Novel Approach to Real Polynomial Root-finding and Matrix Eigen-solving

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Abstract

Univariate polynomial root-finding is both classical and important for modern computing. Frequently one seeks just the real roots of a polynomial with real coefficients. They can be approximated at a low computational cost if the polynomial has no nonreal roots, but typically nonreal roots are much more numerous than the real ones. We dramatically accelerate the known algorithms in this case by exploiting the correlation between the computations with matrices and polynomials, extending the techniques of the matrix sign iteration, and exploiting the structure of the companion matrix of the input polynomial. We extend some of the proposed techniques to the approximation of the real eigenvalues of a real nonsymmetric matrix.

Keywords: Polynomials, Real roots, Matrices, Matrix sign iteration, Companion matrix, Frobenius algebra, Square root iteration, Root squaring, Real eigenvalues, Real nonsymmetric matrix

1 Introduction

Assume a univariate polynomial of degree $n$ with real coefficients,

$$p(x) = \sum_{i=0}^{n} p_i x^i = p_n \prod_{j=1}^{n} (x - x_j), \quad p_n \neq 0, \quad (1.1)$$

which has $r$ real roots $x_1, \ldots, x_r$ and $s = (n - r)/2$ pairs of nonreal complex conjugate roots. In some applications, e.g., to algebraic and geometric optimization, one seeks just the $r$ real roots, which make up just a small fraction of all roots. This is a well studied subject (see [15] Chapter 15, [28], [34], and the bibliography therein), but we dramatically accelerate the known algorithms by combining and extending the techniques of [31] and [27]. At first our iterative Algorithm 1.1 reduces the original problem of real root-finding to the same problem for an auxiliary polynomial of degree $r$ having $r$ real roots. Our iterations converge with quadratic rate, and so we need only $k = O(b + d)$ iterations, assuming the tolerance $2^{-b}$ to the error norm of the approximation to the auxiliary polynomial (we denote it $v_k(x)$) and the minimal distance $2^{-d}$ of the nonreal roots from the real axis. The values $d$ and $k$ are large for the input polynomials with nonreal roots lying very close to the real axis, but our techniques of Remark 1.4 enable us to handle such harder inputs as
well. The known algorithms approximate the roots of \(v_k(x)\) at a low arithmetic cost, and having these approximations computed, we recover the \(r\) real roots of the input polynomial \(p(x)\). Overall we perform \(O(kn \log(n))\) arithmetic operations. This arithmetic cost bound is quite low, but in the case of large degree \(n\), the algorithm is prone to numerical problems, and so we devise dual Algorithms 4.2 and 4.3 to avoid the latter problems. This works quite well according to our test results, but formal study of the issue and of the Boolean complexity of the algorithm is left as a research challenge.

Let us comment briefly on the techniques involved and the complexity of the latter algorithms. They perform computations in the Frobenius matrix algebra generated by the companion matrix of the input polynomial. By using FFT and exploiting the structure of the matrices in the algebra, one can operate with them as fast as with polynomials. Real polynomial root-finding is reduced to real eigen-solving for the companion matrix. Transition to matrices and the randomization techniques, extended from [27, Section 5], streamline and simplify the iterative process of Algorithm 4.1. Now this process outputs an auxiliary \(r \times r\) matrix \(L\) whose eigenvalues are real and approximate the \(r\) real eigenvalues of the companion matrix. It remains to apply the QR algorithm to the matrix \(L\), at the arithmetic cost \(O(r^3)\) (cf. [11, page 359]), dominated if \(r^3 = O(k n \log(n))\).

The algorithm can be immediately applied to approximating all the real eigenvalues of a real nonsymmetric \(n \times n\) matrix by using \(O(kn^3)\) arithmetic operations. We point out a direction to potential decrease of this complexity bound to \(O((k+n)n^2)\) by means of similarity transformation to rank structured representation. Maintaining such representation would require additional research, however, and we propose a distinct novel algorithm. It approximates all real eigenvalues of an \(n \times n\) matrix by using \(O(m n^2)\) arithmetic operations (see Algorithm 5.1), and this bound decreases to \(O(m n)\) for the companion and various generalized companion matrices. Here \(m\) denotes the number of iterations required for the convergence of the basic iteration of the algorithm. Generally this number grows versus Algorithm 4.2 but remains reasonable for a large class of input matrices.

We engage, extend, and combine the number of efficient methods available for complex polynomial root-finding, particularly the ones of [31] and [27], but we also propose new techniques and employ some old methods in novel and nontrivial ways. Our Algorithm 4.1 streamlines and substantially modifies [31, Algorithm 9.1] by avoiding the stage of root-squaring and the application of the Cayley map. Some techniques of Algorithm 4.2 are implicit in [27, Section 5], but we specify a distinct iterative process, employ the Frobenius matrix algebra, extend the matrix sign iteration to real eigen-solving, employ randomization and the QR algorithm, and include the initial acceleration by scaling. Our Algorithm 4.4 naturally extends Algorithms 4.1 and 4.2 but we prove that this extension is prone to the problems of numerical stability, and our finding can be applied to the similar iterations of [8] and [8] as well. Algorithm 4.5 can be linked to Algorithm 4.1 and hence to [27, Section 5], but incorporates some novel promising techniques. Our simple recipe for real root-finding by means of combining the root radii algorithm with Newton’s iteration in Algorithm 4.6 and even the extension of our Algorithm 4.2 to the approximation of real eigenvalues of a real nonsymmetric matrix are also novel and promising. Some of our algorithms take advantage of combining the power of operating with matrices and polynomials (see Remarks 4.9 and 4.12). Finding their deeper synergistic combinations is another natural research challenge, traced back to [18] and [2]. Our coverage of the complex plane geometry and various rational transformations of the variable and the roots can be of independent interest.

Hereafter “flops” stands for “arithmetic operations”, “lc(p)” stands for “the leading coefficient of \(p(x)\)”, \(D(X, r) = \{x : |x - X| \leq r\}\) and \(C(X, r) = \{x : |x - X| = r\}\) denote a disc and a circle on the complex plane, respectively. We write \(\|\sum_i v_i x^i\|_q = (\sum_i |v_i|^q)^{1/q}\) for \(q = 1, 2\) and \(\|\sum_i v_i x^i\|_{\infty} = \max_i |v_i|\). A function is in \(\tilde{O}(f(bc))\) if it is in \(O(f(bc))\) up to polylogarithmic factors in \(b\) and \(c\). \(\text{agcd}(u, v)\) denotes an approximate greatest common divisor of two polynomials \(u(x)\) and \(v(x)\) (see [1] on definitions and algorithms).
2 Some Basic Results for Polynomial Computations

2.1 Mappings of the Variables and the Roots

Some important maps of the roots of a polynomial can be computed at a linear or nearly linear cost.

**Theorem 2.1.** (Root Inversion, Shift and Scaling, cf. [22].) Given a polynomial \( p(x) \) of \((1.1)\) and two scalars \( a \) and \( b \), we can compute the coefficients of the polynomial \( q(x) = p(ax + b) \) by using \( O(n \log(n)) \) flops. We need only \( 2n - 1 \) flops if \( b = 0 \). Reversing a polynomial inverts all its roots involving no flops, that is, \( p_{rev}(x) = x^n p(1/x) = \sum_{i=0}^{n} p_i x^{n-i} = p_n \prod_{j=1}^{n} (1 - xx_j) \).

**Theorem 2.2.** (Root Squaring, cf. [12,].) (i) Let a polynomial \( p(x) \) of \((1.1)\) be monic. Then \( q(x) = (-1)^n p(\sqrt{x})p(-\sqrt{x}) = \prod_{j=1}^{n} (x - x_j^2) \), and (ii) one can evaluate \( p(x) \) at the \( k \)-th roots of unity for \( k > 2n \) and then interpolate to \( q(x) \) by using \( O(n \log(n)) \) flops.

Recursive root-squaring is prone to numerical problems because the coefficients of the iterated polynomials very quickly span many orders of magnitude. One can counter this deficiency by using a special tangential representation of the coefficients and intermediate results (cf. [16]).

**Theorem 2.3.** (Cayley Maps.) The maps \( y = (x - \sqrt{-1}i)/(x + \sqrt{-1}i) \) and \( x = \sqrt{-1}(y + 1)/(y - 1) \) send the real axis \( \{ x : x \text{ is real} \} \) onto the unit circle \( C(0, 1) = \{ y : |y| = 1 \} \), and vice versa.

**Theorem 2.4.** (Möbius Maps.) (i) The maps \( y = \frac{1}{2}((\hat{x} + 1/\hat{x}), \hat{x} = \hat{y} + \sqrt{\hat{y}^2 - 1} \) and \( y = \frac{1}{2}(x - 1/x) \), \( x = y + \sqrt{y^2 - 1} \) send the unit circle \( C(0, 1) = \{ x : |x| = 1 \} \) to the line intervals \([-1,1] \) \{ \hat{y} : \Re[y] = 0, -1 \leq \hat{y} \leq 1 \} \) [14, equation (14)] and \( y = p(x)p(-x) = \prod_{j=1}^{n} (y - \hat{y}) \) (cf. [3, equation (14)]). Fix a complex \( \phi \) and interpolation at the Chebyshev nodes, and then the application of the algorithms of [17] or [20] yields the claimed cost bounds, even though the paper [17] slightly overestimates the cost bound of its interpolation algorithm.

**Theorem 2.5.** (Error of Möbius Iteration.) Fix a complex \( x = x^{(0)} \) and define the iterations

\[
x^{(h+1)} = \frac{1}{2}(x^{(h)} + 1/x^{(h)}) \quad \text{and} \quad \gamma = \sqrt{-1} \quad \text{for} \quad h = 0, 1, \ldots, (2.1)
\]

\[
x^{(h+1)} = \frac{1}{2}(x^{(h)} - 1/x^{(h)}) \quad \text{and} \quad \gamma = 1 \quad \text{for} \quad h = 0, 1, \ldots, (2.2)
\]

The values \( x^{(h)}, \gamma \) are real for all \( h \) if \( x^{(0)} \gamma \) is real. Otherwise \( |x^{(h)} - \text{sign}(x)\sqrt{-1}/\gamma| \leq \frac{2x^{(h)}}{1 - \tau} \) for \( \tau = \frac{|x - \text{sign}(x)}{x + \text{sign}(x)} \) and \( h = 0, 1, \ldots \).

**Proof.** The bound is from [3, page 500]) under (2.1), that is, for \( \gamma = \sqrt{-1} \), and is readily extended to the case of (2.2), that is, for \( \gamma = 1 \).

2.2 Root Radii Approximation and Proximity Tests

**Theorem 2.6.** (Root Radii Approximation.) Assume a polynomial \( p(x) \) of \((1.1)\) and two real scalars \( c > 0 \) and \( d \). Define the \( n \) root radii \( r_j = |x_k| \) for \( j = 1, \ldots, n \), distinct \( k_1, \ldots, k_n \), and \( r_1 \geq r_2 \geq \cdots \geq r_n \). Then, by using \( O(n \log^2(n)) \) flops, we can compute \( n \) approximations \( \tilde{r}_j \) such that \( \tilde{r}_j \leq r_j \leq (1 + c/n^d)\tilde{r}_j \), for \( j = 1, \ldots, n \).
Proof. (Cf. [33, Section 4], [15 Section 15.4].) At first fix a sufficiently large integer \(k\) and apply \(k\) times the root-squaring of Theorem 2.2 by using \(O(kn \log (n))\) flops. Then apply the algorithm of [33] to approximate all root radii \(r_j^{(k)} = r_j^{2^k}, j = 1, \ldots, n\), of the output polynomial \(p_k(x)\) within a factor of \(2n\) by using \(O(n)\) flops. Hence the root radii \(r_1, \ldots, r_n\) are approximated within a factor of \((2n)^{1/2^k}\), which is \(1 + c/n^d\) for \(k\) of order \(\log(n)\).

Alternatively one can estimate the root radii by applying Gerschgorin theorem to the companion matrix of a polynomial \(p(x)\), defined in Section 4.2 (see [7]) or by using heuristic methods (see [3]). Next we approximate the largest root radius \(r_1\) of \(p(x)\) at a lower cost. Applying the same algorithms to the reverse polynomial \(p_{rev}(x)\) yields the smallest root radius \(r_n\) of \(p(x)\) (cf. Theorem 2.1).

Theorem 2.7. (See [32].) Assume a polynomial \(p(x)\) of degree \(n\). Write \(r_1 = \max_{j=1}^n |x_j|, r_n = \min_{j=1}^n |x_j|, \) and \(\gamma^+ = \max_{i=1}^n |p_{n-i}/p_n|\). Then \(\gamma^+ / n \leq r_1 \leq 2\gamma^+\).

Theorem 2.8. (See [23].) For \(\epsilon = 1/2^b > 0\), one only needs \(a(n, \epsilon) = O(n + b \log(b))\) flops to compute an approximation \(r_{1, \epsilon}\) to the root \(r_1\) radii of \(p(x)\) such that \(r_{1, \epsilon} \leq r_1 \leq 5(1 + \epsilon)r_{1, \epsilon}\). In particular, \(a(n, \epsilon) = O(n)\) for \(b = O(n/\log(n))\), and \(a(n, \epsilon) = O(n \log(n))\) for \(b = O(n)\).

The latter theorem and the heuristic proximity test below can be applied even where a polynomial \(p(x)\) is defined by a black box subroutine for its evaluation rather than by its coefficients.

By shifting and scaling the variable (cf. Theorem 2.1), we can move all roots of \(p(x)\) into a fixed disc, e.g., \(D(0, 1) = \{x : |x| \leq 1\}\). The smallest root radius \(r_n\) of the polynomial \(q(x) = p(x - c)\) for a complex point \(c\) denotes the minimum distance of the roots from this point. Approximation of this distance is called proximity test at the point \(c\). Besides Theorems 2.7 and 2.8 one can apply heuristic proximity test at a point \(c\) by means of Newton’s iteration,

\[
y_0 = c, \quad y^{(h+1)} = y^{(h)} - p(y^{(h)}/p(y^{(h)}), \quad h = 0, 1, \ldots
\]

(2.3)

If \(c\) approximates a simple isolated root, the iteration refines this approximation very fast.

Theorem 2.9. (See [32, Corollary 4.5].) Suppose both discs \(D(y_0, r)\) and \(D(y_0, r/s)\) for \(s \geq 5n^2\) contain a single simple root \(y\) of a polynomial \(p = p(x)\) of degree \(n\). Then Newton’s iteration \(y_{k+1}\) converges to this root right from the start, so that \(|y_k - y| \leq 8|y_0 - y|/2^k\).

By exploiting the correlations between the coefficients of a polynomial and the power sums of its roots, the paper [30] had weakened the above assumption that \(s \geq 5n^2\) to allow any constant \(s > 1\). By recursively squaring the variable and the roots \(O(\log(n))\) times (as in the proof of Theorem 2.6), one can allow any \(s\) below \(1 + c/n^d\), for any pair of real constants \(c > 0\) and \(d\).

2.3 Two Auxiliary Algorithms for the First Polynomial Root-finder

Theorem 2.10. (Root-finding Where All Roots Are Real.) The modified Laguerre algorithm of [10] converges to all roots of a polynomial \(p(x)\) of degree \(n\) right from the start, uses \(O(n)\) flops per iteration, and therefore approximates all \(n\) roots within \(\epsilon = 1/2^b\) by using \(O(\log(b))\) iterations and performing \(O(n \log(b))\) flops overall. This asymptotic cost bound is optimal and is also supported by the alternative algorithms of [6] and [4].

Theorem 2.11. (Splitting a Polynomial into Two Factors Over a Circle, cf. [23] or [15], Chapter 15.) Suppose a polynomial \(t(x)\) of degree \(n\) has \(r\) roots inside the circle \(C(0, \rho)\) and \(n - r\) roots outside the circle \(C(0, R)\) for \(R/\rho \geq 1 + 1/n\). Let \(c = 1/2^b\) for \(b \geq n\). Then by performing \(O((\log^2(n) + \log(b) \log(n))\) flops (that is, \(O(n \log^2(n))\) flops for \(b = O(\log^2(n))\)), with a precision of \(O(b)\) bits, we can compute two polynomials \(\tilde{f}\) and \(\tilde{g}\) such that \(|p - \tilde{f}\tilde{g}|_q \leq \epsilon|p|_q\) for \(q = 1, 2\) or \(\infty\), the polynomial \(\tilde{f}\) of degree \(r\) has \(r\) roots inside the circle \(C(0, 1)\), and the polynomial \(\tilde{g}\) of degree \(n - r\) has \(n - r\) roots outside this circle. (iii) By recursively squaring the variable and the roots \(O(\log(n))\) times (by using \(O(n \log^2(n))\) flops), one can extend the result of part (ii) to the case where \(R/\rho \leq 1 + 1/n\), for any pair of positive constants \(c\) and \(d\).
3 Root-finding As Eigen-solving and Basic Definitions and Results for Matrix Computations

3.1 Some Basic Definitions for Matrix Computations

\( M^T = (m_{ji})_{i,j=1}^{m,n} \) is the transpose of a matrix \( M = (m_{ij})_{i,j=1}^{m,n} \). \( M^H \) is its Hermitian transpose. 
\( I = I_n = (e_1 | e_2 | \ldots | e_n) \) is the \( n \times n \) identity matrix, whose columns are the \( n \) coordinate vectors \( e_1, e_2, \ldots, e_n \). \( \text{diag}(b_j)_{j=1}^{s} = \text{diag}(b_1, \ldots, b_s) \) is the \( s \times s \) diagonal matrix with the diagonal entries \( b_1, \ldots, b_s \). \( R(M) \) is the range of a matrix \( M \), that is, the linear space generated by its columns. A matrix of full column rank is a matrix basis of its range.

A matrix \( Q \) is unitary if \( Q^HQ = I \) or \( QQ^H = I \). \( (Q, R) = (Q(M), R(M)) \) for an \( m \times n \) matrix \( M \) of rank \( n \) denotes a unique pair of unitary \( m \times n \) matrix \( Q \) and upper triangular \( n \times n \) matrix \( R \) such that \( M = QR \) and all diagonal entries of the matrix \( R \) are positive [1] Theorem 5.2.2.

\( M^+ \) is the Moore–Penrose pseudo inverse of \( M \) [1] Section 5.5.4. An \( n \times m \) matrix \( X = M^{(l)} \) is a left inverse of an \( n \times n \) matrix \( M \) if \( XM = I_n \). \( M^{(i)} = M^+ \) for a matrix \( M \) of full rank. \( M^{(i)} = M^H \) for a unitary matrix \( M \). \( M^{(i)} = M^+ = M^{-1} \) for a nonsingular matrix \( M \).

Definition 3.1. \( S \) is the invariant subspace of a square matrix \( M \) if \( M \mathbb{S} = \{Mv : v \in \mathbb{S} \} \subseteq \mathbb{S} \). A scalar \( \lambda \) is an eigenvalue of a matrix \( M \) associated with an eigenvector \( v \) if \( Mv = \lambda v \). All eigenvectors associated with an eigenvalue \( \lambda \) of \( M \) form an eigenspace \( \mathbb{S}(M, \lambda) \), which is an invariant space. Its dimension \( d \) is the geometric multiplicity of \( \lambda \). The eigenvalue is simple if its multiplicity is 1. The set \( \Lambda(M) \) of all eigenvalues of a matrix \( M \) is called its spectrum.

3.2 The Companion Matrix and the Frobenius Algebra

\[
C_p = \begin{pmatrix}
0 & -p_0/p_n \\
1 & -p_1/p_n \\
\vdots & \vdots \\
0 & -p_{n-1}/p_n \\
1 & -p_{n-2}/p_n \\
\end{pmatrix}
\]

is the companion matrices of the polynomial \( p(x) \) of [1]. \( p(x) = cC_p(x) = \det(xI_n - C_p) \) is the characteristic polynomial of \( p(x) \). Its roots form the spectrum of \( C_p \), and so real root-finding for the polynomial \( p(x) \) turns into real eigen-solving for the matrix \( C_p \).

Theorem 3.1. (The Cost of Computations in the Frobenius Matrix Algebra, cf. [3] or [2].) The companion matrix \( C_p \in \mathbb{C}^{n \times n} \) of a polynomial \( p(x) \) of [1] generates Frobenius matrix algebra. One needs \( O(n) \) flops for addition, \( O(n \log(n)) \) flops for multiplication, and \( O(n \log^2(n)) \) flops for inversion in this algebra. One needs \( O(n \log(n)) \) flops to multiply a matrix in this algebra by a vector.

3.3 Decreasing the Size of an Eigenproblem

Next we reduce eigen-solving for the matrix \( C_p \) to the study of its invariant space generated by the \( r \) eigenspaces associated with the \( r \) real eigenvalues. The following theorem is basic for this step.

Theorem 3.2. (Decreasing the Eigenproblem Size to the Dimension of an Invariant Space, cf. [3], Section 2.1.) Let \( U \in \mathbb{C}^{n \times r} \), \( R(U) = \mathcal{U} \), and \( M \in \mathbb{C}^{n \times n} \). Then (i) \( \mathcal{U} \) is an invariant space of \( M \) if and only if there exists a matrix \( L \in \mathbb{C}^{k \times k} \) such that \( MU = UL \) or equivalently if and only if \( L = U^{(l)} MU \), (ii) the matrix \( L \) is unique (that is, independent of the choice of the left inverse \( U^{(l)} \)) if \( U \) is a matrix basis for the space \( \mathcal{U} \), (iii) \( \Lambda(L) \subseteq \Lambda(M) \), (iv) \( L = U^{H} MU \) if \( U \) is a unitary matrix, and (v) \( MUv = \lambda Uv \) if \( Lv = \lambda v \).

By virtue of the following theorem, a matrix function shares its invariant spaces with the matrix \( C_p \), and so we can facilitate the computation of the desired invariant space of \( C_p \) if we reduce the task to the case of an appropriate matrix function, for which the solution is simpler.
Theorem 3.3. (The Eigenproblems for a Matrix and Its Function.) Suppose $M$ is a square matrix, a rational function $f(\lambda)$ is defined on its spectrum, and $M\mathbf{v} = \lambda \mathbf{v}$. Then (i) $f(M)\mathbf{v} = f(\lambda)\mathbf{v}$. (ii) Let $U$ be the eigenspace of the matrix $f(M)$ associated with its eigenvalue $\mu$. Then this is an invariant space of the matrix $M$ generated by its eigenspaces associated with all its eigenvalues $\lambda$ such that $f(\lambda) = \mu$. (iii) The space $U$ is associated with a single eigenvalue of $M$ if $\mu$ is a simple eigenvalue of $f(M)$.

Proof. We readily verify part (i), which implies parts (ii) and (iii).  \square

Suppose we have computed a matrix basis $U \in \mathbb{C}^{n \times r}$ for an invariant space $U$ of a matrix function $f(M)$ of an $n \times n$ matrix $M$. By virtue of Theorem 3.3, this is a matrix basis of an invariant space of the matrix $M$. We can first compute a left inverse $U^{(l)}$ or the orthogonalization $Q = Q(U)$ and then approximate the eigenvalues of $M$ associated with this eigenspace as the eigenvalues of the $r \times r$ matrix $L = U^{(l)}MU = QHMQ$ (cf. Theorem 3.2).

Given an approximation $\tilde{\mu}$ to a simple eigenvalue of a matrix function $f(M)$, we can compute an approximation $\tilde{\mathbf{u}}$ to an eigenvector $\mathbf{u}$ of the matrix $f(M)$ associated with this eigenvalue, recall from part (iii) of Theorem 3.3 that this is also an eigenvector of the matrix $M$, associated with its simple eigenvalue, and approximate this eigenvalue by the Rayleigh Quotient $\frac{\tilde{\mathbf{u}}^T M \tilde{\mathbf{u}}}{\tilde{\mathbf{u}}^T \tilde{\mathbf{u}}}$.

3.4 Some Maps in the Frobenius Matrix Algebra

Part (i) of Theorem 3.3 implies that for a polynomial $p(x)$ of (1.11) and a rational function $f(x)$ defined on the set $\{x_i\}_{i=1}^n$ of its roots, the rational matrix function $f(C_p)$ has the spectrum $\Lambda(f(C_p)) = \{f(x_i)\}_{i=1}^n$. In particular, the maps

$$C_p \rightarrow C_p^{-1}, \quad C_p \rightarrow aC_p + bI, \quad C_p \rightarrow C_p^2, \quad C_p \rightarrow \frac{C_p + C_p^{-1}}{2}, \quad and \quad C_p \rightarrow \frac{C_p - C_p^{-1}}{2}$$

induce the maps of the eigenvalues of the matrix $C_p$, and thus induce the maps of the roots of its characteristic polynomial $p(x)$ given by the equations

$$y = \frac{1}{x}, \quad y = ax + b, \quad y = x^2, \quad y = 0.5(x + 1/x), \quad and \quad y = 0.5(x - 1/x),$$

respectively. By using the reduction modulo $p(x)$, define the five dual maps

$$y = (1/x) \mod p(x), \quad y = ax + b \mod p(x), \quad y = x^2 \mod p(x), \quad y = 0.5(x + 1/x) \mod p(x), \quad and \quad y = 0.5(x - 1/x) \mod p(x),$$

where $y = y(x)$ denotes polynomials. Apply the two latter maps recursively, to define two iterations with polynomials modulo $p(x)$ as follows, $y_0 = x,$ $y_{n+1} = 0.5(y_n + 1/y_n) \mod p(x)$ (cf. (2.11)) and $y_0 = x,$ $y_{n+1} = 0.5(y_n - 1/y_n) \mod p(x)$ (cf. (2.22)), $h = 0, 1, \ldots$, More generally, define the iteration $y_0 = x,$ $y_{n+1} = ay_n + b/y_n \mod p(x),$ $h = 0, 1, \ldots$, for any pair of scalars $a$ and $b$.

4 Real Root-finders

4.1 Möbius Iteration

Theorem 2.5 implies that right from the start of iteration (2.2) the values $x^{(h)}$ converge fast to $\pm \sqrt{-1}$ unless the initial value $x^{(0)}$ is real, in which case all iterates $x^{(h)}$ are real. It follows that right from the start the values $y^{(h)} = (x^{(h)})^2 + 1$ converge fast to 0 unless $x^{(0)}$ is real, whereas all values $y^{(h)}$ are real and exceed 1 if $x^{(0)}$ is real. Write $t_h(y) = \prod_{j=1}^h (y - (x_j^{(h)})^2 - 1)$ and $v_h(y) = \prod_{j=1}^h (y - (x_j^{(h)})^2 - 1)$ for $h = 1, 2, \ldots$. The roots of the polynomials $t_h(y)$ and $v_h(y)$ are the images of all roots and of the real roots of the polynomial $p(x)$ of (1.11), respectively, produced by the composition of the maps (2.2) and $y^{(h)} = (x^{(h)})^2 + 1$. Therefore $t_h(y) \approx y^2 v_h(y)$ for large integers $h$ where the polynomial $v_h(y)$ has degree $r$ and has exactly $r$ real roots, all exceeding 1, and so for large integers $h$, the sum of the
The $r+1$ leading terms of the polynomial $t_h(y)$ closely approximates the polynomial $y^{2s}v_h(y)$. (To verify that the $2s$ trailing coefficients nearly vanish, we need just $2s$ comparisons.) The above argument shows correctness of the following algorithm. (One can similarly apply and analyze iteration (2.1).)

**Algorithm 4.1.** Möbius iteration for real root-finding.

**Input:** two integers $n$ and $r$, $0 < r < n$, and the coefficients of a polynomial $p(x)$ of equation (1.1) where $p(0) \neq 0$.

**Output:** approximations to the real roots $x_1, \ldots, x_r$ of the polynomial $p(x)$.

**Computations:**

1. Write $p_0(x) = p(x)$ and recursively compute the polynomials $p_{h+1}(y)$ such that $p_{h+1}(y) = p_h(x)p_h(-1/x)$ for $y = (x-1/x)/2$ and $h = 0, 1, \ldots$ (Part (ii) of Theorem 2.4 combined with Theorem 4.10 defines the images of the real and nonreal roots of the polynomial $p(x)$ for all $h$.)

2. Periodically, at some selected Stages $k$, compute the polynomials

$$t_h(y) = (-1)^nq_k(\sqrt{y+1}) q_h(-\sqrt{y+1})$$

where $q_k(y) = p_k(y)/l_0(p_k)$ (cf. Theorems 2.1 and 2.2). When the integer $k$ becomes large enough, so that $2s$ trailing coefficients of the polynomial $q_k(x)$ vanish or nearly vanish, delete these coefficients and divide the resulting polynomial by $x^{2s}$, to obtain a polynomial $v_k(x)$ of degree $r$, which is an approximate factor of the polynomial $t_k(x)$ and has $r$ real roots on the ray $\{x: x \geq 1\}$.

3. Apply one of the algorithms of [8], [2], and [10] (cf. Theorem 2.10) to approximate the $r$ roots of the polynomial $v_k(x)$.

4. Extend the descending process from [19], [24] and [3] to recover approximations to the $r$ roots $x_1, \ldots, x_r$ of the polynomial $p_0(x) = p(x)$. At first, having the $r$ roots $w_j$ of the polynomial $v_k(x)$ approximated, compute the $2r$ values $\pm w_j^2 - 1$, $j = 1, \ldots, r$. Then select among them the $r$ values $x_j^{(k)}$, $j = 1, \ldots, r$, by applying one of the proximity tests of Section 2.2 to the polynomial $q_k(y)$ at all of these $2r$ values. (The $r$ selected values approximate the $r$ common real roots of the polynomials $q_k(y)$ and $p_k(y)$.) Compute the $2r$ values $x_j^{(k)} \pm \sqrt{(x_j^{(k)})^2 + 1}$, $j = 1, \ldots, r$. By virtue of part (i) of Theorem 2.4, $r$ of these values approximate the $r$ real roots of the polynomial $p_{k-1}(x)$. Select these approximations by applying one of the proximity tests of Section 2.2 to the polynomial $p_{k-1}(x)$ at all of the $2r$ candidate values. Continue recursively to descend down to the $r$ real roots of $p_0(x) = p(x)$. The process is not ambiguous because only $r$ roots of the polynomial $p_0(x)$ are real for each $h$, by virtue of Theorem 2.4.

Like lifting Stage 1, descending Stage 4 involves order of $kn \log(n)$ flops, which also bounds the overall cost of performing the algorithm.

**Remark 4.1.** (Refinement by means of Newton’s iteration.) For every $h, k, k-1, \ldots, 0$, one can apply Newton’s iteration $x_{j,i+1}^{(h)} = x_{j,i}^{(h)} - p(x_j^{(h)})/p'(x_j^{(h)}), h = 0, 1, \ldots, i = 0, 1, \ldots, l$, concurrently at the $r$ approximations $x_j^{(h)}$, $j = 1, \ldots, r$, to the $r$ real roots of the polynomial $p_h(x)$. We can perform $l$ iteration loop by using $O(nl \log^2(r))$ flops, that is $O(n \log^2(r))$ flops per loop (cf. [22], Section 3.1), adding this to the overall arithmetic cost of order $kn \log(n)$ for performing the algorithm. We can perform the proximity tests of Stage 4 of the algorithm by applying Newton’s iteration at all $2r$ candidate approximation points. Having selected $r$ of them, we can continue applying the iteration at these points, to refine the approximations.

**Remark 4.2.** (Countering Degeneracy.) If $p(0) = p_0 = \cdots = p_m = 0 \neq p_{m+1}$, then we should output the real root $x_0 = 0$ of multiplicity $m$ and apply the algorithm to the polynomial $p(x)/x^m$ to approximate the other real roots. Alternatively we can apply the algorithm to the polynomial $q(x) = p(x-s)$ for a shift value $s$ such that $q(0) \neq 0$. With probability 1, $q(0) \neq 0$ for Gaussian random variable $s$, but we can approximate the root radii of the polynomial $p(x)$ (cf. Theorem 2.6) and then deterministically find a scalar $s$ such that $q(x)$ has no roots near 0.
Remark 4.3. (Saving the Recursive Steps of Stage 1.) The first goal of the algorithm is the computation of a polynomial $v_k(x)$ of degree $r$ that has $r$ real roots and is an approximate factor of the polynomial $t_k(x)$. If the assumptions of Theorem 2.11 are satisfied for $t(x) = t_k(x)$ for a smaller integer $k$ we can compute a polynomial $v_k(x)$ for this $k$ decreasing the overall computational cost. For a fixed $k$ we can verify the assumptions by using $O(n \log^2(n))$ flops (by applying the root radii algorithm of Theorem 2.6), and so it is not too costly to test even all integers $k$ in the range, unless the range is large. By using the binary search for the minimum integer $k$ satisfying Theorem 2.11 we would need only $O(\log(n))$ tests, that is, $O(n \log^3(n))$ flops.

Remark 4.4. (Handling the Nearly Real Roots.) The integer parameter $k$ and the overall arithmetic cost of performing the algorithm are large if the value $2^{-d} = \min_{j=r+1}^{n} |3x_j|$ is small. We can counter this deficiency by splitting out from the polynomial $t_k(x)$ its factor $v_{k,+}(x)$ of degree $r_+ > r$ that has $r_+$ real and nearly real roots if the other nonreal roots lie sufficiently far from the real axis. Our convergence analysis and the recipes for splitting out the factor $v_k(x)$ (including the previous remark) can be readily extended. If the integer $r_+$ is small, we can compute all the $r_+$ roots of the polynomial $v_{k,+}(x)$ at a low cost and then select the $r$ real roots among them. Even if the integer $r_+$ is large, but all of $r_+$ roots of the polynomial $v_{k,+}(x)$ lie on or close enough to the real axis, we can approximate these roots at a low cost by using the modified Laguerre algorithm of [10].

Remark 4.5. (The Number of Real Roots.) We assume that we know the number $r$ of the real roots (e.g., supplied by noncostly algorithms of computer algebra), but we can compute this number as a by-product of Stage 2, and similarly for our other algorithms. With a proper policy we can compute the integer $r$ by testing at most $2 + 2 \lceil \log_2(r) \rceil$ candidates in the range $[0, 2r - 1]$.

4.2 An Extended Matrix Sign Iteration

The known upper bounds on the condition numbers of the roots of the polynomials $p_k(y)$ grow exponentially as $k$ grows large (cf. [3 Section 3]). If the bounds are actually sharp, Algorithm 4.1 is prone to numerical stability problems already for moderately large integers $k$. We can avoid this potential deficiency by replacing the iteration of Stages 1 and 2 by the dual matrix iteration

$$Y_0 = C_p, \quad Y_{h+1} = 0.5(Y_h - Y_h^{-1}) \quad \text{for } h = 0, 1, \ldots, \quad (4.1)$$

It extends the matrix sign iteration $\hat{Y}_{h+1} = 0.5(\hat{Y}_h + \hat{Y}_h^{-1})$ for $h = 0, 1, \ldots$ (cf. [2.1], [2.2], part (ii) of our Theorem 2.3 and [13]) and maps the eigenvalues of the matrix $Y_0 = C_p$ according to (2.2).

So Stage 1 of Algorithm 4.1 maps the characteristic polynomials of the above matrices $Y_h$. Unlike the case of the latter map, working with matrices enables us to recover the desired real eigenvalues of the matrix $C_p$ by means of our recipes of Section 3 without recursive descending.

Algorithm 4.2. Matrix sign iteration modified for real eigen-solving.

**Input and Output** as in Algorithm 4.1, except that FAILURE can be output with a probability close to 0.

**Computations:**

1. Write $Y_0 = C_p$ and recursively compute the matrices $Y_{h+1}$ of (4.1) for $h = 0, 1, \ldots$ (2s eigenvalues of the matrix $Y_h$ converge to $\pm \sqrt{-1}$ as $h \to \infty$, whereas its $r = n - 2s$ other eigenvalues are real for all $h$, by virtue of Theorem 2.5.)

2. Fix a sufficiently large integer $k$ and compute the matrix $Y = Y_k^2 + I_n$. (The map $Y_0 = C_p \to Y$ sends all nonreal eigenvalues of $C_p$ into a small neighborhood of the origin 0 and sends all real eigenvalues of $C_p$ into the ray $\{ x : x \geq 1 \}$.)

3. Apply the randomized algorithms of [14] to compute the numerical rank of the matrix $Y$. The rank is at least $r$, and if it exceeds $r$, then go back to Stage 1. If it is equal to $r$, then generate a standard Gaussian random $n \times r$ matrix $G$ and compute the matrices $H = YQ(G)$ and $Q = Q(H)$. (The analysis of pre-processing with Gaussian random multipliers in [14], Section
Section 5.3 shows that, with a probability close to 1, the columns of the matrix \( Q \) closely approximate a unitary basis of the invariant space of the matrix \( Y \) associated with its \( r \) absolutely largest eigenvalues, which are the images of the real eigenvalues of the matrix \( C_p \).

Having this approximation is equivalent to having a small upper bound on the residual norm \( \| Y - Q Q^H Y \| \). Verify the latter bound. If the verification fails (which is unlikely), output FAILURE and stop the computations.

4. Otherwise compute and output approximations to the \( r \) eigenvalues of the \( r \times r \) matrix \( L = Q^H C_p Q \). They approximate the real roots of the polynomial \( p(x) \). (Indeed, by virtue of Theorem 3.3, \( Q \) is an approximate matrix basis for the invariant space of the matrix \( C_p \) associated with its \( r \) real eigenvalues. Therefore, by virtue of Theorem 3.2, the \( r \) eigenvalues of the matrix \( L \) approximate the \( r \) real eigenvalues of the matrix \( C_p \).)

Stages 1 and 2 involve \( O(k n \log^2(n)) \) flops by virtue of Theorem 3.1. This exceeds the estimate for Algorithm 4.1 by a factor of \( \log(n) \). Stage 3 adds \( O(n r^2) \) flops and the cost \( a_{rn} \) of generating \( n \times r \) standard Gaussian random matrix. The cost bounds are \( O(r^3) \) at Stage 4 and \( O((k n \log^2(n) + n r^2) + a_{rn}) \) overall.

**Remark 4.6.** (Counting Real Eigenvalues.) The binary search can produce the number of real eigenvalues as the numerical rank of the matrices \( Y_k^2 + I \) when this rank stabilizes.

**Remark 4.7.** (Acceleration by Using Random Circulant Multiplier.) We can decrease the arithmetic cost of Stage 3 to \( a_{rn} + O(n \log(n)) \) and can perform only \( O(k n \log^2(n) + n r^2) + a_{rn} \) flops overall if we replace an \( n \times r \) standard Gaussian random multiplier by the product \( \Omega P \) where \( \Omega \) and \( C \) are \( n \times n \) matrices, \( \Omega \) is the matrix of the discrete Fourier transform, \( C \) is a random circulant matrix, and \( P \) is an \( n \times 1 \) random permutation matrix, for a sufficiently large \( l \) order \( r \log(r) \). See [14, Section 11], [26, Section 6] for the analysis and for the supporting probability estimates. They are only slightly less favorable than in the case of a Gaussian random multiplier.

**Remark 4.8.** (Acceleration by Means of Scaling.) We can dramatically accelerate the initial convergence of Algorithm 4.4 by applying determinantal scaling (cf. [13]), that is, by computing the matrix \( Y_1 \) as follows, \( Y_1 = 0.5(\nu Y_0 - (\nu Y_0)^{-1}) \) for \( \nu = 1/| \det(Y_0)|^{1/n} = |p_n|/p_0 \), \( Y_0 = C_p \).

**Remark 4.9.** (Hybrid Matrix and Polynomial Algorithms.) Can we modify Algorithm 4.4 to keep its advantages but to decrease the arithmetic cost of its Stage 1 to the level \( kn \log(n) \) of Algorithm 4.1? Let us do this for a large class of input polynomials by applying a hybrid algorithm that combines the power of Algorithms 4.1 and 4.2. First note that we can replace iteration (4.1) by any of the iterations \( Y_{h+1} = 0.5(Y_h^3 + 3Y_h) \) and \( Y_{h+1} = -0.125(3Y_h^3 + 10Y_h^3 + 15Y_h) \) for \( h = 0, 1, \ldots \) provided that all or almost all nonreal roots of the polynomial \( p(x) \) lie in the discs \( D(\pm \sqrt{-1}, 1/2) \). Indeed right from the start, the iterations send the nonreal roots lying in these discs toward the two points \( \pm \sqrt{-1} \) with quadratic and cubic convergence rates, respectively. (To prove this, extend the proof of [3, Proposition 4.1].) Both iterations keep the real roots real, involve no inversions, and use \( O(n \log(n)) \) flops per loop. These observations suggest the following policy. Perform the iterations of Algorithm 4.1 as long as the outputs are not corrupted by rounding errors. (Choose the number of iterations of Algorithm 4.1 heuristically.) For a large class of inputs, the iterations (in spite of the above limitation on their number) bring the images of the nonreal eigenvalues of \( C_p \) into the basin of convergence of the inversion-free matrix iterations above. Now let \( q_h(x) \) denote the auxiliary polynomial output by Algorithm 4.1. Then approximate its real roots by applying one of the inversion-free iterations above to its companion matrix \( C_{q_h} \). Descend from these roots to the real roots of the polynomial \( p(x) \) as in Algorithms 4.4.

### 4.3 Numerical Stabilization of the Extended Matrix Sign Iteration

The images of nonreal eigenvalues of the matrix \( C_p \) converge to \( \pm \sqrt{-1} \) in the iteration of Stage 1 of Algorithm 4.2, but the images of some real eigenvalues of \( C_p \) can come close to 0, and then the next step of the iteration would involve an ill conditioned matrix \( Y_h \). This would be a complication unless
we are applying an inversion-free variant of the iteration of the previous remark. We can detect that the matrix $Y_k$ is ill conditioned by encountering difficulty in its numerical inversion or by computing its smallest singular value (e.g., by applying the Lanczos algorithm [11, Proposition 9.1.4]). In such cases we can try to avoid problems by shifting the matrix (and its eigenvalues), that is, by adding to or subtracting from the current matrix $Y_k$ the matrix $sI$ for a reasonably small positive scalar $s$. We can select this scalar by applying Theorem [2.6] heuristic methods, or randomization.

Towards a more radical recipe, apply the following modification of Algorithm 4.2.

**Algorithm 4.3.** Numerical stabilization of an extended matrix sign iteration.

**Input, Output and Stages 3 and 4 of Computations** are as in Algorithm 4.2 except that the input includes a small positive scalar $\alpha$ such that no eigenvalues of the matrix $C_p$ have imaginary parts close to $\pm \alpha \sqrt{-1}$ (see Remark 4.10 below), the set of $r$ real roots $x_1, \ldots, x_r$ of the polynomial $p(x)$ is replaced by the set of its $r_+$ roots having the imaginary parts in the range $[-\alpha, \alpha]$, and the integer $r$ is replaced by the integer $r_+$ throughout.

**Computations:**

1. Apply Stage 1 of Algorithm 4.2 to the two matrices $Y_{0, \pm} = \alpha \sqrt{-1} I \pm C_p$, producing two sequences of the matrices $Y_{h, +}$ and $Y_{h, -}$ for $h = 0, 1, \ldots$.

2. Fix a sufficiently large integer $k$ and compute the matrix $Y = Y_{k, +} + Y_{k, -}$.

Because of the assumed choice of $\alpha$, the matrices $\alpha \sqrt{-1} I \pm C_p$ have no real eigenvalues, and so the images of all their eigenvalues, that is, the eigenvalues of the matrices $Y_{h, +}$ and $Y_{h, -}$, converge to $\pm \sqrt{-1}$ as $k \to \infty$. Moreover, one can verify that the eigenvalues of the matrix $Y_{k, +} + Y_{k, -}$ converge to 0 unless they are the images of the $r_+$ eigenvalues of the matrix $C_p$ having the imaginary parts in the range $[-\alpha, \alpha]$. The latter eigenvalues of the matrix $Y_{k, +} + Y_{k, -}$ converge to $2\sqrt{-1}$. This shows correctness and numerical stability of Algorithm 4.3.

The algorithm approximates the $r_+$ roots of $p(x)$ by using $O(kn \log^2(n) + nr_+^2) + a_{+n}$ flops, versus $O(kn \log^2(n) + nr^2) + a_{rn}$ involved in Algorithm 4.2.

**Remark 4.10.** One can choose a positive $\alpha$ of Algorithm 4.3 by applying heuristic methods or as follows: map the two lines $\{x : \exists x = \pm \alpha\}$ into the unit circle $C(0, 1)$, extend these two maps to the two maps of the polynomial $p(x)$ into the polynomials $q_{\pm}(x) = p(x \pm \alpha \sqrt{-1})$, and apply the algorithm of Theorem 2.6 to these two polynomials.

### 4.4 Square Root Iteration (a Modified Modular Version)

Next we describe another dual polynomial version of Algorithm 4.2. It extend the square root iteration $y_{h+1} = \frac{1}{2}(y_h + 1/y_h)$, $h = 0, 1, \ldots$. Compared to Algorithm 4.2 we first replace all rational functions in the matrix $C_p$ by the same rational functions in the variable $x$ and then reduce every function modulo the input polynomial $p(x)$. The reduction does not affect the values of the functions at the roots of $p(x)$, and so these values are precisely the eigenvalues of the rational matrix functions involved in Algorithm 4.2.

**Algorithm 4.4.** Square root modular iteration modified for real root-finding.

**Input and Output** as in Algorithm 4.2.

**Computations:**

1. Write $y_0 = x$ and (cf. 4.1) compute the polynomials

\[
y_{h+1} = \frac{1}{2}(y_h + 1/y_h) \mod p(x), \quad h = 0, 1, \ldots. \tag{4.2}
\]

2. Periodically, for selected integers $k$, compute the polynomials $t_k = y_k^2 + 1 \mod p(x)$ and $g_k(x) = \text{aged}(p, t_k)$.
3. If \( \deg(g_h(x)) = n - r = 2s \), compute the polynomial \( v_k \approx p(x)/g_h(x) \) of degree \( r \). Otherwise continue the iteration of Stage 1.

4. Apply one of the algorithms of [6], [3], and [10] (cf. Theorem 2.10) to approximate the \( r \) roots \( y_1, \ldots, y_r \) of the polynomial \( v_k \). Output these approximations.

By virtue of our comments preceding this algorithm, the values of the polynomials \( t_k(x) \) at the roots of \( p(x) \) are equal to the images of the eigenvalues of the matrix \( C_p \) in Algorithm 4.2. Hence the values of the polynomials \( t_k(x) \) at the nonreal roots of \( p(x) \) converge to 0 as \( k \to \infty \), whereas their values at the real roots of \( p(x) \) stay far from 0. Therefore, for sufficiently large integers \( k \), \( \text{agcd}(p, t_k) \) turn into the polynomial \( \prod_{j=r+1}^n (x - x_j) \). This implies correctness of the algorithm. Its asymptotic computational cost is \( O(kn \log^2(n)) \) plus the cost of computing \( \text{agcd}(p, t_k) \) and choosing the integer \( k \) (see our next remark).

Remark 4.11. Compared to Algorithm 4.2, the latter algorithm reduces real root-finding essentially to the computation of \( \text{agcd}(p, t_k) \), but the complexity of this computation is not easy to estimate [11]. Moreover, let us reveal serious problems of numerical stability for this algorithm and for the similar algorithms of [5] and [3]. Consider the case where \( r = 0 \). Then the polynomial \( t(x) \) has degree at most \( n - 1 \), and its values at the \( n \) nonreal roots of the polynomial \( p(x) \) are close to 0. This can only occur if \( ||t_k(x)|| \approx 0 \).

Remark 4.12. We can concurrently perform Stages 1 of both Algorithms 4.2 and 4.4. The information about the numerical rank at Stage 3 of Algorithm 4.2 can be a guiding rule for the choice of the integer parameter \( k \) and computing the polynomials \( t_k, g_k \) and \( v_k \) of Algorithm 4.4. Having the polynomial \( v_k \) available, Algorithm 4.4 produces the approximations to the real roots more readily than Algorithm 4.2 does this at its Stage 4.

4.5 Cayley Map and Root-squaring

The following algorithm is somewhat similar to Algorithm 4.1 but employs repeated squaring of the roots instead of mapping them into their square roots.

**Algorithm 4.5.** Real root-finding with Cayley map and repeated root-squaring.

**Input and Output** as in Algorithm 4.1 except that we require that \( p(1)p(\sqrt{-1}) \neq 0 \).

**Computation:**

1. Compute the polynomial \( q(x) = (\sqrt{-1} (x - 1)^n + 1) = \sum_{i=0}^n q_i x^i \). (This is the Cayley map of Theorem 2.3. It moves the real axis, in particular the real roots of \( p(x) \), onto the unit circle \( C(0,1) \).)

2. Write \( q_0(x) = q(x)/q_n \), fix a sufficiently large integer \( k \), and apply the \( k \) squaring steps of Theorem 2.2, \( q_{h+1}(x) = (-1)^n q_h(\sqrt{x})q_h(-\sqrt{x}) \) for \( h = 0, 1, \ldots, k - 1 \). (These steps keep the images of the real roots of \( p(x) \) on the circle \( C(0,1) \) for all \( k \), while sending the images of every other root of \( p(x) \) toward either the origin or the infinity.)

3. For a sufficiently large integer \( k \), the polynomial \( q_k(x) \) approximates the polynomial \( x^r u_k(x) \) where \( u_k(x) \) is a polynomial of degree \( r \) whose all \( r \) roots lie on the unit circle \( C(0,1) \). Extract an approximation to this polynomial from the coefficients of the polynomial \( q_k(x) \).

4. Compute the polynomial \( w_k(x) = u_k(\sqrt{-1} \frac{x + 1}{x - 1}) \). (This Cayley map sends the images of the real roots of \( p(x) \) from the unit circle \( C(0,1) \) back to the real line.)

5. Apply one of the algorithms of [6], [3], and [10] to approximate the \( r \) real roots \( z_1, \ldots, z_r \) of the polynomial \( w_k(x) \) (cf. Theorem 2.10).

6. Apply the Cayley map \( w_j^{(k)} = (z_j + \sqrt{-1})/(z_j - \sqrt{-1}) \) for \( j = 1, \ldots, r \) to extend Stage 5 to approximating the \( r \) roots \( x_j^{(k)} \) of the polynomials \( u_k(x) \) and \( y_k(x) = x^r u_k(x) \) lying on the unit circle \( C(0,1) \).
7. Apply the descending process (similar to the ones of [14], [24], and of our Algorithm 4.1) to approximate the \( r \) roots \( x_1^{(h)}, \ldots, x_r^{(h)} \) of the polynomials \( q_h(x) \) lying on the unit circle \( C(0,1) \) for \( h = k - 1, \ldots, 0 \).

8. Approximate the \( r \) real roots \( x_j = \sqrt{-1}(x_j^{(0)} + 1)/(x_j^{(0)} - 1), j = 1, \ldots, r \), of the polynomials \( p(x) \).

Our analysis of Algorithm 4.1 (including its complexity estimates and the comments and recipes in Remarks 4.2–4.5) can be extended to Algorithm 4.5.

### 4.6 A Tentative Approach to Real Root-finding by Means of Root-radii Approximation

**Algorithm 4.6.** (Real root-finding by means of root radii approximation.)

**Input and Output** as in Algorithm 4.4

**Computations:**

1. Compute approximations \( \tilde{r}_1, \ldots, \tilde{r}_n \) to the root radii of a polynomial \( p(x) \) of \([14]\) (see Theorem 2.6). (This defines \( 2n \) candidates points \( \pm \tilde{r}_1, \ldots, \pm \tilde{r}_n \) for the approximation of the \( r \) real roots \( x_1, \ldots, x_r \).)

2. At all of these \( 2n \) points, apply one of the proximity tests of Section 2.2 to select \( r \) approximations to the \( r \) real roots of the polynomial \( p(x) \).

3. Apply Newton’s iteration \( x^{(h+1)} = x^{(h)} - p(x^{(h)})/p'(x^{(h)}) \), \( h = 0, 1, \ldots \), concurrently at these \( r \) points, expecting to refine quickly the approximations to the isolated simple real roots.

### 5 Real Eigen-solving for a Real Nonsymmetric Matrix

Suppose we are seeking the real eigenvalues of a real nonsymmetric \( n \times n \) matrix \( M \). We can substitute this matrix for the input matrix \( C_p \) of Algorithm 4.2 or 4.3 and apply the algorithm with no further changes. The overall arithmetic complexity would grow to \( O(kn^3) \) flops, but may still be competitive if the integer \( k \) is small, that is, if the algorithm converges fast for the input matrix \( M \).

Seeking acceleration, one can first define a similarity transformation of the matrix \( M \) into a rank structured matrix whose all subdiagonal blocks have rank at most 1 [30], [9]. Then one would only need \( O(n^2) \) flops to perform the first iteration (4.1), but each new iteration (4.1) would double the upper bound on the maximal rank of the subdiagonal blocks and thus would increase the estimated complexity of the next iteration accordingly. So the overall arithmetic cost would still be of order \( kn^3 \) flops, unless the integer \( k \) is small. One is challenged to devise a similarity transformation of a matrix that would decrease the maximal rank of its subdiagonal block, say, from 2 to 1, by using quadratic arithmetic time. This would decrease the overall arithmetic cost bound to \( O(kn^2) \).

Now consider extension of Algorithm 4.5 to real eigen-solving. We must avoid using high powers of the input and auxiliary matrices because these powers tend to have numerical rank 1. The following algorithm, however, involves such powers implicitly, when it computes the auxiliary matrix \( P^\omega P^{-m} \) as the product \( \prod_{i=0}^{m-1} (P - \omega_m^i P^{-1}) \) where \( P = (M + \sqrt{-1} I)(M - \sqrt{-1} I)^{-1}, m \) denotes a fixed reasonably large integer, and \( \omega_m = \exp(2\pi \sqrt{-1}/m) \) is a primitive \( m \)th root of unity.

**Algorithm 5.1.** Real eigen-solving by means of factorization.

**Input:** a real \( n \times n \) matrix \( M \) having \( r \) real eigenvalues and \( s = (n - r)/2 \) pairs of nonreal complex conjugate eigenvalues, neither of them is equal to \( \sqrt{-1} \).

**Output:** approximations to the real eigenvalues \( x_1, \ldots, x_r \) of the matrix \( M \).

**Computations:**
1. Compute the matrix $P = (M + \sqrt{-1}I)(M - \sqrt{-1}I)^{-1}$. (This is the matrix version of a Cayley map of Theorem 2.2. It moves the real and only the real eigenvalues of the matrix $M$ into the eigenvalues of the matrix $P$ lying on the unit circle $C(0, 1)$.)

2. Fix a sufficiently large integer $m$ and compute the matrix $Y = (P^m - P^{-m})^{-1}$ in the following factorized form $\prod_{i=0}^{m-1}(P - \omega_i^mP^{-1})^{-1}$ where $\omega_m = \exp(2\pi\sqrt{-1}/m)$. (For any integer $m$ the images of all real eigenvalues of the matrix $M$ have absolute values at least $1/2$, whereas the images of all nonreal eigenvalues of that matrix converge to 0 as $m \to \infty$.)

3. Complete the computations as at Stages 3 and 4 of Algorithm 4.2.

The arithmetic complexity of the algorithm is $O(mn^3)$ flops for general matrix $M$, but decreases to $O(mn^2)$ if $M$ is a Hessenberg matrix or if the rank of all its subdiagonal blocks is bounded by a constant. For $M = C_p$ the complexity decreases to $O(mn)$, which makes the algorithm attractive for real polynomial root-finding, as long as it converges for a reasonably small integers $m$.

**Remark 5.1.** (Scaling and the simplification of the factorizations.) One can apply the algorithm to a scaled matrix $\theta M/||M||$ for a fixed matrix norm $||.||$ and a fixed scalar $\theta$, $0 < \theta < 1$, say, for $\theta = 0.5$. In this case the inversion at Stage 1 is applied to a diagonally dominant matrix. Towards more radical simplification of the algorithm, one can avoid computing and inverting the matrix $P$ and can instead compute the matrix $Y$ in one of the following two equivalent factorized forms,

$$
Y = \prod_{i=0}^{m-1}((M^2 + I) F_i(M)^{-1}G_i(M)^{-1}) = \prod_{i=0}^{m-1} (\alpha_iF_i(M)^{-1} + \beta_iG_i(M)^{-1})
$$

for

$$F_i(M) = M + \sqrt{-1}I + \omega_{2m}(M - \sqrt{-1}I) = (1 + \omega_{2m}^i)M + \sqrt{-1}(1 - \omega_{2m}^i)I,$$

$$G_i(M) = M + \sqrt{-1}I - \omega_{2m}(M - \sqrt{-1}I) = (1 - \omega_{2m}^i)M + \sqrt{-1}(1 + \omega_{2m}^i)I,$$

some complex scalars $\alpha_i$ and $\beta_i$, and $i = 0, \ldots, m - 1$. Then again, one can apply the algorithm to a scaled matrix $\gamma M$ for an appropriate scalar $\gamma$ to simplify the solution of linear systems of equations with the matrices $F_i(M)$ and $G_i(M)$.

**Remark 5.2.** One can adapt the integer $m$ by doubling it to produce the desired eigenvalues if the computations show that the current integer $m$ is not large enough. The previously computed matrices $F_i(M)$ and $G_i(M)$ can be reused.

## 6 Numerical Tests

Three series of numerical tests have been performed in the Graduate Center of the City City University of New York by Ivan Retamoso and Liang Zhao. In all three series they tested Algorithm 4.2, and the results of the test are quite encouraging.

In the first series of tests, Algorithm 4.2 has been applied to one of the Mignotte benchmark polynomials, namely to $p(x) = x^n + (100x - 1)^3$. It is known that this polynomial has three ill conditioned roots clustered about 0.01 and has $n - 3$ well conditioned roots. In the tests, Algorithm 4.2 has output the roots within the error less than $10^{-6}$ by using 9 iterations for $n = 32$ and $n = 64$ and by using 11 iterations for $n = 128$ and $n = 256$.

In the second series of tests, polynomials $p(x)$ of degree $n = 50, 100, 150, 200, 250$ have been generated as the products $p(x) = f_1(x)f_2(x)$. Here $f_1(x)$ was the $r$th degree Chebyshev polynomial (having $r$ real roots) for $r = 8, 12, 16$, and $f_2(x) = \sum_{i=0}^{n-r} a_i x^i$, $a_i$ being i.i.d. standard Gaussian random variables, for $j = 0, \ldots, n - r$. Algorithm 4.2 (performed with double precision) was applied to 100 such polynomials $p(x)$ for each pair of $n$ and $r$. Table 6.1 displays the output data, namely, the average values and standard deviation of the numbers of iterations and of the maximum difference between the output values of the roots and their values produced by MATLAB root-finding function ”roots()”.

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In the third series of tests, Algorithm 4.2 approximated the real eigenvalues of a random real symmetric matrix $A = U^T \Sigma U$, where $U$ was an orthogonal $n \times n$ standard Gaussian random matrix, $\Sigma = \text{diag}(x_1, \ldots, x_r, y_1, \ldots, y_{n-r})$, and $x_1, \ldots, x_r$ (resp. $y_1, \ldots, y_{n-r}$) were i.i.d. standard Gaussian real (resp. non-real) random variables. Table 6.2 displays the mean and standard deviation of the number of iterations and the error bounds in these tests for $n = 50, 100, 150, 200, 250$ and $r = 8, 12, 16$.

Table 6.1: Number of Iterations and Error Bounds for Algorithm 4.2 on Random Polynomials

| $n$ | $r$ | Iter-mean | Iter-std | Bound-mean | Bound-std |
|-----|-----|-----------|----------|------------|-----------|
| 50  | 8   | 7.44      | 1.12     | $4.18 \times 10^{-6}$ | $1.11 \times 10^{-6}$ |
| 100 | 8   | 8.76      | 1.30     | $5.90 \times 10^{-6}$ | $1.47 \times 10^{-6}$ |
| 150 | 8   | 9.12      | 0.88     | $2.61 \times 10^{-5}$ | $1.03 \times 10^{-5}$ |
| 200 | 8   | 9.64      | 0.86     | $1.48 \times 10^{-6}$ | $5.93 \times 10^{-6}$ |
| 250 | 8   | 9.96      | 0.73     | $1.09 \times 10^{-6}$ | $5.23 \times 10^{-6}$ |
| 50  | 12  | 7.16      | 0.85     | $3.45 \times 10^{-4}$ | $9.20 \times 10^{-4}$ |
| 100 | 12  | 8.64      | 1.15     | $1.34 \times 10^{-3}$ | $2.67 \times 10^{-3}$ |
| 150 | 12  | 9.12      | 2.39     | $3.38 \times 10^{-4}$ | $1.08 \times 10^{-3}$ |
| 200 | 12  | 9.76      | 2.52     | $6.89 \times 10^{-6}$ | $1.75 \times 10^{-5}$ |
| 250 | 12  | 10.04     | 1.17     | $1.89 \times 10^{-5}$ | $4.04 \times 10^{-5}$ |
| 50  | 16  | 7.28      | 5.06     | $3.67 \times 10^{-3}$ | $7.62 \times 10^{-3}$ |
| 100 | 16  | 10.20     | 5.82     | $1.44 \times 10^{-3}$ | $4.51 \times 10^{-3}$ |
| 150 | 16  | 15.24     | 6.33     | $1.25 \times 10^{-3}$ | $4.90 \times 10^{-3}$ |
| 200 | 16  | 13.36     | 5.38     | $1.07 \times 10^{-3}$ | $4.72 \times 10^{-3}$ |
| 250 | 16  | 13.46     | 6.23     | $1.16 \times 10^{-4}$ | $2.45 \times 10^{-4}$ |

Table 6.2: Number of Iterations and Error Bounds for Algorithm 4.2 on Random Matrices

| $n$ | $r$ | Iter-mean | Iter-std | Bound-mean | Bound-std |
|-----|-----|-----------|----------|------------|-----------|
| 50  | 8   | 10.02     | 1.83     | $5.51 \times 10^{-11}$ | $1.65 \times 10^{-10}$ |
| 100 | 8   | 10.81     | 2.04     | $1.71 \times 10^{-12}$ | $5.24 \times 10^{-12}$ |
| 150 | 8   | 14.02     | 2.45     | $1.31 \times 10^{-13}$ | $3.96 \times 10^{-13}$ |
| 200 | 8   | 12.07     | 0.94     | $2.12 \times 10^{-11}$ | $6.70 \times 10^{-11}$ |
| 250 | 8   | 13.59     | 1.27     | $2.75 \times 10^{-10}$ | $8.14 \times 10^{-10}$ |
| 50  | 12  | 10.46     | 1.26     | $1.02 \times 10^{-12}$ | $2.61 \times 10^{-12}$ |
| 100 | 12  | 10.60     | 1.51     | $1.79 \times 10^{-10}$ | $3.66 \times 10^{-10}$ |
| 150 | 12  | 11.25     | 1.32     | $5.69 \times 10^{-8}$  | $1.80 \times 10^{-7}$  |
| 200 | 12  | 12.36     | 1.89     | $7.91 \times 10^{-10}$ | $2.50 \times 10^{-9}$  |
| 250 | 12  | 11.72     | 1.49     | $2.53 \times 10^{-12}$ | $3.84 \times 10^{-12}$ |
| 50  | 16  | 10.10     | 1.45     | $1.86 \times 10^{-9}$  | $5.77 \times 10^{-9}$  |
| 100 | 16  | 11.39     | 1.70     | $1.37 \times 10^{-10}$ | $2.39 \times 10^{-10}$ |
| 150 | 16  | 11.62     | 1.78     | $1.49 \times 10^{-11}$ | $4.580 \times 10^{-11}$ |
| 200 | 16  | 11.88     | 1.32     | $1.04 \times 10^{-12}$ | $2.09 \times 10^{-12}$ |
| 250 | 16  | 12.54     | 1.51     | $3.41 \times 10^{-11}$ | $1.08 \times 10^{-10}$ |
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