

Numerically Reliable Computation of Characteristic Polynomials

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Abstract

In this paper, we present an algorithm for computing the characteristic polynomial of the pencil $(A - sE)$. It is shown that after a preliminary reduction of the matrices A and E to, respectively, an upper Hessenberg and an upper triangular matrix, the problem of computing the characteristic polynomial is transformed to the solution of certain triangular systems of linear algebraic equations. We show that the computed characteristic polynomial corresponds exactly to perturbed matrices $A + \Delta A$ and $E + \Delta E$ and we derive bounds for ΔA and ΔE . We also suggest how to improve on this backward error via iterative refinement.

1. Introduction

In several engineering problems e.g., computation of transfer functions of linear dynamical systems [8] and applied mathematical problems e.g., computation of functions of a matrix [1], one needs to compute the characteristic polynomial of a matrix, $\det(A - sI)$ or that of a matrix pair, $\det(A - sE)$. Some of the common methods currently in use for computing the characteristic polynomial of a matrix include: reduction to Frobenius canonical form, use of Hyman's method for computing the determinant of a Hessenberg matrix [16], Faddeev-LeVerrier recursion [3], finding the polynomial by first computing the eigenvalues of the matrix, etc. Most of these methods have also been extended to computing the characteristic polynomial of matrix pairs.

Unfortunately, none of the above techniques has been proved to be numerically stable in a strict sense. While it is true that the computation of the eigenvalues of a matrix is numerically stable, forming the characteristic polynomial from them is not. The purpose of this note is to develop a numerically reliable technique for the computation of $\det(A - sE)$. We would like to emphasize here that if the eventual aim is to compute the eigenvalues of a matrix or the zeros of a matrix pencil, then the use of the QR or QZ algorithms, respectively, is advocated due to its numerical reliability. However, if the characteristic polynomial is explicitly required, then the algorithm in the sequel will provide a faster and reliable mean to determine it.

The layout of this paper is as follows: In Section 2, we present the numerical algorithm for computation of $\det(A - sE)$ by reducing the problem to solution of triangular systems of equations. In Section 3, we derive the backward error bounds

for solution of linear systems of equations. The bounds are further refined by taking into account the structure of the problem discussed in Section 2. Numerical results for several experiments with large size problems are presented in Section 4.

2. Computation of Characteristic Polynomial

Hessenberg Triangular Reduction

Given a matrix pair (E, A) , $E, A \in \mathbb{R}^{n \times n}$, there exist orthogonal matrices Q and $Z \in \mathbb{R}^{n \times n}$, such that $\bar{E} := Q^T E Z$ is an upper triangular matrix ($e_{i,j} = 0, i > j$) and $\bar{A} := Q^T A Z$ is an upper Hessenberg matrix ($a_{i,j} = 0, i > j + 1$) [4].

Further, it can be assumed without any loss of generality that \bar{A} is an *unreduced* upper Hessenberg matrix ($a_{i,i-1} \neq 0, i = 2, \dots, n$). If indeed \bar{A} is not unreduced, then the problem of computing the characteristic polynomial can be decomposed into smaller problems.

Hyman's Method for Computing the Determinant of A

Given an *unreduced* upper Hessenberg matrix $A \in \mathbb{R}^{n \times n}$, it is always possible to find an elementary transformation matrix T such that

$$A := AT = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1,n-1} & a_{1,n} \\ a_{21} & a_{22} & \cdots & a_{2,n-1} & 0 \\ & a_{32} & \cdots & a_{3,n-1} & 0 \\ & & \ddots & \vdots & \vdots \\ & & & a_{n,n-1} & 0 \end{bmatrix}. \quad (2.1)$$

Then, the determinant of A is given by

$$\det(A) = (-1)^{n-1} a_{1n} \prod_{i=2}^n a_{i,i-1}$$

The above result was used in [9], [10] to compute the characteristic polynomial $\det(A - sE)$. This was achieved by determining a *unimodular* transformation matrix $T(s)$ (with determinant normalized to 1) such that

$$\begin{aligned} A(s) &:= (A - sE)T(s) \\ &= \begin{bmatrix} a_{11}(s) & a_{12}(s) & \cdots & a_{1,n-1}(s) & d(s) \\ a_{21} & a_{22}(s) & \cdots & a_{2,n-1}(s) & 0 \\ & a_{32} & \cdots & a_{3,n-1}(s) & 0 \\ & & \ddots & \vdots & \vdots \\ & & & a_{n,n-1} & 0 \end{bmatrix} \end{aligned} \quad (2.2)$$

where E is an upper triangular matrix and A is an unreduced upper Hessenberg matrix. Similar to (2.1), the characteristic polynomial $\det(A - sE)$ is given by $(-1)^{n-1} d(s) \prod_{i=2}^n a_{i,i-1}$. Note that, in (2.2) $T(s)$ can be chosen as follows

$$T(s) = \begin{bmatrix} I & \\ & t(s) \end{bmatrix}$$

where $t(s) = [t_1(s) \ t_2(s) \ \dots \ t_{n-1}(s) \ 1]^T$. For the actual computation of the characteristic polynomial of the matrix $A(s)$, one only needs to compute the vector $t(s)$. Equation (2.2) then simplifies to

$$(A - sE)t(s) = \begin{bmatrix} d(s) \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (2.3)$$

In (2.3), since $t_n(s)$ is assumed to be 1, the polynomial vector $t(s)$ can be determined completely by solving the following systems (of polynomial equations)

$$\begin{bmatrix} a_{21} & a_{22}(s) & \dots & a_{2,n-1}(s) & a_{2,n}(s) \\ & a_{32} & \dots & a_{3,n-1}(s) & a_{3,n}(s) \\ & & \ddots & \vdots & \vdots \\ & & & a_{n,n-1} & a_{n,n}(s) \end{bmatrix} \begin{bmatrix} t_1(s) \\ t_2(s) \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (2.4)$$

subsequently, $d(s)$ is computed as the product

$$d(s) := [a_{11}(s) \ a_{12}(s) \ \dots \ a_{1,n-1}(s) \ a_{1,n}(s)] t(s) \quad (2.5)$$

Using the fact that $t_n(s) = 1$, Equations (2.4) and (2.5) can be rewritten as

$$\begin{bmatrix} -1 & a_{11}(s) & \dots & a_{1,n-1}(s) \\ & a_{21} & \dots & a_{2,n-1}(s) \\ & & \ddots & \vdots \\ & & & a_{n,n-1} \end{bmatrix} \begin{bmatrix} d(s) \\ t_1(s) \\ \vdots \\ t_{n-1}(s) \end{bmatrix} = - \begin{bmatrix} a_{1,n}(s) \\ a_{2,n}(s) \\ \vdots \\ a_{n,n}(s) \end{bmatrix} = s \begin{bmatrix} e_{1,n} \\ e_{2,n} \\ \vdots \\ e_{n,n} \end{bmatrix} - \begin{bmatrix} a_{1,n} \\ a_{2,n} \\ \vdots \\ a_{n,n} \end{bmatrix} \quad (2.6)$$

Notice that it follows from this triangular system that $\deg(t_{n-i}(s)) \leq i$. By equating the like powers of s on both sides, Equation (2.6) can be expanded to the following block bidiagonal matrix vector equation

$$\begin{bmatrix} F & -G & & \\ & F & -G & \\ & & \ddots & \ddots \\ & & & F & -G \\ & & & & F \end{bmatrix} \begin{bmatrix} x_n \\ x_{n-1} \\ \vdots \\ x_1 \\ x_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ g_n \\ -f_n \end{bmatrix} \quad (2.7)$$

where,

$$F = \begin{bmatrix} -1 & a_{11} & \dots & a_{1,n-1} \\ & a_{21} & \dots & a_{2,n-1} \\ & & \ddots & \vdots \\ & & & a_{n,n-1} \end{bmatrix}, f_n = \begin{bmatrix} a_{1,n} \\ a_{2,n} \\ \vdots \\ a_{n,n} \end{bmatrix}$$

$$G = \begin{bmatrix} 0 & e_{11} & \dots & e_{1,n-1} \\ & 0 & \dots & e_{2,n-1} \\ & & \ddots & \vdots \\ & & & 0 \end{bmatrix}, g_n = \begin{bmatrix} e_{1,n} \\ e_{2,n} \\ \vdots \\ e_{n,n} \end{bmatrix} \quad \text{and} \quad (2.8)$$

$$[d(s) \ (t(s))^T]^T = s^n x_n + s^{n-1} x_{n-1} + \dots + s x_1 + x_0.$$

Remark 2.1 Due to the assumption that A is an unreduced upper Hessenberg matrix, the matrix F is upper triangular with all diagonal terms nonzero. Therefore, (2.7) represents a block bidiagonal system of linear algebraic equations, $Tx = b$, with its diagonal blocks in upper triangular form.

Remark 2.2 Naturally, if implemented as represented in (2.7), the algorithm would require an inordinate amount of memory. However, it is easy to see that Equation (2.7) can be equivalently solved using the following recursion:

$$\begin{aligned} Fx_0 &= -f_n \\ Fx_1 &= Gx_0 + g_n \\ Fx_i &= Gx_{i-1}, \quad i = 2, \dots, n \end{aligned} \quad (2.9)$$

which requires $(n+1)$ solutions of n -th order triangular system of equations and n matrix-vector multiplications of n -th order triangular matrices, requiring $\mathcal{O}(n^3)$ operations. It is possible to reduce this cost further by exploiting the fact that the last $i-1$ components of the vectors $x_i, i = 2, \dots, n$ will be zero. Therefore, the size of the matrices in the previous recursion decreases from the second step by 1 at each step and the cost of the algorithm can be reduced to $\mathcal{O}(n^3/4)$ operations.

3. Backward Error Bounds

In this section and, unless otherwise stated, A , and E will be any general $n \times n$ matrices. Besides, \otimes will stand for the Kronecker product and vec will be the vector operator which stacks the columns of a matrix in a vector. We first recall some classical results about componentwise error analysis (see [11], [12]).

Theorem 3.1 *The normwise backward error*

$$\eta_{E,f}(y) := \min\{\epsilon : (A + \Delta A)y = b + \Delta b, \|\Delta A\| \leq \epsilon \|E\|, \|\Delta b\| \leq \epsilon \|f\|\}$$

is given by

$$\eta_{E,f}(y) = \frac{\|r\|}{\|E\| \|y\| + \|f\|}, \quad (3.1)$$

where $r = b - Ay$. If $\epsilon \|A^{-1}\| \|E\| < 1$ the following bound

$$\frac{\|x - y\|}{\|x\|} = \frac{\epsilon}{1 - \epsilon \|A^{-1}\| \|E\|} \kappa_{E,f}(A, x) \quad (3.2)$$

is attainable to first order in ϵ and the associated condition number is

$$\kappa_{E,f}(A, x) = \frac{\|A^{-1}\| \|f\|}{\|x\|} + \|A^{-1}\| \|E\|. \quad (3.3)$$

Theorem 3.2 *The componentwise backward error*

$$\omega_{E,f}(y) := \min\{\epsilon : (A + \Delta A)y = b + \Delta b, \\ |\Delta A| \leq \epsilon E, |\Delta b| \leq \epsilon f\}$$

where E and f have now nonnegative entries (note that the inequalities on this definition should be considered componentwise) is given by

$$\omega_{E,f}(y) = \max_i \frac{|r_i|}{(E|y| + f)_i}. \quad (3.4)$$

If $\epsilon \| |A^{-1}| E \| < 1$ the following bound

$$\frac{\|x - y\|_\infty}{\|x\|_\infty} = \frac{\epsilon}{1 - \epsilon \| |A^{-1}| E \|} \text{cond}_{E,f}(A, x) \quad (3.5)$$

is attainable to first order in ϵ and the associated condition number is now

$$\text{cond}_{E,f}(A, x) = \frac{\| |A^{-1}| E \|_x + \| |A^{-1}| |f| \|_\infty}{\|x\|_\infty}. \quad (3.6)$$

Similar results also hold for normwise errors. For triangular systems of equations, the following result holds (see [6]).

Theorem 3.3 *Let the triangular system $Tx = b$, where $T \in \mathbb{R}^{n \times n}$ is nonsingular, be solved by back substitution, with any ordering. Then the computed solution y satisfies*

$$(T + \Delta T)y = b, \quad |\Delta T| \leq \gamma_m |T|, \quad |\Delta b| \leq \gamma_m |b| \quad (3.7)$$

where $\gamma_m = mu/(1 - mu)$, m is the bandwidth of the system and u is the unit roundoff of the machine.

From this backward error bound, one obtains (see also [13]):

$$\frac{\|x - y\|_\infty}{\|x\|_\infty} \leq \frac{\text{cond}(T, x) \gamma_m}{1 - \text{cond}(T) \gamma_m} \text{cond}(T, x) \\ = \frac{\| |T^{-1}| |T| \|_\infty}{\|x\|_\infty},$$

where, $\text{cond}(T) = \| |T^{-1}| |T| \|_\infty$. As a direct consequence of Theorem 3.3, the solution of the block bidiagonal matrix vector equation in (2.7) and, therefore, the coefficients of the characteristic polynomial, are computed in a backward stable manner. However, this neglects an important fact: the structure exhibited by system (2.7). In [15], [2], [5], it is shown that the structure can affect both the conditioning and the stability of many problems and thus it has to be taken into account.

Error Bounds due to the Structure of the Problem

In [5], [15], definitions for the *structured componentwise backward error* and the *structured condition number* are presented. We make use of these results and apply them to our particular problem. Consider the linear system $A_s x = b$, $A_s \in \mathbb{R}^{n \times n}$, $x, b \in \mathbb{R}^n$ where the structured matrix A_s belongs to a set S whose members depend on t real parameters i.e., $A_s = A_s[p]$. The following theorem from [5] defines the *structured backward error* for this linear system.

Theorem 3.4 *Assume that*

$$\Delta p = D_1 v, \quad D_1 = \text{diag}(g_i), \quad \Delta b = D_2 w, \quad D_2 = \text{diag}(f_i),$$

where $g \in \mathbb{R}^t$ and $f \in \mathbb{R}^n$ are nonnegative vectors of tolerances. Then, with $A_s + \Delta A_s = A_s[p + \Delta p]$, the *structured componentwise backward error* is defined as

$$\mu(y) := \min \left\{ \left\| \begin{bmatrix} v \\ w \end{bmatrix} \right\|_\infty : (A_s + \Delta A_s)y = b + \Delta b, \right. \\ \left. \|\Delta p\| = D_1 v, \quad \|\Delta b\| = D_2 w \right\}.$$

It is important to note that this constrained nonlinear minimization problem has no closed solution in general. Therefore, the results provided in [5] only apply to the special case where S is a linear subspace of $\mathbb{R}^{n \times n}$. This happens to be the case for Toeplitz matrices [15], which is what we need here. It is possible to compute the vector $[v^T \ w^T]^T$ from the minimal ∞ -solution of the system

$$[(I_n \otimes y^T) B D_1, -D_2] \begin{bmatrix} v \\ w \end{bmatrix} = b - A_s y \equiv Cz = r \quad (3.8)$$

where B satisfies $\text{vec}(\Delta A_s^T) = B \Delta p$. If C is rank-deficient, then there may be no solution to the system (3.8) and the *structured componentwise backward error* can be regarded as being infinite. Otherwise, this system has to be solved in the ∞ -norm sense. It is also possible to obtain an approximate solution by minimizing in the 2-norm. Moreover, the bound

$$\mu(y) \leq \|r\|_2 \|C^+\|_2 = \frac{\|r\|_2}{\sigma_{\min}(C)} \quad (3.9)$$

explicitly states the relation between the *structured componentwise backward error* and the conditioning of the matrix C . From the definition in (3.4) the following forward error bound is derived

$$\frac{\|x - y\|_\infty}{\|x\|_\infty} \leq \epsilon \text{cond}_\infty(A_s, x) + O(\epsilon^2) \quad (3.10)$$

where the *structured condition number* satisfies

$$\text{cond}_\infty(A_s, x) = \frac{\| |A_s^{-1}| X B \|_\infty + \| |A_s^{-1}| |f| \|_\infty}{\|x\|_\infty} \\ \leq \theta_\infty(A_s, x) \\ = \frac{\| |A_s^{-1}| X B D_1 \|_\infty + \| |A_s^{-1}| D_2 \|_\infty}{\|x\|_\infty}.$$

Error Bounds for the Proposed Algorithm

Consider the system $Tx = b$ in (2.7) and let y denote the computed solution. From Theorem 3.3,

$$(T + \Delta T_u)y = (b + \Delta b_u), \quad |\Delta T_u| \leq \gamma_{2n} |T|, \quad |\Delta b_u| \leq \gamma_{2n} |T|.$$

The residual of the computed solution is given by

$$r = b - Ty = (T + \Delta T_u)y - \Delta b_u - Ty = \Delta T_u y - \Delta b_u.$$

Therefore,

$$|r| \leq |\Delta T_u| |y| + |\Delta b_u| \leq \gamma_{2n} (|T| |y| + |b|),$$

and the same result holds for any vector norm and its corresponding subordinate matrix norm. In particular, for the vector

2-norm,

$$\begin{aligned}
\|r\|_2 &\leq \|r\|_1 \leq \gamma_{2n} (\|T\|_1 \|\theta\|_1 + \|\delta\|_1) \\
&\leq \gamma_{2n} \left(\left\| \begin{bmatrix} G \\ F \end{bmatrix} \right\|_1 \|\theta\|_1 + \|\delta\|_1 \right) \\
&\leq \gamma_{2n} (\|G\|_1 + \|F\|_1) \|\theta\|_1 + \|\delta\|_1 \\
&= \gamma_{2n} (\|G\|_1 + \|F\|_1) \|\theta\|_1 + \|f_n\|_1 + \|g_n\|_1 \\
&\leq \sqrt{n} \gamma_{2n} (\sqrt{n} (\|G\|_2 + \|F\|_2) \|\theta\|_2 \\
&\quad + \|f_n\|_2 + \|g_n\|_2).
\end{aligned}$$

Consider now the structure of the matrices F and G where, to avoid confusions, we will denote the matrices of the pencil by $(\bar{A} - s\bar{E})$. The previous bound can be simplified if a few conditions are satisfied. Assume that $\|\bar{A}\|_1 \geq 1$ and $\|\theta\|_1 \geq 1$ (this can be obtained by proper scaling of the original pencil), then

$$\begin{aligned}
\|F\|_1 \|\theta\|_1 + \|f_n\|_1 &= (\|F\|_1 + \|f_n\|_1 / \|\theta\|_1) \|\theta\|_1 \\
&\leq \|\bar{A}\|_1 \|\theta\|_1 \\
&\leq n \|\bar{A}\|_2 \|\theta\|_2.
\end{aligned}$$

Using the same idea, if $\|\theta\|_1 \geq 1$ then

$$\|G\|_1 \|\theta\|_1 + \|g_n\|_1 \leq n \|\bar{E}\|_2 \|\theta\|_2,$$

and the bound for the 2-norm of the residual can be expressed in function of the data of the original pencil as

$$\|r\|_2 \leq n \gamma_{2n} (\|\bar{A}\|_2 + \|\bar{E}\|_2) \|\theta\|_2.$$

Finally, from (3.9)

$$\begin{aligned}
\mu(y) &\leq \|r\|_2 \|C^+\|_2 \\
&= n \gamma_{2n} (\|\bar{A}\|_2 + \|\bar{E}\|_2) \|\theta\|_2 \|C^+\|_2,
\end{aligned}$$

where C is constructed for our problem according to (3.8). This inequality gives a bound for the *structured componentwise backward error*. This bound will be small if the condition number of C is small. This fact agrees with the intuitive idea that in such case, the *structured componentwise backward error* will also be small.

We believe that a few steps of iterative refinement applied on the solution will lead to a smaller *structured backward error*. This would be based on computing the structured backward error using (3.8) and then using this in the first order perturbation of equation (2.8). If this process can be shown to be convergent, the backward stability of the algorithm would be guaranteed, [7], [14]. Since these are linear equations we expect this to converge if $u \cdot \mu(y) \ll 1$ (see [16]).

4. Numerical results

We present the results of several experiments carried out on a SUN Sparc-10, using *MATLAB* and double precision ($u \approx 1.11 \times 10^{-16}$). The matrix pairs (\bar{E}, \bar{A}) were generated using a random uniform distribution [0,1]. The infinite matrix norm and infinite vector norm are used unless otherwise stated.

Table 4.1 shows the normwise and componentwise relative backward error when solving the system $Tx = b$ of (2.7) for three large-size problems. In the same table, the normwise and componentwise condition number are also presented. The relative backward errors and relative condition numbers are

n	$\eta_{ T , b }(y)$	$\omega_{ T , b }(y)$	$\kappa_{ A , b }$	$\text{cond}_{ T , b }$
50	$7.192e^{-18}$	$1.266e^{-16}$	$1.067e^4$	$5.064e^1$
100	$2.663e^{-18}$	$1.664e^{-16}$	$3.109e^4$	$9.260e^1$
150	$4.168e^{-18}$	$1.527e^{-16}$	$4.122e^4$	$1.127e^2$

Table 4.1: Comparison of the normwise and componentwise backward relative errors and condition numbers for large-size, generalized problems (\bar{E}, \bar{A}) , $\kappa_{|A|,|b|} = \kappa_{|A|,|b|}(T, y)$ $\text{cond}_{|T|,|b|} = \text{cond}_{|T|,|b|}(T, y)$.

n	$\eta_{ T , b }(y)$	$\omega_{ T , b }(y)$	$\kappa_{ A , b }$	$\text{cond}_{ T , b }$
50	$7.298e^{-18}$	$1.523e^{-16}$	$2.047e^3$	$3.583e^1$
100	$1.432e^{-17}$	$1.835e^{-16}$	$9.350e^4$	$8.403e^1$
150	$8.371e^{-18}$	$2.508e^{-16}$	$2.227e^4$	$1.392e^2$

Table 4.2: Comparison of the normwise and componentwise backward relative errors and condition numbers for large-size problems (I_n, \bar{A}) , $\kappa_{|A|,|b|} = \kappa_{|A|,|b|}(T, y)$ $\text{cond}_{|T|,|b|} = \text{cond}_{|T|,|b|}(T, y)$.

obtained from equations (3.1), (3.3), (3.4) and (3.6) for $E = |T|$, $f = |b|$ and $x = y$.

In Table 4.2, the same experiments are repeated for the matrix pair (I_n, \bar{A}) . In this case the computed characteristic polynomial will be that of the matrix \bar{A} .

In Table 4.3 the normwise, componentwise and structured componentwise relative backward error for small-size problems are shown. The computation of the structured parameters requires the construction of the coefficient matrix described in (3.8) which is a time-consuming process in *MATLAB*. Memory restrictions also appear for moderately large problems. Yet, one should be able to exploit the sparsity of this system to derive efficient solutions. This will be crucial especially when going to iterative refinement based on this system of equations. The structured componentwise relative backward error was approximated by the minimum 2-norm solution of (3.8) considering

n	$\eta_{ T , b }(y)$	$\omega_{ T , b }(y)$	$\mu(y)$
5	$1.204e^{-17}$	$4.254e^{-17}$	$1.824e^{-15}$
10	$8.820e^{-18}$	$1.255e^{-16}$	$5.716e^{-15}$
	$\kappa_{ A , b }(T, y)$	$\text{cond}_{ T , y }(T , y)$	$\theta_\infty(T , b)$
5	80.461	8.391	6.193
10	514476	11.774	11.395

Table 4.3: Comparison of the backward relative errors and the condition numbers for small-size, generalized problems (\bar{E}, \bar{A}) .

$g = \text{vec}_{\neq 0}([\tilde{A}], |\tilde{E}|^T)$ and $f = |b|$. The required operator $\text{vec}_{\neq 0}$ stacks by columns in a long vector only the nonzero entries of a matrix. Thus, the tolerance vector g of Theorem 3.4 only stores those nonzero elements of the matrix pair (\tilde{E}, \tilde{A}) .

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