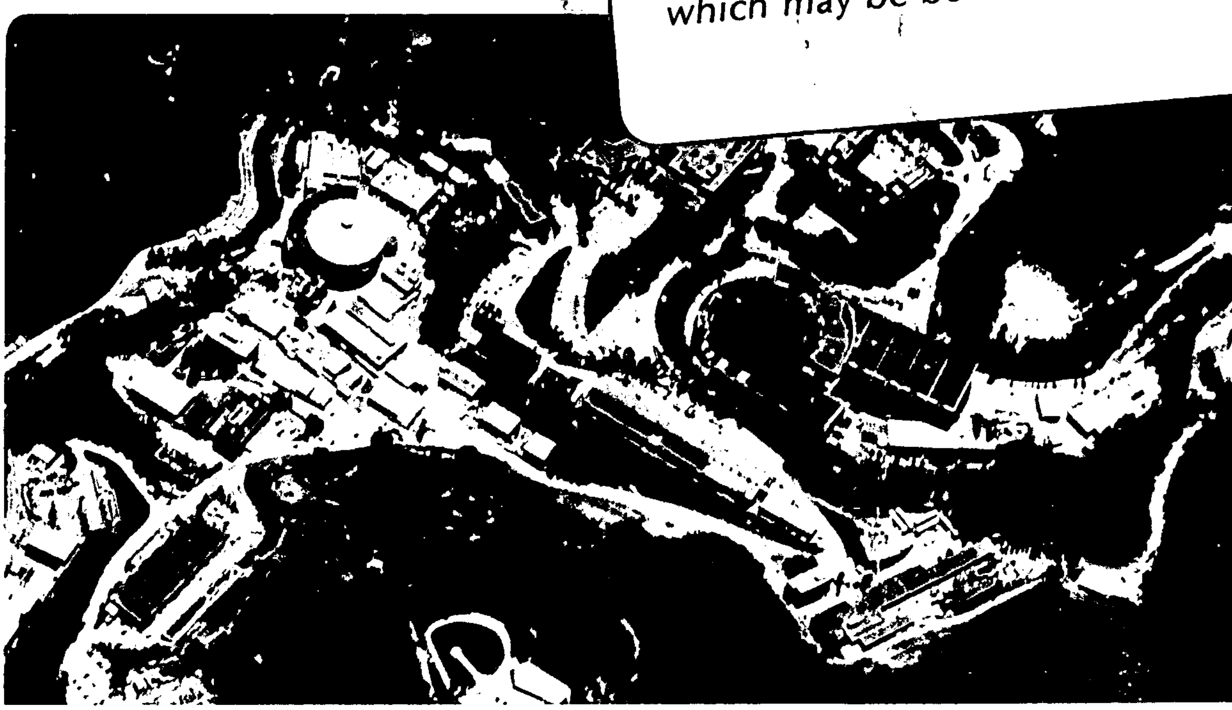

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PRECONDITIONED ITERATIVE METHODS FOR INDEFINITE SYMMETRIC TOEPLITZ SYSTEMS *

Paul Concus† and Paul Saylor‡

Dedicated to David M. Young on the occasion of his 65th birthday

Abstract

Stable fast direct methods for solving symmetric positive-definite Toeplitz systems of linear equations have been known for a number of years. Recently, a conjugate-gradient method with circulant preconditioning has been proposed as an effective means for solving these equations. For the (non-singular) indefinite case, the only stable algorithms that appear to be known are the general $O(n^3)$ direct methods, such as LU decomposition, which do not exploit the Toeplitz structure. We depict here some initial numerical results on the feasibility of circulant preconditioned iterative methods for the indefinite symmetric case.

1. Introduction

The use of iterative methods for the solution of linear systems of equations $Ax = b$ for which A is a Toeplitz matrix has been stimulated by the recent work of G. Strang [14]. It was proposed in [14] that for the symmetric positive definite case the use of a circulant matrix as preconditioner could be particularly effective for the conjugant gradient method. Since circulant systems can be solved rapidly with the Fast Fourier Transform (FFT) and since for a significant class of matrices the spectrum of the preconditioned matrix turns out to have strong clustering with only a few isolated extremal eigenvalues, the conjugate gradient iteration can converge with striking efficiency. Subsequent related work can be found in [7], [8], [9], [10], [15].

We report here on our initial findings for extending the use of circulant preconditioners to the case in which A is a symmetric Toeplitz matrix that is indefinite

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(both some positive and some negative eigenvalues). For this case the need for efficient iterative methods is more pressing than for the positive definite case, because the specialized rapid direct methods for Toeplitz matrices can be unstable when the matrix is indefinite.

2. Toeplitz and Circulant Matrices

Let A denote a real symmetric $n \times n$ Toeplitz matrix. A Toeplitz matrix is constant along its diagonals and thus, in the symmetric case, is determined by the n elements of the first row, $a_0, a_1, \ldots, a_{n-1}$,

$$A = \begin{bmatrix} a_0 & a_1 & \cdots & a_{n-2} & a_{n-1} \\ a_1 & a_0 & a_1 & \cdots & a_{n-2} \\ a_2 & a_1 & a_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & a_1 \\ a_{n-1} & \cdots & a_2 & a_1 & a_0 \end{bmatrix}. \tag{1}$$

Such matrices arise in applications such as time series analysis, Padé approximation, and differential and integral equations.

A circulant matrix, which is a special case of a Toeplitz matrix, is determined by only the first $\frac{n}{2}+1$ elements of the first row if n is even. Each successive row contains the elements of the row above shifted one to the right, with the last element wrapped around to become the first, i.e.,

$$\begin{bmatrix} c_0 & c_1 & \cdots & c_2 & c_1 \\ c_1 & c_0 & c_1 & \cdots & c_2 \\ c_2 & c_1 & c_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & c_1 \\ c_1 & \cdots & c_2 & c_1 & c_0 \end{bmatrix}.$$

Since the eigenvectors of a circulant matrix are given by successive powers of the n^{th} roots of unity, systems with circulant coefficient matrix are amenable to solution by the FFT in $O(n \log n)$ operations.

To obtain a preconditioner S for symmetric positive definite A, Strang proposed keeping the central diagonals of A and replacing the outer diagonals by reflected values from the central ones to complete the circulant. For the matrix A in (1) the circulant preconditioner S is

$$S = \begin{bmatrix} a_0 & a_1 & \dots & a_2 & a_1 \\ a_1 & a_0 & a_1 & \dots & a_2 \\ a_2 & a_1 & a_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & a_1 \\ a_1 & \dots & a_2 & a_1 & a_0 \end{bmatrix}. \tag{2}$$

For n even, element a_{n-j} is replaced with a_j for $j = 1, 2, \dots, \frac{n}{2} - 1$. No arithmetic computation of new elements is required.

The preconditioner S was shown to be extremely effective for use with the conjugate gradient method. Because the FFT can be used to form the matrix-vector products with A in $O(n \log n)$ operations as well as to solve the preconditioning circulant systems in $O(n \log n)$ operations, each conjugate gradient step is very efficient. A remarkable feature is that the eigenvalues of $S^{-1}A$ cluster exceptionally favorably. Suppose that the elements $a_0, a_1, \dots, a_{n-1}$ are part of a sequence $\{a_k\}_{k=0}^{\infty}$, which defines a limiting symmetric positive definite Toeplitz matrix of infinite order. It was proved in [9] by R. Chan & G. Strang that for $n \to \infty$, if the underlying (real-valued) generating function $f(\theta) = \sum_{-\infty}^{\infty} a_{|k|} e^{ik\theta}$ is positive and in the Wiener class $\sum_{-\infty}^{\infty} |a_k| < \infty$, then the $n \times n$ matrices S and S^{-1} are uniformly bounded and positive definite for all sufficiently large n, and the eigenvalues of $S^{-1}A$ cluster at unity. An interesting relationship between this clustering and approximation on the unit circle is discussed in [16].

3. Solution Methods

As part of a general study on iterative methods for solving symmetric indefinite systems of linear equations, we describe here our initial investigations for Toeplitz coefficient matrices. We are interested in methods that work on the original system of equations and avoid transforming to the associated positive-definite normal-equation system.

Numerical methods for solving symmetric Toeplitz systems of equations can be categorized as follows.

A. *General direct methods.* General direct methods such as LU and QR decomposition require $O(n^3)$ operations and can be used for the positive-definite case or, with pivoting, for the indefinite case. They do not take specific advantage of the Toeplitz structure.

B. *Specialized direct methods.* For the positive definite case specialized direct methods have been devised that take advantage of the matrix structure to solve a system in fewer operations than required for general direct methods. The stability of these methods has been studied by Bunch in [6]. Both the "classical" $O(n^2)$ specialized methods of Levinson [11] and Trench [17] and the more recent "fast" $O(n \log^2 n)$ specialized methods (e.g., [1], [4], [5]) are generally unstable if the matrix is not positive definite.

C. *Iterative methods.* For the positive definite case the circulant preconditioned conjugate gradient method proposed by Strang requiring $O(n \log n)$ operations per iteration can be very effective. For the indefinite case, which is the area of our study, iterative methods can be of comparatively greater interest because of instability of the specialized direct methods. Three iterative-method possibilities for consideration are (a) the conjugate residual method on the original system of equations; (b) circulant preconditioning with acceleration, such as adaptive Chebyshev [12] or a conjugate gradient type method [3]; and (c) stabilization of the specialized direct methods with iterative techniques.

We are concerned here with the iterative method possibility (b) of circulant preconditioning for symmetric indefinite Toeplitz matrices and report on some preliminary numerical experiments.

4. Test Matrix Preconditioners

The circulant preconditioners we investigate for our test matrices are the Strang preconditioner S in (2) and the circulant matrix that best approximates A in the Frobenius norm, which was suggested by T. Chan [10].

The optimal Frobenius norm circulant preconditioner is obtained from A by replacing both a_i and a_{n+1-i} by a weighted average. Let C denote the preconditioner. Then there holds

$$C = \begin{bmatrix} a_0 & \bar{a}_1 & \dots & \bar{a}_2 & \bar{a}_1 \\ \bar{a}_1 & a_0 & \bar{a}_1 & \dots & \bar{a}_2 \\ \bar{a}_2 & \bar{a}_1 & a_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \bar{a}_1 \\ \bar{a}_1 & \dots & \bar{a}_2 & \bar{a}_1 & a_0 \end{bmatrix}, \tag{3}$$

where $\bar{a}_i = \frac{n-i}{n}a_i + \frac{i}{n}a_{n-i}$, $i = 1, 2, \dots, \frac{n}{2}$ (for n even). The pairing of the off-diagonal elements of A has the same pattern for C as for S. For S the lower-index element simply replaces the larger, whereas for C a weighted average of the two replaces both.

Recently, R. Chan has proved that the preconditioner C, and others having the same pairing/replacement pattern, enjoy the same asymptotic clustering properties as does S for the same class of matrices—symmetric positive definite Toeplitz matrices with positive generating function in the Wiener class [7]. He showed also that the S preconditioning is the best circulant approximation to A in the 1 and ∞ norms [8]. For non-square matrices, other circulant preconditionings based on Cybenko's QR factorization are considered by Olkin in [13].

Although the asymptotic spectra are the same for the C and S preconditionings, for finite n there are differences that can have practical effects on the relative convergence rates for the preconditioned conjugate gradient method. The S preconditioning appears to cluster eigenvalues more sharply than does the C preconditioning, particularly when a_k decreases rapidly away from the main diagonal, although the C preconditioning appears to result in smaller condition number [10]. The sharper clustering for S results in enhanced convergence for the preconditioned conjugate gradient method for some problems.

5. Test Matrices

The test matrices considered here for the symmetric indefinite case are taken from the positive definite examples used by T. Chan and by Strang, which are then shifted by constant diagonal matrices to make some of the eigenvalues negative. The matrices before shifting are the following.

(i) $a_k = 1/(k+1)$, $k = 0, 1, \ldots, n$. Since the decay away from the diagonal is only arithmetic, the limiting underlying generating function does not belong to the Wiener class and hence would not satisfy the hypotheses for the asymptotic clustering and other results of [7], [9].

(ii) $a_k = \left(\frac{1}{2}\right)^k$, $k = 0, 1, \ldots, n$. This is a matrix studied by Kac, Murdock, and Szegö. Decay away from the diagonal is geometric, and the hypotheses of [7], [9] on the limiting underlying generating function are satisfied. In fact, the S preconditioner is unusually effective for this matrix, which is the inverse of a tridiagonal matrix (not Toeplitz). As pointed out in [15], the preconditioned matrix $S^{-1}A$ has only five distinct eigenvalues (for n even). These are $\frac{1}{1+\frac{1}{2}}$, $\frac{1}{1+(\frac{1}{2})^{n/2}}$, 1, $\frac{1}{1-(\frac{1}{2})^{n/2}}$, $\frac{1}{1-\frac{1}{2}}$. The smallest and largest eigenvalues are simple and independent of n. The eigenvalue 1 is double, and the other two are repeated $\left(\frac{n}{2}-2\right)$ times each. Thus the clustering toward 1 is exponential. These striking properties, well suited for the conjugate gradient method, appear to have encouraged much of the work in [9], [14], and [15].

(iii) $a_k = \frac{\cos k}{k+1}$, $k = 0, 1, \ldots, n$. This is a variation of case (1). The $\cos k$ factor introduces some negative elements in the matrix and alters the smooth arithmetic decay away from the diagonal. As for (1), its limiting underlying generating function does not belong to the Wiener class.

(iv) $a_0 = 2 + \frac{1}{n^2}$, $a_1 = -1$, $a_2 = a_3 = \cdots = a_{n-1} = 0$. This tridiagonal matrix is a discretization of the one-dimensional Helmholtz operator $-u_{xx} + u$ with Dirichlet boundary conditions on a uniform mesh on $[0, 1]$. The limiting matrix A satisfies the hypotheses of [7], [9] so that the results there apply. The preconditioner

S in this case replaces a_{n-1} with -1 and leaves the other a_i, $i = 0, \ldots, n-2$ unchanged. It corresponds to the Helmholtz operator with periodic, instead of Dirichlet, boundary conditions. Since S and A differ only by a rank-two matrix, $S^{-1}A$ has an $(n-2)$-fold eigenvalue of 1. The C preconditioner for this case replaces a_1 and a_{n-1} by their weighted average $\frac{n-1}{n}a_1$, and there holds

$$C = \frac{n-1}{n} S + \frac{1}{n} I.$$

In general, C and A differ by a matrix of full rank.

Note that the discrete Laplace operator $-u_{xx}$, which would result simply in 2 on the diagonal instead of $2 + \frac{1}{n^2}$ as in (iv), would not provide a suitable test matrix, as the S preconditioner, which would correspond to a Laplace operator with periodic boundary conditions, is singular [9]. The generating function of the matrix, in this case, does not satisfy the positivity condition.

For the numerical experiments the above matrices are shifted by a constant diagonal matrix $-\alpha I$, with values of α such that $A - \alpha I$ is indefinite, but nonsingular. As only the diagonal elements of A are changed by the shift, the preconditioners for $A - \alpha I$ are $S - \alpha I$ and $C - \alpha I$, where S and C are the preconditioners for A. Note that if an unshifted preconditioned matrix has an eigenvalue 1 corresponding to eigenvector ϕ, e.g.,

$$A\phi = S\phi,$$

then

$$(A - \alpha I)\phi = (S - \alpha I)\phi,$$

so that the shifted preconditioned matrix also has eigenvalue 1 with eigenvector ϕ. The shifting preserves eigenvalues unity of the preconditioned matrix. There holds, more generally, that shifting preserves eigenvalues of the difference between A and the preconditioner, e.g., if μ and ψ are an eigenvalue-eigenvector pair such that $(A - S)\psi = \mu\psi$, then $[(A - \alpha I) - (S - \alpha I)]\psi = \mu\psi$. This implies that shifting preserves any clustering of the spectrum of $A - S$, for example as in Theorem 2 of [8] (dependence of A and S on the order n is denoted explicitly here): *Let f be a positive function* *in the Wiener class, then for all $\epsilon > 0$, there exist M and $N > 0$ such that for all $n > N$, at most M eigenvalues of $A(n) - S(n)$ have absolute values exceeding ϵ.* If also $(S - \alpha I)$ and $(S - \alpha I)^{-1}$ are uniformly bounded for all $n > N$, then the shifting would preserve the result of [8], [9] that the eigenvalues of $S^{-1}A$ cluster at unity.

6. Computed Spectra

The spectra for $n = 16$, as computed using a public-domain version of MATLAB, are given in Figs. 1–5. For Figs. 1–4 the value $\alpha = \frac{\nu_5(A)+\nu_6(A)}{2}$ is chosen, where $\nu_i(A)$ denotes the i^{th} eigenvalue of A, $0 < \nu_1 \leq \nu_2 \leq \cdots \leq \nu_n$. For Fig. 5, $\alpha = \frac{\nu_4(A)+\nu_5(A)}{2}$ is chosen. For all the test problems, A has distinct eigenvalues, so that $\nu_4 \neq \nu_5 \neq \nu_6$ and $A - \alpha I$ is nonsingular. For these problems $S - \alpha I$ and $C - \alpha I$ are nonsingular also. Our interest is to observe whether the shifted preconditioners yield clustering of the eigenvalues, and to compare the clustering properties. For the standard adaptive Chebyshev method [12], the eigenvalues of the preconditioned matrix must lie in a half-plane. If they do not, then an adaptive Chebyshev method using two disjoint regions—one in each half-plane—to enclose the eigenvalues might be employed, but such techniques are not as highly developed. If the eigenvalues do not lie in a half-plane, then a conjugate-gradient-like acceleration might be employed, but these methods are not robust. They also are not robust if the symmetric part is indefinite, even if the eigenvalues are in a half plane; thus this property is of interest also.

In each figure, the top three rows depict the eigenvalues of A and of the preconditioned matrices $S^{-1}A$ and $C^{-1}A$, with plotting symbols of plusses, circles, and triangles, respectively. The fourth row depicts the spectrum of the shifted matrix $A - \alpha I$. Plotted below are the imaginary vs. real part of the eigenvalues λ of $(S-\alpha I)^{-1}(A-\alpha I)$ and $(C - \alpha I)^{-1}(A - \alpha I)$, using the same plotting symbols as for the unshifted preconditioned matrices.

In Figs. 1–3, the spectra of the unshifted matrices are consistent with those given in [10] for the case $n = 15$. (We have chosen n to be even so that the property for case (ii) of only 5 distinct eigenvalues holds.) As observed in [10], for these cases the C preconditioning results in a spectrum that lies strictly within that for the S preconditioning. However, for examples such as (ii) (Fig. 2), the eigenvalue clustering is smeared out. For example (iv) (Fig. 4) the spectrum for the C preconditioning does not lie strictly within that for the S preconditioning, but the condition number for C is still smaller. For this case the C preconditioning smears out the clustering considerably. For the shifted matrices, behavior of the two preconditionings can differ more appreciably.

In Fig. 1 (the arithmetic decay case), one sees that for the shifted matrices the S preconditioning spectrum lies within that for the C preconditioning, in contrast to the case for the unshifted matrices. The imaginary parts for the S preconditioning are much smaller than for the C preconditioning, and the real parts are all positive. The complex conjugate pair of eigenvalues for the C preconditioning to the left of the imaginary axis would pose difficulties for, say, adaptive Chebyshev acceleration that would not be present for the S preconditioning.

In Fig. 2 (the geometric decay case), the strong clustering at 1 for the S preconditioning for the unshifted matrix can be seen. Even though the order of the matrix is only 16, the separation between the double eigenvalue at 1 and the seven-fold ones at $\left(1+\left(\frac{1}{2}\right)^8\right)^{-1}$ and $\left(1-\left(\frac{1}{2}\right)^8\right)^{-1}$ can be distinguished as only a slight thickening of the circle designating the eigenvalue at 1. For the shifted matrices, both the C and S preconditionings yield eigenvalues entirely in the right half plane. The S preconditioning yields much stronger clustering. Some eigenvalues have departed only slightly from the real axis, whereas for the C preconditioning significant imaginary parts have appeared. Again, the C preconditioning would appear less favorable for acceleration than the S preconditioning.

In Fig. 3 (the altered arithmetic decay case) the S preconditioning does not cluster the eigenvalues as well as the C preconditioning does for the unshifted matrices. For the shifted matrices the real parts of the C preconditioning eigenvalues are interior to the interval of the real parts of the S preconditioning eigenvalues, but the imaginary parts are larger. An adaptive acceleration method that estimates an ellipse enclosing the eigenvalues might deal with the S preconditioning matrix more easily, although with other shifts for this problem we observed that neither preconditioning suggested itself as being substantially better than the other.

In Fig. 4 (the Helmholtz equation case) the special spectral properties for the S preconditioning can be observed. For both the shifted and unshifted case this preconditioning differs from the original matrix by only the rank two matrix whose elements are equal to -1 in the $(1, n)$ and $(n, 1)$ positions and zero elsewhere. Thus, the preconditioned matrix has an $(n-2)$-fold eigenvalue of unity. For this case the C preconditioned spectrum for the unshifted matrix does not lie interior to the S preconditioned spectrum, as for the other cases, but overlaps it. (But it does have smaller condition number.) For the shifted matrices, the C preconditioned matrix has a complex-conjugate pair.

Fig. 5 illustrates the different behavior for the Helmholtz-equation test matrix if four rather than five eigenvalues of A are shifted to be negative. In the experiments for this matrix, we observed that there was some correlation between the behavior of the spectrum and whether an odd or an even number of eigenvalues of A had been shifted to be negative. Fig. 5 is representative of even shift cases (except for a shift of $\alpha = \frac{\nu_8(A)+\nu_9(A)}{2}$, for which matrices become singular). The eigenvalues of the preconditioned shifted matrix are not all in the right-half plane, as for the odd-shift case of Fig. 4, and for the S preconditioning they are all real. The property that the interior eigenvalues of the circulant preconditioners are double (the two extremal ones are simple) may have some bearing on the odd vs. even shift behavior that was observed.

For the examples, circulant preconditioning appears to be of benefit for conditioning the spectra of the shifted matrices. The S preconditioning seems to be of greater benefit than the C preconditioning in yielding compact spectra, particularly for the examples satisfying the conditions of [7], [9] that the limiting underlying generating function be positive and in the Wiener class. For the conjugate gradient type accelerations that rely on the symmetric part of the preconditioned matrix being positive definite, we note that this was generally not the case in the experiments—symmetric parts were indefinite. This suggests that an adaptive Chebyshev acceleration would be preferable, particularly when the spectrum of the preconditioned matrix lies in a half plane, which is satisfied often but not always in the experiments; the standard adaptive algorithm packages [2] could then be used. If the preconditioned spectrum does not lie in a half plane, then the preconditioning might be effective in conjunction with Chebyshev acceleration employing two disjoint spectra-enclosing regions or with the conjugate gradient method applied to the normal equations of the preconditioned system.

As a final note, we remark that the unshifted preconditioners, which are positive definite, were generally not nearly as effective in conditioning the spectra of the shifted matrices as were the shifted preconditioners. We believe that the numerical results are sufficiently encouraging to warrant further consideration of circulant preconditioning for the iterative solution of symmetric indefinite Toeplitz systems of linear equations.

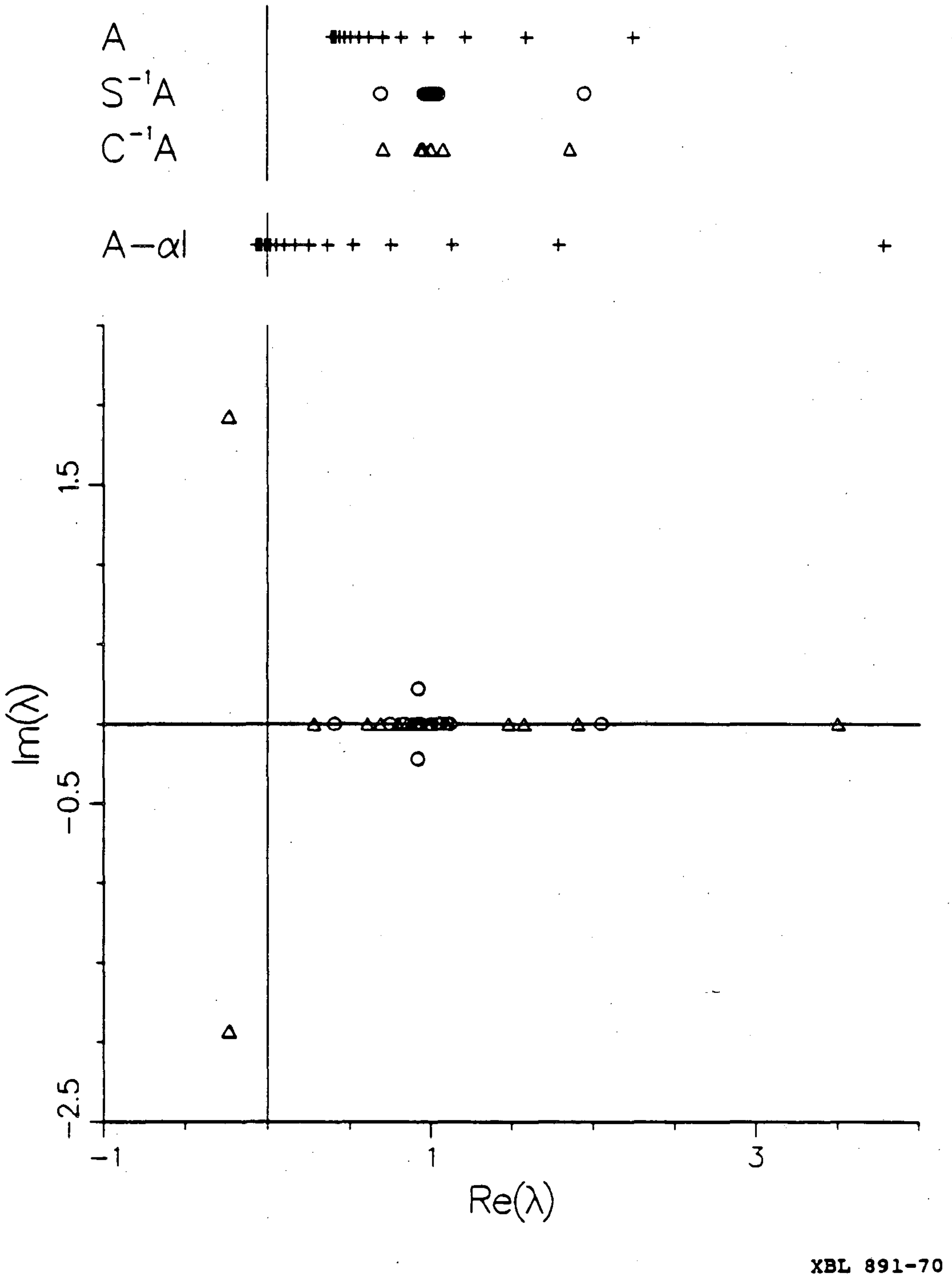

Fig. 1. Spectra for $a_k = \frac{1}{k+1}$ and $\alpha = \frac{1}{2}(\nu_5(A) + \nu_6(A))$.

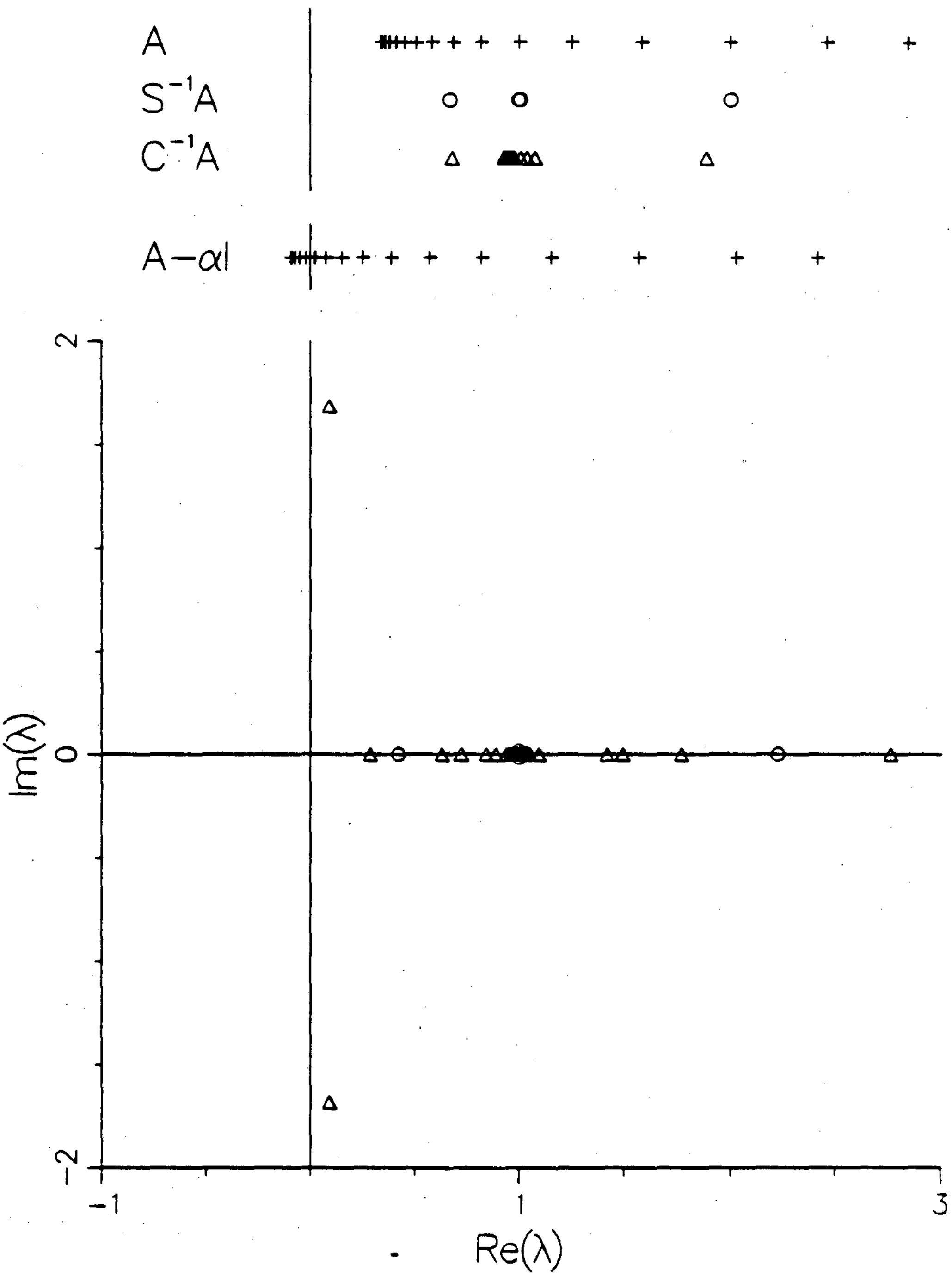

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Fig. 2. Spectra for $a_k = \left(\frac{1}{2}\right)^k$ and $\alpha = \frac{1}{2}(\nu_5(A) + \nu_6(A))$.

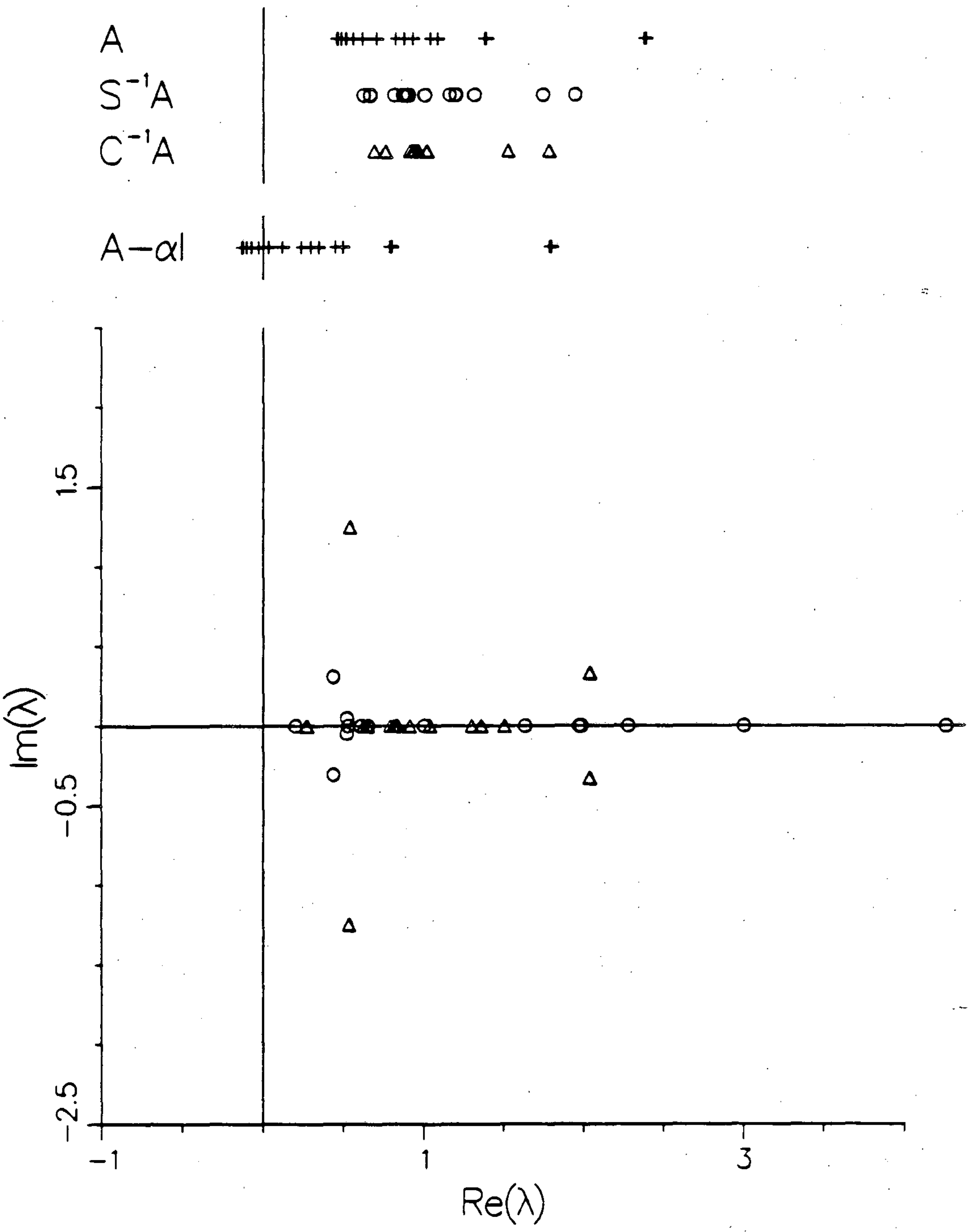

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Fig. 3. Spectra for $a_k = \frac{\cos k}{k+1}$ and $\alpha = \frac{1}{2}(\nu_5(A) + \nu_6(A))$.

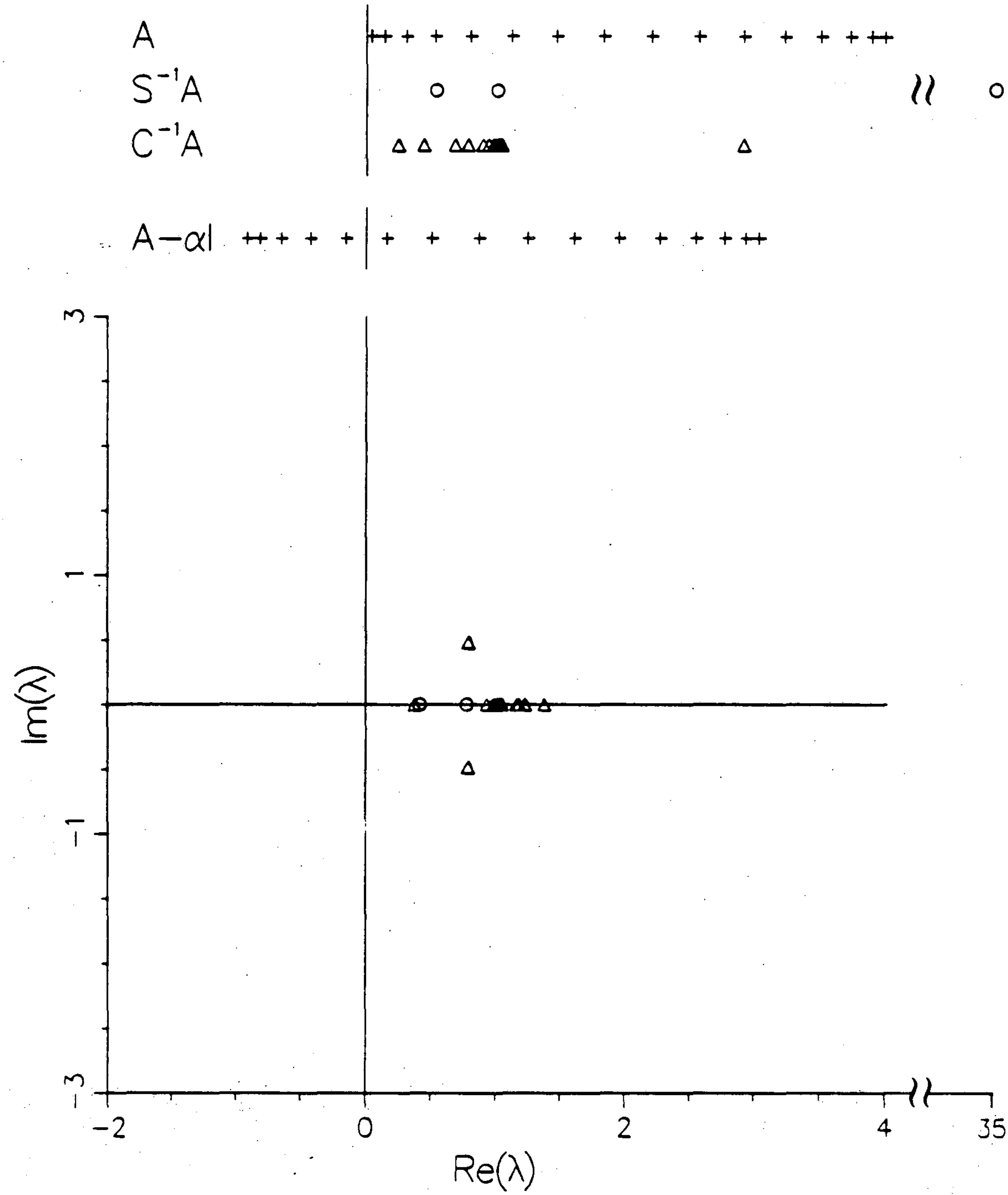

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Fig. 4. Spectra for $A(1,\cdot) = (2 \ -1 \ 0 \ \cdots \ 0)$ and $\alpha = \frac{1}{2}(\nu_5(A) + \nu_6(A))$.

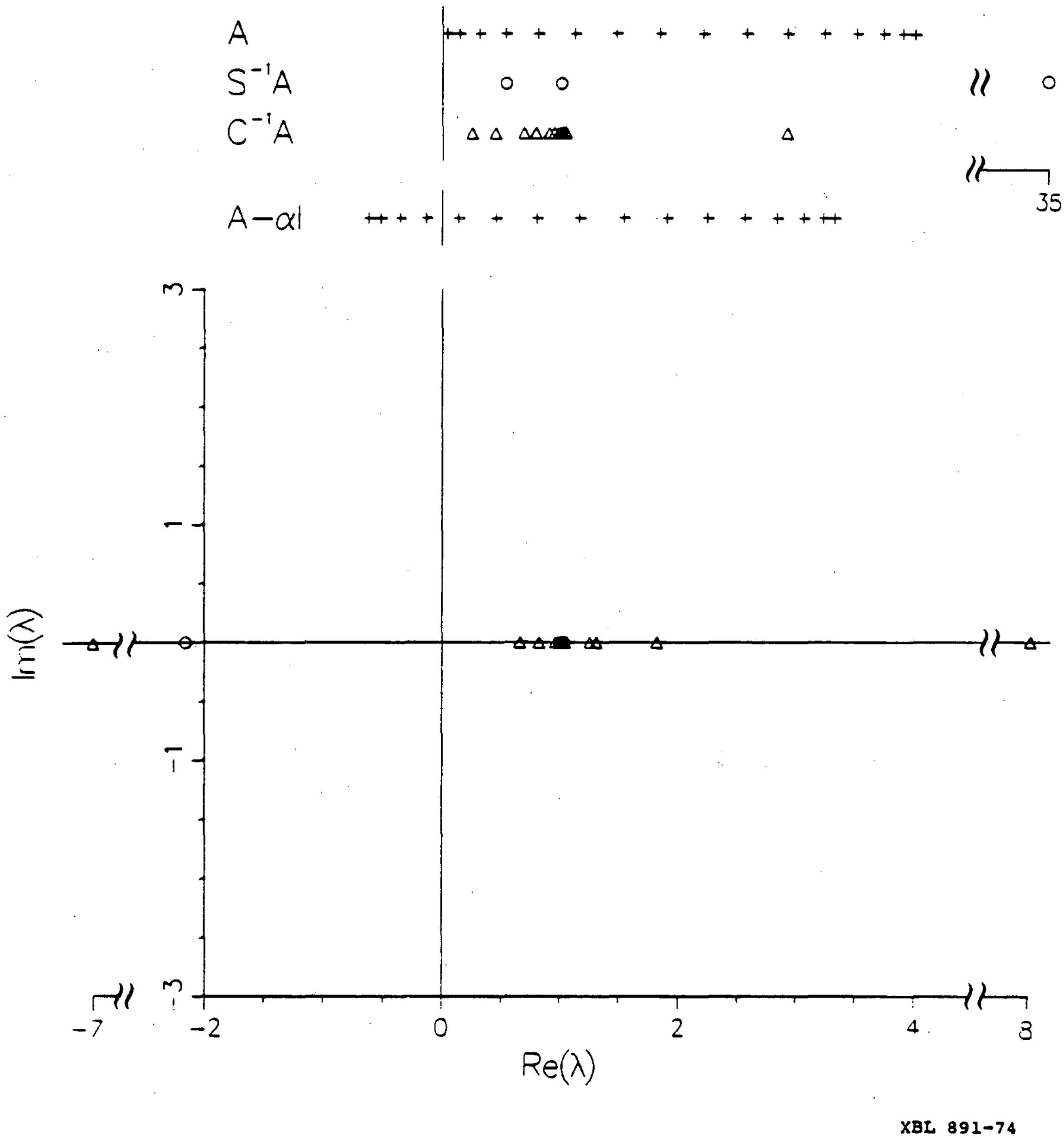

Fig. 5. Spectra for $A(1,\cdot) = (2\ \ -1\ 0\ \cdots\ 0)$ and $\alpha = \frac{1}{2}(\nu_4(A) + \nu_5(A))$.

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