Forward stable computation of roots of real polynomials with only real distinct roots

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Abstract

As showed in (Fiedler, 1990), any polynomial can be expressed as a characteristic polynomial of a complex symmetric arrowhead matrix. This expression is not unique. If the polynomial is real with only real distinct roots, the matrix can be chosen real. By using accurate forward stable algorithm for computing eigenvalues of real symmetric arrowhead matrices from (Jakovčević Stor, Slapničar, Barlow, 2015), we derive a forward stable algorithm for computation of roots of such polynomials in $O(n^2)$ operations. The algorithm computes each root to almost full accuracy. In some cases, the algorithm invokes extended precision routines, but only in the non-iterative part. Our examples include numerically difficult problems, like the well-known Wilkinson’s polynomials. Our algorithm compares favourably to other method for polynomial root-finding, like MPSolve or Newton’s method.

Keywords Roots of polynomials; Generalized companion matrix; Eigenvalue decomposition; Arrowhead matrix; High relative accuracy; Forward stability

MSC 65F15, 65G50, 15-04, 15B99

1 Introduction and Preliminaries

Polynomials appear in many areas of scientific computing and engineering. Developing fast algorithms and reliable implementations of polynomial solvers are of challenging interest. Famous example by James H. Wilkinson in 1963 [12], usually referred to as Wilkinson’s polynomial, is often used to illustrate difficulties when finding the roots of a polynomial. The polynomial of order $n$ is defined by a simple formula:

$$W_n(x) = \prod_{i=1}^{20} (x - i) = (x - 1)(x - 2) \cdots (x - n).$$

For example, the location of the roots of $W_{20}$ is very sensitive to perturbations in the coefficients, so that in [13], Wilkinson said: "Speaking for myself, I regard it as the most traumatic
experience in my career as a numerical analyst.” Many methods for finding roots of polynomials with ever increasing accuracy have been developed since (see for example [1], [5]).

In [4], Miroslav Fiedler showed that any polynomial can be expressed as a characteristic polynomial of a complex symmetric arrowhead matrix. This expression is not unique. If the polynomial is real with only real distinct roots, the matrix can be chosen real. We have the following theorem:

**Theorem 1.** [4, Theorem 3] Let \( u(x) \) be a polynomial of degree \( n \),

\[
    u(x) = x^n + px^{n-1} + r(x),
\]

Let

\[
    D = \text{diag}(d_1, \ldots, d_{n-1}),
\]

where \( d_j \) are all distinct and \( u(d_j) \neq 0 \). Let

\[
    v(x) = \prod_{j=1}^{n-1} (x - d_j),
\]

\[
    \alpha = -p - \sum_{j=1}^{n-1} d_j,
\]

\[
    z = \begin{bmatrix} \zeta_1 & \zeta_2 & \cdots & \zeta_{n-1} \end{bmatrix}^T,
\]

where

\[
    \zeta_j^2 = \frac{-u(d_j)}{v'(d_j)} = \frac{-u(d_j)}{\prod_{i=1}^{n-1} (d_j - d_i)}.
\]

Then the symmetric arrowhead matrix

\[
    A = \begin{bmatrix} D & z \\ z^T & \alpha \end{bmatrix},
\]

has characteristic polynomial \((-1)^nu(x)\).

If \( u(x) \) has only real distinct roots and the \( d_j \)'s interlace them, then \( A \) is real.

Fiedler concludes his paper by stating “One can hope to obtain, by some sophisticated special choice of the numbers \( d_j \), stable or even universal algorithms for solving algebraic equations.”

In [8] the authors developed a forward stable algorithm for computing eigendecomposition of a real symmetric irreducible arrowhead matrix, which is exactly the matrix \( A \) given by Theorem

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1In a report by Corless and Litt [2], the matrix \( A \) from theorem [1] is referred to as generalized companion matrix not expressed in monomial basis. In this case, the basis is the Newton basis.
More precisely, the algorithm from [8] computes each eigenvalue and all individual components of the corresponding eigenvector of a given arrowhead matrix of floating-point numbers to almost full accuracy in \(O(n)\) floating point-operations, a feature which no other method has.

In this case, we are interested only in the roots of \(u\), that is, in the eigenvalues of \(A\) from (5), each of which is computed independently of the others in \(O(n)\) operations. This, together with independent computation of elements of \(z\), makes our algorithm suitable for parallel computing.

In this paper, we propose a new two-step algorithm: given a polynomial \(u\) of the form (1) whose coefficients are given floating-point numbers,

1. compute the generalized companion matrix \(A\) from (5), where the elements of \(z\) and \(\alpha\) need to be computed in double the working precision, and then

2. compute the roots of \(u\) as the eigenvalues of \(A\) by using modified version of the forward stable algorithm \textit{aheig} from [8, Algorithm 5].

The organization of the paper is the following. In Section 2 we describe our algorithm named \textit{polyaheig} (POLYnomial roots via ArrowHead EIGenvalues). In Section 3 we analyse the accuracy of the algorithm and give forward error bounds – in Section 3.1 we analyse the accuracy of the computed matrix \(A\), and in Section 3.2 we analyse the accuracy of the computed inverse of the shifted matrix \(A\). In Section 3.3 we discuss possible ways to find the diagonal elements of the matrix \(D\) which interpolate the roots of \(u\). In Section 3.4 we discuss different implementations of the double the working precision, including extended precision routines from [3] and the Compensated Horner scheme from [5, Algorithm 4]. Finally, in Section 4 we illustrate our algorithm with two numerically demanding examples and compare it to the methods from [1] and [5].

2 The algorithm

The eigenvalues of the arrowhead matrix \(A\) from (5) are the zeros of the function

\[ \varphi_A(\lambda) = \alpha - \lambda - z^T(D - \lambda I)^{-1}z. \]

The forward stable algorithm for solving EVP of arrowhead matrices [8] computes all eigenvalues to almost full accuracy. The algorithm is based on shift–and–invert strategy. Let \(d_i\) be the pole which is nearest to \(\lambda\). Let \(A_i\) be the shifted matrix,

\[
A_i = A - d_iI = \begin{bmatrix} D_1 & 0 & 0 & z_1 \\ 0 & 0 & 0 & \zeta_i \\ 0 & 0 & D_2 & z_2 \\ z_1^T & \zeta_i & z_2^T & a \end{bmatrix}
\]  

\[ (6) \]

\(^2\)In [8], the arrowhead matrix \(A\) is called “irreducible” if \(d_j\) are all distinct and \(z_j \neq 0, j = 1, \ldots, n - 1.\)
where

\[ D_1 = \text{diag}(d_1 - d_i, \ldots, d_{i-1} - d_i), \]
\[ D_2 = \text{diag}(d_{i+1} - d_i, \ldots, d_{n-1} - d_i), \]
\[ z_1 = [ \zeta_1 \, \zeta_2 \, \cdots \, \zeta_{i-1} ]^T, \]
\[ z_2 = [ \zeta_{i+1} \, \zeta_{i+2} \, \cdots \, \zeta_{n-1} ]^T, \]
\[ a = \alpha - d_i. \]

Then,

\[ \lambda = \frac{1}{\nu} + d_i, \]

where \( \nu \) is either largest or smallest (first or last) eigenvalue of the matrix

\[ A_i^{-1} \equiv (A - d_i I)^{-1} \equiv \begin{bmatrix} D_1^{-1} & w_1 & 0 & 0 \\
 w_1^T & b & w_2^T & 1/\zeta_i \\
 0 & w_2 & D_2^{-1} & 0 \\
 0 & 1/\zeta_i & 0 & 0 \end{bmatrix}, \]

where

\[ w_1 = -D_1^{-1} z_1 \frac{1}{\zeta_i}, \]
\[ w_2 = -D_2^{-1} z_2 \frac{1}{\zeta_i}, \]
\[ b = \frac{1}{\zeta_i^2} (-a + z_1^T D_1^{-1} z_1 + z_2^T D_2^{-1} z_2). \]

Notice that all elements of the matrix \( A_i^{-1} \) are computed with high relative accuracy, except that in some cases the element \( b \) needs to be computed in double the working precision (for details see [8]). Also, the elements of \( z \) (the Horner scheme) and \( \alpha \) (the trace preservation formula) of \( A \) need to be computed in double the working precision. Notice that our algorithm requires computation in higher precision only in the finite part, unlike algorithms from [1, 5], which require usage of higher precision in the iterative part.

The described procedure is implemented in the algorithm \textit{poly.aheig}. 

4
Algorithm 1

\[
\lambda = \text{poly\_aheig}(u, D)
\]

% Computes the roots \(\lambda\) of the polynomial \(u(x)\) from (1) of order \(n\), with
% distinct real roots. \(D\) is defined by (2) and its entries interlace the roots
% of \(u(x)\), see Section 3.3 for details.

% Compute the values of \(u(x)\) in the interpolating points \(d_j\) using double
% the working precision.
\begin{verbatim}
for j = 1 : n - 1
    s_{double}(j) = u(d(j))
end
\end{verbatim}

% Compute vector \(v\) from Theorem 1 using double the working precision.
\begin{verbatim}
for j = 1 : n - 1
    v_{double}(j) = \prod(d(j) - d(1 : j - 1, j + 1 : n - 1))
end
\end{verbatim}

% compute \(\alpha\) from Theorem 1 using double the working precision.
\[
\alpha_{double} = -p - \sum_{j=1}^{n-1} d_j
\]

% compute vector \(z\) from Theorem 1 using double the working precision.
\begin{verbatim}
for j = 1 : n - 1
    \zeta_{double}(j) = \sqrt{-s_{double}(j)/v_{double}(j)}
end
\end{verbatim}

% call modified algorithm aheig
\begin{verbatim}
for k = 1 : n
    \lambda(k) = \text{aheig\_mod}(D, z_{double}, \alpha_{double}, k)
end
\end{verbatim}
Remark 1. The algorithm $aheig_{mod}$ is a simple modification of the algorithm $aheig$ from [8, Algorithm 5]. The accuracy of the algorithm $aheig$ is essentially based on the assumption that all elements of the matrix $A_i^{-1}$ from (8) can be computed with high relative accuracy, that is, $fl([A_i^{-1}]_{jl}) = [A_i^{-1}]_{jl}(1 + \kappa_{jl}\varepsilon_M)$, for some modest $\kappa_{jl}$. For all elements of $A_i^{-1}$ but $b$, this accuracy is achieved by computing them in standard precision using the standard precision copies of $z$ and $\alpha$. If, according to the theory from [8], the element $b$ needs to be evaluated in double the working precision, formula (9) is evaluated using $z_{\text{double}}$ and $\alpha_{\text{double}}$ in order to obtain full possible accuracy. The details of the analysis follow.

3 Accuracy of the algorithm

The error analysis of the algorithm $aheig$ is given in [8, Sections 3 and 4]. This analysis assumes that $A$ is the given matrix of floating-point numbers. Here, however, $A$ is computed by using formulas (1-5), which must be taken into account. We assume that computations are performed either in the standard floating-point arithmetic with the machine precision $\varepsilon_M = 2^{-53} \approx \approx 1.1102 \cdot 10^{-16}$ (see [6, Chapter 2] for details) or with double the working precision with the machine precision $\varepsilon^2_M = 2^{-106} \approx 1.2326 \cdot 10^{-32}$.

Let us first consider the errors in the polynomial evaluation. The standard method for evaluating polynomial $u(x)$ is the Horner’s method [6, Section 5.1]. Let

$$u(x) = \sum_{i=0}^{n} a_i x^{n-i}, \quad a_0 \equiv 1,$$

and let

$$\text{cond}(u, x) = \frac{\sum_{i=0}^{n} |a_i| |x|^{n-i}}{\sum_{i=0}^{n} a_i x^{n-i}} = \frac{\bar{u}(x)}{u(x)}.$$  \hspace{1cm} (11)

Notice that $\text{cond}(u, x) \geq 1$. Let $\text{Horner}(u, x)$ denote the value of $u(x)$ computed in floating point accuracy by the Horner scheme. Then, the relative error in the computed value is bounded by [6, Section 5.1] \footnote{Thus, the floating-point numbers have approximately 16 significant decimal digits. The term “double the working precision” means that the computations are performed with numbers having approximately 32 significant decimal digits, or with the machine precision equal to $\varepsilon^2_M$.}

$$\frac{|u(x) - \text{Horner}(u, x)|}{|u(x)|} \leq \text{cond}(u, x) \times 2n\varepsilon_M.$$  \hspace{1cm} (10)

Thus, when $\text{Horner}(u, x)$ is evaluated in double the working precision, the relative error is bounded by

$$\frac{|u(x) - \text{Horner}_{\text{double}}(u, x)|}{|u(x)|} \leq \text{cond}(u, x) \times 2n\varepsilon^2_M.$$  \hspace{1cm} (11)

Therefore,

$$\text{Horner}_{\text{double}}(u, x) = (1 + \kappa x^2\varepsilon^2_M)u(x).$$  \hspace{1cm} (12)

\footnote{In [6, 5], the bounds are expressed in terms of quantities $\gamma_k = \frac{k\varepsilon_M}{1-k\varepsilon^2_M}$. For the sake of simplicity, we use standard first order approximations $\gamma_k \approx k\varepsilon_M$.}
where
\[ |\kappa_x| \leq \text{cond}(u, x) \times 2n. \]  \hspace{1cm} (13)

Notice that, if \( \text{cond}(u, x) \) is uniformly bounded,
\[ \text{cond}(u, x) \leq \frac{1}{\varepsilon_M}, \]  \hspace{1cm} (14)

then
\[ |\kappa_x| \leq 2n. \]  \hspace{1cm} (15)

Other two options to obtain bounds similar to (12,13) are to evaluate all parts of the respective formulas by using extended precision routines from [3] or compensated Horner scheme from [5, Algorithm 4] (see Section 3.4 for details).

We now consider the accuracy of the computed matrices \( A, A_i \) and \( A_i^{-1} \) from (5), (6) and (8).

### 3.1 Accuracy of \( A \)

Let \( \hat{A} \) denote the matrix \( A \) computed according to Algorithm 1,
\[
\hat{A} = \begin{bmatrix} D & \hat{\zeta}(d) \\ (\hat{\zeta}(d))^T & \hat{\alpha}(d) \end{bmatrix}.
\]

Here \( \hat{\zeta}(d) \) and \( \hat{\alpha}(d) \) are computed in double the working precision which we denote by superscript \( (d) \). Let
\[
\hat{\zeta}(d) = \begin{bmatrix} \hat{\zeta}_1(d) \\ \hat{\zeta}_2(d) \\ \vdots \\ \hat{\zeta}_{n-1}(d) \end{bmatrix}^T.
\]

By combining (4) and (12), the standard first order error analysis in double the working precision, gives
\[
\hat{\zeta}_j(d) = \frac{-u(d_j)(1 + \kappa_{d_j}\varepsilon_M^2)}{\prod_{i=1}^{n-1} (d_j - d_i)(1 + \varepsilon_1)(1 + (n-3)\varepsilon_2)}(1 + \varepsilon_3)(1 + \varepsilon_4),
\]  \hspace{1cm} (16)

where \(|\varepsilon_{1,2,3,4}| \leq \varepsilon_M^2\). Therefore,
\[
\hat{\zeta}_j(d) = \zeta_j(1 + \kappa_{\zeta_j}\varepsilon_M^2),
\]  \hspace{1cm} (17)

where, by using (13),
\[
\left| \kappa_{\zeta_j}(d) \right| \leq \frac{|\kappa_{d_j}| + (n - 1)}{2} + 1 \leq n \cdot \text{cond}(u, d_j) + \frac{n + 1}{2}.
\]

Similarly, applying the standard first order error analysis in double the working precision to (3), gives
\[
\hat{\alpha}(d) = \alpha(1 + \kappa_{\alpha}(d)\varepsilon_M^2),
\]
where
\[
|\kappa^{(d)}_{\alpha}| \leq \left| a_1 \right| + \sum_{j=1}^{n-1} |d_j| \left( n - 1 \right) \equiv K_{\alpha} (n - 1) .
\] (18)

### 3.2 Accuracy of \( A_i^{-1} \)

Let \( \hat{A}_i^{-1} \) denote the matrix \( A_i^{-1} \) computed according to Algorithm 1 from the matrix \( \hat{A} \). All elements of \( A_i^{-1} \) but possibly \( b_i \), are computed in standard precision using the standard precision copies of \( \hat{z}^{(d)} \) and \( \hat{\alpha}^{(d)} \). Let \( \hat{\zeta}_j \) and \( \hat{\alpha} \) denote \( \hat{\zeta}_j^{(d)} \) and \( \hat{\alpha}^{(d)} \) rounded to the nearest standard precision number, respectively. Then
\[
\hat{\zeta}_j = \zeta_j \left( 1 + \kappa_{\zeta} \varepsilon_M \right), \quad j = 1, \ldots, n - 1,
\]
\[
\hat{\alpha} = \alpha \left( 1 + \kappa_{\alpha} \varepsilon_M \right),
\]
where, by using (17)-(18),
\[
|\kappa_{\zeta_j}| \leq \left( \frac{|\kappa_{d_j}| + (n - 1)}{2} \right) \varepsilon_M + 1, \quad j = 1, \ldots, n - 1,
\]
\[
|\kappa_{\alpha}| \leq K_{\alpha} (n - 1) \varepsilon_M + 1.
\]

Further, according to (13)-(15), if
\[
\text{cond}(u, d_j) \leq \frac{1}{\varepsilon_M}, \quad j = 1, \ldots, n - 1,
\]
then (19) holds with
\[
|\kappa_{\zeta_j}| \leq n + 2, \quad j = 1, \ldots, n - 1,
\]
and if
\[
K_{\alpha} \leq \frac{1}{\varepsilon_M} ,
\]
then (20) holds with
\[
|\kappa_{\alpha}| \leq n.
\]

For \( j \notin \{i, n\} \), similarly as in [8, Proof of Theorem 4], the standard first order error analysis gives
\[
[\hat{A}_i^{-1}]_{jj} = fl \left( \frac{1}{d_j - d_i} \right) = \frac{1}{d_j - d_i} (1 + \kappa_{jj} \varepsilon_M), \quad |\kappa_{jj}| \leq 2.
\]
Similarly, assuming that (21) and (22) hold, for \( j \notin \{i, n\} \) we have
\[
[\hat{A}_i^{-1}]_{ji} = fl([\hat{A}_i^{-1}]_{ij}) = fl \left( \frac{-\zeta_j (1 + \kappa_{\zeta} \varepsilon_M)}{(d_j - d_i) \zeta_i (1 + \kappa_{\zeta} \varepsilon_M)} \right)
\]
\[
= \frac{-\zeta_j}{(d_j - d_i) \zeta_i} (1 + \kappa_{ji} \varepsilon_M), \quad |\kappa_{ji}| \leq (2n + 7).
Finally,

\[
[\hat{A}_i^{-1}]_{ni} = fl([\hat{A}_i^{-1}]_{in}) = fl\left(\frac{1}{\zeta_i(1 + \kappa_i \varepsilon_M)}\right)
= \frac{1}{\zeta_i}(1 + \kappa_{ni} \varepsilon_M), \quad |\kappa_{ni}| \leq (n + 3).
\]

We now analyze the accuracy of the computed element \(b\). Let

\[
K_b = |\alpha| + |d_i| + |z_1^T D_1^{-1} z_1| + |z_2^T D_2^{-1} z_2| - a \left[ 1 + \sum_{j=1}^{n-1} \frac{\zeta_j^2(1 + \kappa_j \varepsilon_M)^2}{d_j - d_i} \right], \quad (25)
\]

where \(D_1, D_2, z_1, z_2\) and \(a\) are defined by (7). We have two cases. First, if

\[ K_b \gg 1, \]

then \(b\) is computed in standard precision using \(\hat{\zeta}_j\) and \(\hat{\alpha}\). Let \(\hat{b}\) denote the computed \(b\). The standard first order error analysis of (9) gives

\[
\hat{b} = fl\left(\frac{1}{\zeta_i^2(1 + \kappa_i \varepsilon_M)^2} \left(\alpha(1 + \kappa_{\alpha} \varepsilon_M) - d_i + \sum_{j=1}^{n-1} \frac{\zeta_j^2(1 + \kappa_j \varepsilon_M)^2}{d_j - d_i} \right)\right)
= b(1 + \kappa_{b} \varepsilon_M),
\]

where

\[ |\kappa_{b}| \leq (n + 2 + \max\{2 \max_{j \neq i} |\kappa_j|, |\kappa_{\alpha}|\}) \cdot K_b + 2|\kappa_{\zeta_i}| + 3. \]

Additionally, if (21) and (23) hold, then (22) and (24) hold, as well, and

\[ |\kappa_{b}| \leq (3n + 6) \cdot K_b + 2n + 7. \]

Second, if

\[ K_b \gg 1, \]

then, according to the theory from (8), the element \(b\) needs to be computed in double the working precision using \(\hat{\zeta}^{(d)}_j\) and \(\hat{\alpha}^{(d)}\) in order to obtain full possible accuracy. The standard first order error analysis of (9) in double the working precision gives

\[
\hat{b}^{(d)} = fl\left(\frac{1}{\zeta_i^2(1 + \kappa_{\zeta_i}^{(d)} \varepsilon_{M}^{2})^2} \left(\alpha(1 + \kappa_{\alpha}^{(d)} \varepsilon_{M}^{2}) - d_i + \sum_{j=1}^{n-1} \frac{\zeta_{j}^{(d)}^2(1 + \kappa_{\zeta_j}^{(d)} \varepsilon_{M}^{2})^2}{d_j - d_i} \right)\right)
= b(1 + \kappa_{b}^{(d)} \varepsilon_{M}^{2}),
\]

where

\[ |\kappa_{b}^{(d)}| \leq (n + 2 + \max\{2 \max_{j \neq i} |\kappa_j^{(d)}|, |\kappa_{\alpha}^{(d)}|\}) \cdot K_b + 2|\kappa_{\zeta_i}^{(d)}| + 3. \]
Finally, let
\[ \kappa^{(d)}_{A_i} = \max \{ 2 \max \{ |\kappa^{(d)}_{c_j}|, |\kappa^{(d)}_{\alpha}| \} \}. \tag{26} \]

If, in addition to (21) and (23),
\[ K_b \leq \frac{1}{\varepsilon_M}, \tag{27} \]
and
\[ \kappa^{(d)}_{A_i} \cdot K_b \leq \frac{1}{\varepsilon_M}, \tag{28} \]
then
\[ \hat{b} = fl(\hat{b}^{(d)}) = b(1 + \kappa_b \varepsilon_M), \]
where
\[ |\kappa_b| \leq n + 5. \]

The above results are summarized in the following lemma:

**Lemma 1.** Let (21) and (23) hold, and let \( K_b \) be defined by (25). For all non-zero elements of the matrix \( A_i^{-1} \) from (8) computed according to Algorithm 1 and Remark 1, except for the element \([A_i^{-1}]_{ii}\), we have
\[ [\hat{A}_i^{-1}]_{kl} = [A_i^{-1}]_{kl}(1 + \kappa_{kl} \varepsilon_M), \quad |\kappa_{kl}| \leq (2n + 7). \]

For the computed element \( b = [A_i^{-1}]_{ii} \) we have the following: if \( K_b \gg 1 \), then
\[ \hat{b} = b(1 + \kappa_b \varepsilon_M), \quad |\kappa_b| \leq (3n + 6) \cdot K_b + 2n + 7. \]

If \( K_b \gg 1 \) and if (27) and (28) hold, then
\[ \hat{b} = b(1 + \kappa_b \varepsilon_M), \quad |\kappa_b| \leq n + 5. \]

The forward error of the computed roots is bounded as follows:

**Theorem 2.** Let (21) and (23) hold, and let \( K_b \) be defined by (25). Let
\[ \hat{\lambda} = \lambda(1 + \kappa_\lambda \varepsilon_M) \]
be the root of \( u(x) \) computed according to Algorithm 1 and Remark 1. If \( K_b \gg 1 \), then
\[ |\kappa_\lambda| \leq 3\sqrt{n}((3n + 6) \cdot K_b + 2n + 7) + 3.18n \left( \sqrt{n} + 1 \right) + 4, \]
and if \( K_b \gg 1 \) and (27) and (28) hold, then
\[ |\kappa_\lambda| \leq (6n + 21)\sqrt{n} + 3.18n \left( \sqrt{n} + 1 \right) + 4. \]

**Proof.** Using the same notation as in [8, §3], the first summand in the above bound for \( \kappa_\lambda \) follows from [8, Theorems 5 and 6], while the second summand is the error bound for bisection from [10, §3.1]. \( \square \)
3.3 Choosing $d_j$

Finding values of $d_j$ which interpolate roots is not an easy task. Articles dealing with computing roots of polynomials usually assume that the initial approximations of the roots are known (see [5], [11]). Another approach, used in [1], is to define the polynomial neighborhood of $u(x)$ as the set of all polynomials with coefficients having $d_{in}$ common digits with the corresponding coefficients of $u(x)$, where $d_{in}$ is predefined input precision. Then, the root neighborhood is the set of the roots of all polynomials in the polynomial neighborhood of $u(x)$.

Since our polynomial is real with only real distinct root our proposal is simpler. Here are some heuristics:

- let $\bar{u}(x)$ be the reverse polynomial of the polynomial $u(x)$ from (10),

$$\bar{u}(x) = x^n u(1/x) = a_0 x^n + a_1 x^{n-1} + a_2 x^{n-2} + \cdots + a_{n-2} x^2 + a_{n-1} x + 1.$$ 

Since the roots of $\bar{u}(x)$ are the reciprocals of the roots of $u(x)$, we have two options for the values $d_j$:

- use the roots of $u'(x)$, or
- use the reciprocals of the roots of $\bar{u}'(x)$.

Depending on the magnitude of the roots, their distribution and relative gaps, one of the methods, or a combination, is expected to work, see Section 4 for examples.

3.4 Implementation of double the working precision

We tested three different implementations of double the working precision:

- convert all quantities to variable precision by Matlab command `sym` with parameter ‘f’, and then evaluate the respective formulas – this is 300 to 1000 times slower than standard precision.

- convert all quantities from standard 64 bit REAL(8) to 128 bit REAL(16) in Intel ifort [7], and then evaluate the respective formulas – this is only 3 times slower,

- evaluate respective formulas by using extended precision routines add2, sub2, mul2, div2, and sqrt2 from [3] – this is $O(10)$ times slower. In these routines double the working precision is simulated by keeping each number as a pair consisting of higher and lower part of mantissa. For example, let

$$[z, zz] = add2(x, xx, y, yy)$$

where all quantities are floating-point numbers with $t$ binary-digits mantissa. Then

$$|z + zz - [(x + xx) + (y + yy)]| \leq (|x + xx| + |y + yy|)2^{-2(t-1)}.$$ 

If $xx = 0$ and $yy = 0$, then (exactly) $z + zz = x + y$. We see that this is nearly equivalent to using double the working precision (the precision is $\frac{1}{2}\varepsilon^2_M$ instead of $\varepsilon^2_M$).

The evaluation of the polynomial $u(x)$ can also be successfully performed by Compensated Horner scheme from [5, Algorithm 4], where both quantities $h$ and $c$ from this algorithm must be preserved for subsequent computations by extended precision routines.
4 Numerical Examples

We illustrate our algorithm with two numerically demanding examples. Here double the working precision in Algorithm 1 was implemented with extended precision routines from [3].

Example 1. The coefficients of Wilkinson polynomial $W_{18}$ are, row-wise:

$$
\begin{align*}
1 & \quad -171 & \quad 13566 \\
-662796 & \quad 2232382 & \quad -549789282 \\
10246937272 & \quad -147560703732 & \quad 1661573386473 \\
-1417053408923 & \quad 102417740732 & \quad -557921681547048 \\
2353125040549984 & \quad -7551527592063024 & \quad 17950712280921504 \\
-30321254007719424 & \quad 34012249593822720 & \quad -22376988058521600 \\
6402373705728000 & & \\
\end{align*}
$$

In this example the interpolating points $d_j$ can be computed by both ways described in Section 3.3, as roots of $u'(x)$ or as the reciprocals of the roots of $\bar{u}'(x)$. For example, in the latter case we have

$$
\max K_b = 214.5 \gg 1, \quad \max_j \{\text{cond}(u, d_j)\} = 2.62 \cdot 10^{14}, \quad K_\alpha = 26.8,
$$

so by Theorem 2, the roots of $W_{18}$ are computed by Algorithm 1 to (almost) full accuracy, in a forward stable manner.

The roots computed by Matlab [9] routine roots, MPSolve [1] (with 16 decimal digits), Algorithm 1 and Mathematica [14] with 100 digits of precision (properly rounded to 16 decimal digits), are, respectively:

| $\lambda^{(\text{roots})}$ | $\lambda^{(\text{MPSolve})}$ | $\lambda^{(\text{polyaheig,Math})}$ |
|-----------------------------|-----------------------------|-----------------------------|
| 18.00001193040660          | 18.0000000000000000        | 18                          |
| 16.99987506992020          | 16.99999999999993         | 17                          |
| 16.00057853967064          | 15.99999999999559         | 16                          |
| 14.99841877954789          | 15.00000000000043         | 15                          |
| 14.0028266587300           | 13.99999999999777         | 14                          |
| 12.99649084561071          | 12.99999999999819         | 13                          |
| 12.0030890986650           | 12.00000000000329         | 12                          |
| 10.99809154207482          | 11.00000000000163         | 11                          |
| 10.00081885564820          | 9.99999999998594          | 10                          |
| 8.999776556759201          | 9.00000000000055          | 9                           |
| 8.000029705840132          | 7.9999999999923           | 8                           |
| 7.000002735870642          | 7.0000000000000000        | 7                           |
| 5.999998227088450          | 5.99999999999999         | 6                            |
| 5.000000283698958          | 5.0000000000000000       | 5                           |
| 3.999999981972712          | 4.0000000000000000       | 4                           |
| 3.000000000132610          | 3.0000000000000000       | 3                           |
| 2.000000000018936          | 2.0000000000000000       | 2                           |
| 0.99999999999808           | 1.0000000000000000       | 1                           |

---

5 We use $W_{18}$ since all its coefficients are exactly stored as 64-bit floating-point numbers.
Table 1: Interpolating points $d_j$ and $\text{cond}(u,d_j)$.

| $j$ | $d_j$ | $\text{cond}(u,d_j)$ |
|-----|-------|----------------------|
| 1   | 5.277655813324802e+13 | 4                   |
| 2   | 1.75921860441599e+13  | $3.58 \cdot 10^{16}$ |
| 3   | 6.253878705847983e-16  | 12.4                |
| 4   | 2.627905491153268e-16  | 46.4                |

Since for every root, the corresponding quantity $K_b \gg 1$, the algorithm $\text{poly}\_a\_heig$ computes fully accurate roots, using only standard working precision to compute the corresponding matrix $\hat{A}^{-1}$ and its absolutely largest eigenvalue.

MPSolve requires input to be defined as integers. Also, MPSolve uses 21 decimal digits to guarantee and obtain relative accuracy of $10^{-13}$, and it uses 234 decimal digits to guarantee and obtain 30 accurate digits.

The Accurate Newton’s method from [5, Algorithm 6] also computes the roots of $W_{18}$ to full accuracy as described in [5, Theorem 6]. However, the starting points $x_0$ which satisfy the conditions of [5, Theorem 6], must be chosen with greater care and must be relatively close to the desired root (for example, $x_0 = 17.1$ to obtain $\lambda_2 = 17$, or $x_0 = 1.1$ to obtain $\lambda_{18} = 1$. Since the Accurate Newton’s method takes on average 6 steps to convergence for each root, it needs approximately $12n^2$ effective extended precision computations, while our algorithm needs in this case $5n^2$ extended precision computations to compute the matrix $\hat{A}$.

The results for $W_{20}$ are similar.

Example 2. Consider the polynomial $u$ of degree 5 with the coefficients

$$
\begin{align*}
1.000000000000000e + 00 \\
-2.028240960365167e + 31 \\
7.136238463529799e + 44 \\
-6.277101735386680e + 57 \\
4.181389724724491e + 42 \\
-6.189700196426900e + 26
\end{align*}
$$

or $\text{sym}(u,'f')$

$$
\begin{align*}
1 & \\
-20282409603651670423947251286016 \\
713623846352979940529142984724747568191373312 \\
-62771017353866800669375019691256932431111159424202737451008 \\
4181389724724490601097907890741292883247104 \\
-618970019642690000010608640
\end{align*}
$$

In this example the interpolating points $d_j$ are efficiently computed as the reciprocals of the roots of $\bar{u}'(x)$. The values $d_j$ and $\text{cond}(u,d_j)$ from (11) are given in Table 1.

For the decreasingly ordered roots of $u$, $\lambda_k$, $k = 1, 2, 3, 4, 5$, the corresponding quantities $K_k$ from (25), $\kappa_{\hat{A}_i}^{(d)}$ from (26) and their respective products from (28), all rounded up, are given in Table 2.
Table 2: Values $K_b$, $\kappa_{A_i}^{(d)}$ and $\kappa_{A_i}^{(d)} \cdot K_b$.

| $k$ | $K_b$ | $\kappa_{A_i}^{(d)}$ | $\kappa_{A_i}^{(d)} \cdot K_b$ |
|-----|-------|----------------------|-------------------------------|
| 1   | 1     | $3.6 \cdot 10^{17}$  | $3.6 \cdot 10^{17}$          |
| 2   | $3.01 \cdot 10^{15}$ | $4.7 \cdot 10^2$  | $1.42 \cdot 10^{18}$         |
| 3   | $3.01 \cdot 10^{15}$ | $4.7 \cdot 10^2$  | $1.42 \cdot 10^{18}$         |
| 4   | 12.6  | $3.58 \cdot 10^{17}$ | $4.48 \cdot 10^{18}$         |
| 5   | 12.6  | $3.58 \cdot 10^{17}$ | $4.48 \cdot 10^{18}$         |

We see that the condition (27) is always fulfilled. Also, $K_\alpha = 1$ from (18), so (23) is fulfilled.

The condition (28) does not hold literally. However, we have $\kappa_{A_i}^{(d)} \cdot K_b \gg \frac{1}{\varepsilon_M}$, which is sufficient to obtain almost full accuracy.

The roots computed by Matlab [9] routine roots, MPSolve [1] (with 16 decimal digits), Algorithm [1] and Mathematica [14] with 100 digits of precision (properly rounded to 16 decimal digits), are, respectively:

| $\lambda^{\text{roots}}$ | $\lambda^{\text{MPSolve}}$ | $\lambda^{\text{poly,aheig,Math}}$ |
|-------------------------|----------------------------|-----------------------------------|
| $2.028240960365167e+31$ | $2.028240960365167e+31$   | $2.028240960365167e+31$           |
| $1.759218604441600e+13 + 1.538e+8i$ | $1.759218604441608e+13$ | $1.759218623050247e+13$          |
| $1.759218604441600e+13 - 1.538e+8i$ | $1.759218604441591e+13$ | $1.759218585832953e+13$          |
| 0                        | $4.440892098500624e-16$ | $4.440892098500624e-16$          |
| 0                        | $2.220446049250314e-16$ | $2.220446049250314e-16$          |

We see that the roots computed by Algorithm [1] coincide fully with roots computed by Mathematica. Here, in addition to the elements $\hat{z}^{(d)}$ and $\hat{\alpha}^{(d)}$ of the matrix $\hat{A}$, the element $b$ of $\hat{A}^{-1}$ was computed in double the working precision.

Again, MPSolve requires input to be defined as integers, and it uses 21 decimal digits to guarantee and obtain relative accuracy of $10^{-14}$, and uses 234 decimal digits to guarantee 30 accurate digits.

Here the Accurate Newton’s method from [5] Algorithm 6] also computes the roots to full accuracy, provided the respective starting points are chosen with greater care. However, the conditions of [5] Theorem 6] cannot be used - for example, for the largest root $\lambda_1$, there is no starting point $x_0$ which satisfies the conditions, except $\lambda_1$ itself. For $\lambda_2$, the starting point $x_0$ which satisfies the conditions can differ from $\lambda_2$ in just last digit.

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