Real Polynomial Root-finding by Means of Matrix and Polynomial Iterations^{*}

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Abstract

Univariate polynomial root-finding is a classical subject, still 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. The subject of devising efficient real root-finders has been long and intensively studied. Nevertheless, we propose some novel ideas and techniques and obtain dramatic acceleration of the known numerical algorithms. In order to achieve our progress we exploit the correlation between the computations with matrices and polynomials, randomized matrix computations, and complex plane geometry, extend the techniques of the matrix sign iterations, and use the structure of the companion matrix of the input polynomial. The results of our extensive numerical tests with benchmark polynomials and random matrices are quite encouraging. In particular in these tests we have consistently computed accurate approximations of the real roots of benchmark polynomials of degree up to 1024 by using the IEEE standard double precision. Moreover the number of iterations required for convergence of our algorithms grew very slowly (if at all) as we increased the degree of the univariate input polynomials and the dimension of the input matrices from 64 to 1024.

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

1 Introduction

Assume a univariate polynomial of degree n with real coefficients,

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

^{*}This work appeared in Theoretical Computer Science, 2017, http://dx.doi.org/10.1016/j.tcs.2017.03.032. It has been supported by NSF Grants CCF 1116736 and CCF-1563942 and PSC CUNY Award 67699-00 45. Some of its results have been presented at CASC 2014.

which typically make up just a small fraction of all roots.¹ The design of efficient real root-finders is a well studied subject (see [19, Section 10.3.5], [47], [54], and the bibliography therein), but the most popular packages of subroutines for root-finding such as MPSolve 2000 [5], Eigensolve 2001 [21], and MPSolve 2012 [10] approximate the r real roots about as fast and as slow as all the ncomplex roots. It can be surprising, but we present some novel methods that accelerate the known numerical real root-finders by a factor of n/r, which is dramatic in various important applications.

The springboard for our real root-finders is the matrix sign iterations, which we apply to the companion matrix of an input polynomial. It is a well known technique for matrix computations [24], and we make it particularly efficient for real polynomial root-finding, although it has never been used for this purpose so far. By combining it with a number of known and novel techniques we ensure fast convergence of the iterations and their efficiency in numerical implementation with the IEEE standard double precision.

Our numerical tests confirm the efficiency of this approach. In particular, we closely approximate the real roots of various benchmark polynomials of degree up to 1024 by using double precision. Moreover the number of iterations required for convergence was typically quite small and grew very slowly (if it grew at all) as the polynomial degree increased from 64 to 1024.

Some of our techniques should be of independent interest, e.g., our numerical stabilization in Section 3.3, our exploitation of matrix functions and randomized matrix computations in Algorithm 3.1, and the combination of our maps of the complex plane with rational transformations of the variable and the roots. Some of our algorithms (e.g., the ones of Section 3.4) combine operations with matrices and polynomials, demonstrating once again the value of synergistic combinations of this kind, which we have been advocating since [33] and [6].

Our goal in this paper is to present a novel approach to real root-finding for a polynomial and to demonstrate the promise of this approach by performing some preliminary tests. We hope that we have advanced toward our goals substantially, and there are promising directions for substantial improvement of the implementation of our algorithms. For example, Stage 3 of our Algorithm 3.1 is reduced to the inversion or orthogonalizaton of Toeplitz-like matrices, and the customary numerical algorithms, currently available for these operations, can be dramatically accelerated by means of the techniques of the papers [62] and [63].

We organize our paper as follows. In the next section we cover some background material. We present a variety of our real polynomial root-finders in Section 3. In Section 4 (the contribution of the second author) we present the results of our numerical tests. In the Appendix we cover some auxiliary results.

2 Basic Definitions and Results

Hereafter "flop" stands for "floating point arithmetic operation", assumed to be performed numerically, with bounded precision, e.g., the standard IEEE double precision.

2.1 Some Basic Definitions for Matrix Computations

- $\mathbb{C}^{m \times n}$ denotes the linear space of complex $m \times n$ matrices. $\mathbb{R}^{m \times n}$ is its subspace of $m \times n$ real matrices.
- $M^T = (m_{ji})_{i,j=1}^{m,n}$ is the transpose of a matrix $M = (m_{ij})_{i,j=1}^{m,n} \in \mathbb{C}^{m \times n}$. M^H is its Hermitian transpose. $M^H = M^T$ for a real matrix M.
- $||M|| = ||M||_2$ denotes its spectral norm.

¹Recall the following excerpt from [14]: "A celebrated result due to Erdös and Turán [20] says that, for a univariate polynomial over C whose middle coefficients are not too big with respect to its extremal coefficients, the arguments of its roots are approximately equidistributed. Combined with a recent result of Hughes and Nikeghbali [27], this shows that the roots of such a polynomial clustered near the unit circle." This result does not apply to some classes of polynomials of practical importance, but the study in [17] (also see the earlier papers [28] and [18]) shows that the expected number r of the real roots of random real polynomials of various such classes stays in the range between orders of $\log(n)$ and \sqrt{n} ;

- $I = I_n$ is the $n \times n$ identity matrix.
- diag $(b_i)_{i=1}^s$ = diag (b_1, \ldots, b_s) is the $s \times s$ diagonal matrix with the diagonal entries b_1, \ldots, b_s .
- $\mathcal{R}(M)$ 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 $Q^H Q = I$ or $QQ^H = I$, and such a matrix is called *orthogonal* if it is real.
- Suppose an $m \times n$ matrix M has rank n (and so $m \ge n$). Write (Q, R) = (Q(M), R(M)) to denote a unique pair of a unitary $m \times n$ matrix Q and an upper triangular $n \times n$ matrix R such that M = QR and all diagonal entries of the matrix R are positive [22, Theorem 5.2.3].
- M^+ is the unique Moore–Penrose pseudo inverse of M [22, Section 5.5.2], equal to M^H if and only if the matrix M is unitary.
- An $m \times n$ matrix M has an $n \times m$ left inverse matrix $X = M^{(I)}$ such that $XM = I_n$ if and only if it has full column rank n. In this case M^+ is a left inverse. The left inverse is unique if and only if M is a nonsingular matrix, in which case m = n and $M^{(I)} = M^{-1}$.
- The ϵ -rank of a matrix M is the minimal rank of the matrices in its ϵ -neighborhood. Numerical rank nrank(M) is the ϵ -rank where ϵ is small in context.

Definition 2.1. Eigenvalues, eigenvectors and eigenspaces.

- A scalar x is an eigenvalue of a matrix M associated with an eigenvector \mathbf{v} if $M\mathbf{v} = x\mathbf{v}$.
- The eigenvectors associated with an eigenvalue x or, more generally, with any set of the eigenvalues $\mathcal{X} \in \mathcal{X}(M)$ form the eigenspaces $\mathcal{S}(M, x)$ and $\mathcal{S}(M, \mathcal{X})$, respectively, associated with the eigenvalue x and the set \mathcal{X} of eigenvalues, respectively. A linear subspace \mathcal{S} of $\mathbb{C}^{n \times n}$ is an eigenspace of a matrix M if and only if $M\mathcal{S} = \{M\mathbf{v} : \mathbf{v} \in \mathcal{S}\} \subseteq \mathcal{S}$ (see [53, Definition 4.1.1]).
- An eigenvalue x of a matrix M is a root of the characteristic polynomial det(xI M). The multiplicity of this root is the algebraic multiplicity of the eigenvalue x, denoted am(x). The dimension $gm(x) = \dim(\mathcal{S}(M, x))$ is the geometric multiplicity of x, never exceeding am(x). An eigenvalue x is simple if gm(x) = 1.

2.2 The Companion Matrix and the Frobenius Algebra

Let $\mathbf{e}_n^T = (0, 0, \dots, 0, 1)$ denote the *n*th coordinate vector and write $\mathbf{p} = (p_i/p_n)_{i=0}^{n-1}$,

$$Z = C_0 = \begin{pmatrix} 0 & & & 0 \\ 1 & \ddots & & & 0 \\ & \ddots & & \ddots & & \vdots \\ & & \ddots & 0 & 0 \\ & & & & 1 & 0 \end{pmatrix} \text{ and } C_p = \begin{pmatrix} 0 & & & -p_0/p_n \\ 1 & \ddots & & & -p_1/p_n \\ & \ddots & \ddots & & \vdots \\ & & \ddots & 0 & -p_{n-2}/p_n \\ & & & 1 & -p_{n-1}/p_n \end{pmatrix} = Z - \mathbf{p}^T \mathbf{e}_n. \quad (2.1)$$

Z is the down-shift matrix. C_p is the *companion matrix* of the polynomial p(x) of (1.1), which is the characteristic polynomial of this matrix. Hence real root-finding for the polynomial p(x) turns into real eigen-solving for this matrix.

 $Z\mathbf{v} = (v_{i-1})_{i=1}^n$, for a vector $\mathbf{v} = (v_i)_{i=1}^n$ and for $v_0 = 0$.

Theorem 2.1. (The Cost of Computations in the Frobenius Matrix Algebra.) The companion matrix $C_p \in \mathbb{R}^{n \times n}$ of a polynomial p(x) of (1.1) generates the Frobenius matrix algebra \mathcal{A}_p . One needs O(n) flops for addition and $O(n \log(n))$ for multiplication and inversion in this algebra as well as for multiplication of a matrix in this algebra by a vector. These cost bounds hold both for exact computation with no errors and numerically stable approximate computations.

Proof. The estimates for the exact computation can be readily deduced from the following expressions from [44] for a matrix $C(\mathbf{p}, \mathbf{c})$ in the algebra \mathcal{A}_p defined by its first column $\mathbf{c} = (c_i)_{i=0}^{n-1}$,

$$C(\mathbf{p}, \mathbf{c}) = \sum_{i=0}^{n-1} c_i C_p^i = \sum_{i=0}^{n-1} c_i Z^i + \mathbf{p} \mathbf{u}^T,$$
(2.2)

for **p** of equation (2.1), $\mathbf{u} = (u_i)_{i=0}^{n-1}$, $u_0 = 0$, $u_i = \sum_{k=n-i}^{n-1} c_k \rho^{k-n+i}$, for $i = 1, \ldots, n-1$ and $\rho = -p_{n-1}/p_n$, so that $\rho = 0$ if $p_{n-1} = 0$. (If $c_0 = 0$, then invert the matrix $C(\mathbf{q}, \mathbf{c}_s) = C(\mathbf{p}, \mathbf{c})$ for q(x) = p(x - s) and a random real or complex shift s.) The algorithm of [12], using the transition to the so called "Horner's basis", performs numerically stable multiplication in the algebra \mathcal{A}_p , [62] performs numerically stable inversion by using $O(n \log^2(n))$ flops, which is accelerated by a factor of $\log(n)$ in [43, Section 9.8].

2.3 Decreasing the Size of an Eigenproblem

An eigenvalue x of a matrix M as well as a set of eigenvalues \mathcal{X} are *dominant* if they are absolutely larger than all the other eigenvalues. An eigenspace is called *dominant* if it is associated with a dominant eigenvalue or a dominant set of eigenvalues.

The set $\mathcal{X}(M)$ of all eigenvalues of a matrix M is called its *spectrum*.

The Power Method [22, Section 7.3.1] computes the vector $M^k \mathbf{v}$, for a random vector \mathbf{v} and a sufficiently large integer k. The 1-dimensional vector space $\{tM^k\mathbf{v}\}$, for $t \in \mathbb{C}$, is expected to approximate the eigenspace associated with an eigenvalue x if it is dominant and simple. This would not work only if the vector \mathbf{v} has an absolutely small component along the eigenvector associated with this eigenvalue x, but such an event is unlikely, for a random vector \mathbf{v} . One can choose k = 1 if the domination of the eigenvalue x in the spectrum of M is strong. Let us extend the Power Method for k = 1 to the approximation of a strongly dominant eigenspace of a dimension r.

Algorithm 2.1. Approximation of the dominant eigenspace.

INPUT: an $n \times n$ matrix M, the dimension r of its dominant eigenspace \mathcal{U} , 0 < r < n, and two tolerance bounds: a positive integer K and a positive ϵ .

OUTPUT: FAILURE (with a low probability) or a unitary matrix U whose range approximates the eigenspace U.

COMPUTATIONS:

- 1. Apply the randomized algorithm of [23], which at first generates a standard Gaussian random $n \times r_+$ matrix G for a proper integer $r_+ > r$ and then computes the matrix H = MG and the numerical rank nrank(H).
- 2. Unless $\operatorname{nrank}(H) = r$, re-apply the algorithm of [23] up to K times until the equation $\operatorname{nrank}(H) = r$ is observed. If it is never observed, output FAILURE (this occurs with a probability near 0).
- 3. If nrank(H) = r, then compute the QR factorization H = Q(H)R(H), output an $n \times r$ unitary matrix U approximating the first r columns of the matrix Q(H), and stop. (The analysis in [23, Section 4], [45, Section 7.4], and [50, Theorem 4.3] shows that, with a probability close to 1, the columns of the matrix U closely approximate a unitary basis of the eigenspace U and that $||M UU^H M|| \leq \epsilon ||M||$. The latter bound would certify correctness of the output.)

The arithmetic cost of performing the algorithm is $O(n^2r_+)$, but decreases to $O(nr_+(r_++\log(n)))$, for $M = C_P$, by virtue of Theorem 2.1. It increases by a factor of $\log(r)$ if the dimension rof the eigenspace \mathcal{U} is not available, but is computed by using binary search that begins with recursive doubling of the candidate integer values 1, 2, 4, etc. The algorithm generates nr_+ random parameters, but its modification using the structured (so called SRFT) multipliers G involves only nsuch parameters and only $O(n \log(n))$ flops for the computation of the product MG (see [23, Section 11] and [45, Section 7.5]). Alternative application of the orthogonal iterations of [22, Section 7.3.2] requires order of n^2r_+ flops. **Remark 2.1.** Actually the algorithm of [23] works even where the input includes an upper bound r_+ on the dimension r of the dominant eigenspace \mathcal{U} , rather than the dimension itself, and then the algorithm can compute this dimension r within the above computational cost as by-product. (The integer $r = \operatorname{nrank}(H)$ can be obtained, e.g., from rank revealing QR factorization of the matrix H.)

Now suppose that we have an eigenspace generated by r eigenvalues of an $n \times n$ matrix. Then the following simple theorem (extending the recipe of the Rayleigh quotients) enables us to approximate these eigenvalues as the eigenvalues of an auxiliary $r \times r$ matrix.

Theorem 2.2. (Decreasing the Eigenproblem Size to the Dimension of an Eigenspace, cf. [60, Section 2.1].)

Suppose that $M \in \mathbb{C}^{n \times n}$, $U \in \mathbb{C}^{n \times r}$, and the matrix U has full column rank $r \leq n$ and generates the space $\mathcal{U} = \mathcal{R}(U)$. Then

(i) \mathcal{U} is an eigenspace 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 $L = U^{(I)}MU$,

(*ii*) $\mathcal{X}(L) \subseteq \mathcal{X}(M)$,

(iii) $MU\mathbf{v} = xU\mathbf{v}$ if $L\mathbf{v} = x\mathbf{v}$,

(iv) the matrix L is unique, that is, its choice is independent of the choice of a matrix U and its left inverse $U^{(I)}$, and so $L = U^H M U$, for a unitary matrix U.

The algorithm and the theorem enable us to approximate the r real eigenvalues of a matrix as the r dominant eigenvalues of an auxiliary matrix. Theorems 2.2 and 2.3 (below) together suggest a direction to such a reduction, and we achieve it in Sections 3.1 and 3.3.

2.4 Matrix Functions and Eigenspaces

Theorem 2.3. (The Eigenproblems for a Matrix and Its Function.)

Suppose that M is a square matrix and that a rational function f(x) is defined on its spectrum. (i) Then $f(M)\mathbf{v} = f(x)\mathbf{v}$ if $M\mathbf{v} = x\mathbf{v}$.

(ii) Let $\mathcal{U} = \mathcal{U}_{\mu,f}$ denote the eigenspace of the matrix f(M) associated with its eigenvalue μ . Then this is an eigenspace of the matrix M associated with all its eigenvalues x such that $f(x) = \mu$.

(iii) The space \mathcal{U} has dimension 1 and is associated with a single eigenvalue of M if μ is a simple eigenvalue of f(M).

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

Remark 2.2. The matrix Z^k , for $1 \le k \le n$, has the single eigenvalue 0 satisfying am(0) = n and gm(0) = k, and so $\dim(\mathcal{U}_{0,f}) = k$, for M = Z, $f(x) = x^k$, and $k = 1, \ldots, n$.

Suppose that we have computed a matrix basis $U \in \mathbb{C}^{n \times r_+}$, for an eigenspace \mathcal{U} of a matrix function f(M) of an $n \times n$ matrix M. By virtue of Theorem 2.3, this is a matrix basis of an eigenspace of the matrix M. We can first compute a left inverse $U^{(I)}$ 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 $L = U^{(I)}MU = Q^H MQ$ (cf. Theorem 2.2).

If r = 1, then the matrix U turns into an eigenvector **u**, shared by the matrices f(M) and M, while the matrix L turns into the the Rayleigh Quotient $\frac{\mathbf{u}^T M \mathbf{u}}{\mathbf{u}^T \mathbf{u}}$ or the simple quotient $(M \mathbf{u})_i / u_i$, for any i such that $u_i \neq 0$.

2.5 Some Maps in the Frobenius Matrix Algebra

Part (i) of Theorem 2.3 implies that, for a polynomial p(x) of (1.1) 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 $\mathcal{X}(f(C_p)) = \{f(x_i)\}_{i=1}^n$. In particular, the maps

$$C_p \to C_p^{-1}, \ C_p \to aC_p + bI, \ C_p \to C_p^2, \ C_p \to \frac{C_p + C_p^{-1}}{2}, \ \text{and} \ C_p \to \frac{C_p - C_p^{-1}}{2}$$

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

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

respectively. The latter two maps can be only applied if the matrix C_p is nonsingular, so that $x \neq 0$, and similarly for the two dual maps below.

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

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

where y = y(x) denotes polynomials. Apply the two latter maps recursively, to define two iterations with polynomials modulo p(x) as follows, $y_0 = x$, $y_{h+1} = 0.5(y_h + 1/y_h) \mod p(x)$ and $y_0 = 0.5(y_h + 1/y_h)$ x, $y_{h+1} = 0.5(y_h - 1/y_h) \mod p(x)$, $h = 0, 1, \dots$ More generally, define the iteration $y_0 = x$, $y_{h+1} = ay_h + b/y_h \mod p(x), h = 0, 1, \dots$, for any pair of scalars a and b, provided that $y_h = 0$, for none h.

3 Real Root-finders with Modified Matrix Sign Iterations. Variations and Extensions

In this section we present some efficient numerical real root-finders based on modification of the matrix sign classical iterations applied to the companion matrix of the input polynomial.

3.1A Modified Matrix Sign Iterations

Our first algorithm approximates the r real roots of a polynomial p(x) of (1.1) as the real eigenvalues of the companion matrix C_p . It applies the matrix iterations

$$M_0 = C_p, \ M_{h+1} = 0.5(M_h - M_h^{-1}), \ \text{for } h = 0, 1, \dots,$$
 (3.1)

which modify the matrix sign iterations $\widehat{M}_{h+1} = 0.5(\widehat{M}_h + \widehat{M}_h^{-1})$ (cf. [24]).

For every eigenvalue x_j of the matrix $M_0 = C_p$, define its *trajectory* made up of the eigenvalues of the matrices M_h , being its images in the maps $M_0 \to M_h$, for $h = 1, 2, 3, \ldots$ More generally iterations (3.2) below modifying the Möbius classical iterations $x^{(h+1)} = \frac{1}{2}(x^{(h)} + 1/x^{(h)})$, for h = $0, 1, \ldots$, define a trajectory initiated at any complex point $x^{(0)}$.

Hereafter we write $\operatorname{sign}(z) = \operatorname{sign}(\Re(z))$, for a complex number z (cf. [24, page 107]).

Theorem 3.1. (Convergence of the modified Möbius Iterations.) Fix a complex $x = x^{(0)}$ and define the modified Möbius iterations

$$x^{(h+1)} = \frac{1}{2}(x^{(h)} - 1/x^{(h)}), \text{ for } h = 0, 1, \dots$$
 (3.2)

(i) The values $x^{(h)}$ are real, for all h, if $x^{(0)}$ is real. (ii) $|x^{(h)} - \operatorname{sign}(x)\sqrt{-1}| \le \frac{2K^{2^h}}{1-K^{2^h}}$, for $K = |\frac{x-\operatorname{sign}(x)}{x+\operatorname{sign}(x)}|$ and $h = 0, 1, \dots$

Proof. Part (i) is immediately verified. Part (ii) readily extends the similar estimate on [7, page 500].

Theorem 3.1 implies the following result.

Corollary 3.1. As $h \to \infty$, the trajectories of the 2s nonreal eigenvalues of $M_0 = C_p$ converge to $\pm\sqrt{-1}$ with the quadratic rate of convergence right from the start, whereas the trajectories of the r real eigenvalues are real, for all h.

Algorithm 3.1. Matrix sign iterations modified for real eigen-solving.

INPUT: two integers n and r, 0 < r < n, and the coefficients of a polynomial p(x) of equation (1.1). OUTPUT: approximations to the real roots x_1, \ldots, x_r of the polynomial p(x) or FAILURE with a probability close to 0.

COMPUTATIONS:

- 1. Write $M_0 = C_p$ and recursively compute the matrices M_{h+1} of (3.1), for h = 0, 1, ... (cf. Corollary 3.1).
- 2. Fix a sufficiently large integer k and compute the matrix $M = M_k^2 + I_n$.

(By extending Corollary 3.1 observe that the map $M_0 = C_p \rightarrow M$ 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 $\{x : x \ge 1\}$.)

3. Apply our randomized Algorithm 2.1 in order to approximate a unitary matrix U whose columns form a basis for the eigenspace associated with the r dominant eigenvalues of the matrix M.

(By virtue of Theorem 2.3, this is expected to be the eigenspace associated with the real eigenvalues of the matrix C_p , although with a probability close to 0 the algorithm can output FAILURE, in which case we stop the computations.)

4. Compute and output approximations to the r eigenvalues of the $r \times r$ matrix $L = U^H C_p U$. (They approximate the r real eigenvalues of the matrix C_p by virtue of Theorem 2.2 and consequently approximate the r real roots of the polynomial p(x).)

Stages 1 and 2 involve $O(kn \log(n))$ flops by virtue of Theorem 2.1. Stage 3 adds $O(n^2r)$ flops and the cost a_{rn} of generating $n \times r$ standard Gaussian random matrix. Add $O(r^3)$ flops performed at Stage 4 and arrive at the overall arithmetic cost bound $O((kn \log(n) + nr^2) + a_{rn})$.

Remark 3.1. (Counting Real Eigenvalues.) The binary search can produce the number of real eigenvalues as the numerical rank of the matrices $M_k^2 + I$ when this rank stabilizes as k increases. As the number of real roots increases, so does the size of the matrix L. This has consistently implied the decrease of the accuracy of the output approximations in our tests (see the test results in Section 4). One can refine these approximations by applying the inverse Power Method or Newton's iterations, but if the accuracy becomes too low, one must extend the precision of computing.

Remark 3.2. (Acceleration by Means of Scaling.) One can dramatically accelerate the initial convergence of Algorithm 3.1 by applying determinantal scaling (cf. [24]), that is, by replacing the matrix $M_0 = C_p$ by the matrix $M_0 = 0.5(\nu C_p - (\nu C_p)^{-1})$, for $\nu = 1/|\det(C_p)|^{1/n} = |p_n/p_0|$.

Remark 3.3. Real and Nearly Real Roots.

In the presence of rounding errors Algorithm 3.1 and all our other algorithms approximate both r real and $r_+ - r$ nearly real eigenvalues of the matrix M, for some $r_+ \ge r$. The r real eigenvalues, however, are the roots of p(x) and we can refine their approximations very fast (cf. Theorems B.1 and [48]), under some mild assumptions about the isolation of every such a root from the n-1 other roots. (One can partly relax these assumptions by extending the techniques of [48].) Then we can readily select the r real eigenvalues among the r_+ real and nearly real ones.

Generally, however, the distinction between real and nearly real roots is very slim in our numerical algorithms. As this was pointed out in [3], in the course of performing the iterations, the real eigenvalues can become nonreal, due to rounding errors, and then would converge to $\pm \sqrt{-1}$. In our extensive tests we have never observed such a phenomenon, apparently because in these tests the convergence to $\pm \sqrt{-1}$ was much slower for the nearly real eigenvalues than for the eigenvalues with reasonably large imaginary parts.

3.2 Inversion-free Variations of the Modified Matrix Sign Iterations and Hybrid Algorithms

The overall arithmetic cost of the Modified Matrix Sign Iterations is dominated by the cost of k matrix inversions, that is, $O(kn \log^2(n))$ flops (cf. Theorem 2.1). If all nonreal eigenvalues of the matrix M_0 lie in the two discs $D(\pm\sqrt{-1}, 1/2) = \{x : |x \pm \sqrt{-1}| \le 1/2\}$, then we can avoid matrix inversions in the Modified Matrix Sign Iterations by replacing iterations (3.1) with any of the two iteration processes

$$M_{h+1} = 0.5(M_h^3 + 3M_h) \tag{3.3}$$

and

$$M_{h+1} = -0.125(3M_h^5 + 10M_h^3 + 15M_h), ag{3.4}$$

for $h = 0, 1, \ldots$ Right from the start both iterations send the nonreal roots toward the two points $\pm \sqrt{-1}$ with quadratic and cubic convergence rates, respectively. (In order to prove this, extend the proof of [7, Proposition 4.1].) Both iteration processes keep the real roots real and use $O(n \log(n))$ flops per iteration.

What if the nonreal roots do not lie in these discs? We can apply the following combination of iterations (3.1)–(3.4) and Corollary D.1 of Section D.

Algorithm 3.2. A Hybrid Algorithm.

INPUT, OUTPUT as in Algorithm 3.1.

COMPUTATIONS: Perform the iterations of Algorithm 3.1 until a test shows that the 2s nonreal eigenvalues of the input companion matrix are mapped into the discs $D(\pm\sqrt{-1}, 1/2)$. (For testing this condition, apply the algorithm that supports Corollary D.1. To keep the computational cost down, apply this test periodically, according to a fixed policy, based on heuristic rules or the statistics of the previous tests.) Then shift the computations to the inversion-free iterations (3.3) or (3.4) converging faster and using $O(n \log(n))$ flops per iteration.

Let us recall some alternative matrix iterations for real root-finding without inversions. Recall that $sign(M) = M(M^2)^{-0.5}$ and apply the Newton–Schultz iterations for the approximation of the matrix square root [24, equation (6.3)],

$$Y_{k+1} = 0.5 Y_k (3I - Z_k Y_k), \quad Y_0 = M^{-2},$$

and

$$Z_{k+1} = 0.5 (3I - Z_k Y_k) Z_k, \quad Z_0 = I,$$

for k = 0, 1, ... The iterations keep real eigenvalues real and converge if $||I - M^{-2}||_p < 1$, for p = 1, 2, or ∞ . This assumption is easy to satisfy by means of scaling $M \to aM$, which keeps real eigenvalues real, for real a.

The similar coupling technique of [3] is even simpler, because it is applied directly to the modified matrix sign iterations (3.1), preserving its quadratic convergence to $\pm \sqrt{-1}$ right from the start.

In our tests for numerical real root-finding, however, we could perform safely only a small number of these inversion-free iterations at the initial stage, and then the images of the real eigenvalues of the matrix C_p grew very large and the condition numbers of the computed matrices blew up.

3.3 Numerical Stabilization of the Modified Matrix Sign Iterations

The images of nonreal eigenvalues of the matrix C_p converge to $\pm \sqrt{-1}$ in the iterations of Stage 1 of Algorithm 3.1, but if the images of some real eigenvalues of C_p come close to 0, then at the next step we would have to invert an ill-conditioned matrix M_h unless we are applying an inversion-free variant of the iterations of the previous subsection.

We can try to avoid this problem by shifting the matrix (and its eigenvalues), that is, by adding to the current matrix M_h the matrix sI, for a reasonably small positive scalar s or -s. We can select this scalar by applying heuristic methods or randomization. In our tests this policy has preserved convergence quite well, but we have no formal support for this observation. The following stabilization of Algorithm 3.1 involves nonreal values even when the matrix C_p was real, but has both formal and empirical support.

Algorithm 3.3. Numerical stabilization of the modified matrix sign iterations.

INPUT, OUTPUT and Stages 3 and 4 of COMPUTATIONS are as in Algorithm 3.1, except that the input includes a small positive scalar α such that no eigenvalues of the matrix C_p have imaginary parts close to $\pm \alpha \sqrt{-1}$ (see Remark 3.4 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 3.1 to the two matrices $M_{0,\pm} = \alpha \sqrt{-1} I \pm C_p$, thus producing two sequences of the matrices $M_{h,+}$ and $M_{h,-}$, for $h = 0, 1, \ldots$
- 2. Fix a sufficiently large integer k and compute the matrix $M = M_{k,+} + M_{k,-}$.

Because of the assumed choice of α , 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 $M_{k,+}$ and $M_{k,-}$, converge to $\pm\sqrt{-1}$ as $k \to \infty$. Moreover, one can verify that the eigenvalues of the matrix $M_{k,+} + M_{k,-}$ 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 $M_{k,+} + M_{k,-}$ converge to $2\sqrt{-1}$. This shows correctness and numerical stability of Algorithm 3.3.

The algorithm approximates the r_+ roots of p(x) by using $O(kn \log(n) + nr_+^2) + a_{r_+n}$ flops, versus $O(kn \log(n) + nr^2) + a_{r_n}$ involved in Algorithm 3.1.

Remark 3.4. We can test the proximity of the roots to a line in two stages: by at first moving the line into the unit circle $\{x : |x| = 1\}$ (cf. Theorem A.3) and then applying algorithms that supports Theorem D.2 or Corollary D.1.

3.4 Square Root Iterations (a Modified Modular Version)

Next we describe a dual polynomial version of Algorithm 3.1. It extends the square root iterations $y_{h+1} = \frac{1}{2}(y_h + 1/y_h)$, h = 0, 1, ..., and at Stage 2 involves the computation of the polynomial $agcd(p, t_k)$, which denotes an *approximate greatest common divisor* of the input polynomial p = p(x) and an auxiliary polynomial $t_k = t_k(x)$. We refer the reader to [38], [29], [4], [61], [11], and [55] for the definitions of this concept and the algorithms for its computation.

Compared to Algorithm 3.1, we replace all rational functions in the matrix C_p by the same rational functions in the variable x and reduce them modulo the input polynomial p(x). The reduction does not affect the values of the functions at the roots of p(x), and it follows that these values are precisely the eigenvalues of the rational matrix functions computed in Algorithm 3.1.

Algorithm 3.4. Square root modular iterations modified 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). OUTPUT: approximations to the real roots x_1, \ldots, x_r of the polynomial p(x).

COMPUTATIONS:

1. (Cf. (3.1).) Write $y_0 = x$ and compute the polynomials

$$y_{h+1} = \frac{1}{2}(y_h - 1/y_h) \mod p(x), \ h = 0, 1, \dots$$
 (3.5)

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

4. Apply one of the algorithms of [1], [8], and [15] (cf. Theorem C.1) to approximate the r roots y_1, \ldots, y_r of the polynomial v_k . Output these approximations.

Our comments preceding this algorithm show that 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 3.1. 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, $\operatorname{agcd}(p, t_k)$ turns into the polynomial $\prod_{i=r+1}^{n} (x - x_i)$. This implies correctness of the algorithm.

Its asymptotic computational cost is $O(kn \log^2(n))$ plus the cost of computing $\operatorname{agcd}(p, t_k)$ and choosing the integer k (see our next remark).

Remark 3.5. The latter algorithm reduces real root-finding essentially to the computation of $agcd(p, t_k)$. One can apply quite efficient heuristic algorithms for this computation (cf. [38], [29], [4], [61], [11], and [55]), but no good formal estimates are available for their complexity. One can, however, note that $p(x)u_k(x) \approx t_k(x)v_k(x)$, and so, assuming that $v_k(x)$ is a monic polynomial (otherwise we can scale it), can obtain its other coefficients (as well as the coefficients of the polynomial $u_k(x)$) from the least-squares solution to the associated Sylvester linear system of equations. Its well known superfast divide and conquer solution involves order of $n \log^2(n)$ arithmetic operations (cf. [36, Chapter 5]), but the recent numerically stable algorithm of [62] accelerated by a factor of $\log(n)$ in [43, Section 9.8] involves only $O(n \log(n))$ flops.

4 Numerical Tests

Extensive numerical tests of the algorithms of this paper, performed in the Graduate Center of the City University of New York. They are the contribution of the second author (at some points he was assisted by Ivan Retamoso). The tests recorded the number of iterations and the error of the approximation of the real roots of benchmark polynomials to which we applied these algorithms. We have recorded similar data also for the approximation of real eigenvalues of some random matrices M by means of applying Algorithms 3.1 and 3.3. In the latter case the convergence of these algorithms and the number of their iterations depended mostly on the characteristic polynomials of M, even though the estimates for the arithmetic cost of performing each iteration generally grew compared to the special case where $M = C_p$.

In some cases we stopped the iterations already when they produced crude approximation to the roots. This is because, instead of continuing the iterations, we can apply the algorithms of [48] followed by Newton's or Ehrlich–Aberth's iterations (cf. Section B), which refine very fast these crude approximations.

Finally we note that the test results in the present section are quite encouraging (in spite of our caveat in Remark 3.1), e.g., the numbers of iterations required for convergence of our algorithms have grown very slowly (if at all) when we increased the degree of the input polynomials and dimension of the input matrices from 64 to 1024. We performed all tests with the IEEE standard double precision.

The implementation is available upon request.

4.1 Tests for the Modified Matrix Sign Iterations (Algorithm 3.1)

In the first series of the tests, Algorithm 3.1 has been applied to one of the Mignotte benchmark polynomials, namely $p(x) = x^n + (100x - 1)^3$. 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 3.1 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 the tests, polynomials p(x) of degree n = 50, 100, 150, 200, and 250 have been generated as the products $p(x) = p_1(x)p_2(x)$, for the *r*th degree Chebyshev polynomial $p_1(x)$ (having *r* real roots), r = 8, 12, 16, and $p_2(x) = \sum_{i=0}^{n-r} a_i x^i$, a_j being i.i.d. standard Gaussian random variables, for $j = 0, \ldots, n-r$. Algorithm 3.1 (performed with double precision) was applied to 100 such polynomials p(x), for each pair of *n* and *r*. Table 4.1 displays the output data, namely, the average values and the 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()".

In the third series of the tests, Algorithm 3.1 approximated the real eigenvalues x_1, \ldots, x_r of a random complex symmetric matrix $A = U^T \Sigma U$, for $\Sigma = \text{diag}(x_1, \ldots, x_r, y_1, \ldots, y_{n-r})$, r i.i.d. real standard Gaussian random variables x_1, \ldots, x_r , n-r i.i.d. complex (non-real) standard Gaussian random variables y_1, \ldots, y_{n-r} , and a $n \times n$ standard Gaussian random orthogonal matrix U. Table 4.2 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.

In order to estimate the number of iterations required in our algorithms, we periodically estimated the numerical rank of the associated matrix in every k successive iterations, for k = 5 in most of our experiments.

\mathbf{n}	\mathbf{r}	Iteration-mean	Iteration-std	Error-mean	Error-std
50	8	7.44	1.12	4.18×10^{-6}	1.11×10^{-5}
100	8	8.76	1.30	$5.90 imes 10^{-6}$	1.47×10^{-5}
150	8	9.12	0.88	2.61×10^{-5}	1.03×10^{-4}
200	8	9.64	0.86	1.48×10^{-6}	$5.93 imes 10^{-6}$
250	8	9.96	0.73	1.09×10^{-7}	$5.23 imes 10^{-5}$
50	12	7.16	0.85	$3.45 imes 10^{-4}$	$9.20 imes 10^{-4}$
100	12	8.64	1.15	1.34×10^{-5}	2.67×10^{-5}
150	12	9.12	2.39	3.38×10^{-4}	1.08×10^{-3}
200	12	9.76	2.52	6.89×10^{-6}	1.75×10^{-5}
250	12	10.04	1.17	1.89×10^{-5}	4.04×10^{-5}
50	16	7.28	5.06	3.67×10^{-3}	7.62×10^{-3}
100	16	10.20	5.82	1.44×10^{-3}	4.51×10^{-3}
150	16	15.24	6.33	1.25×10^{-3}	4.90×10^{-3}
200	16	13.36	5.38	1.07×10^{-3}	4.72×10^{-3}
250	16	13.46	6.23	$1.16 imes10^{-4}$	2.45×10^{-4}

Table 4.1: Number of Iterations and Error Bounds for Algorithm 3.1 on Random Polynomials

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

Table 4.2: Number of Iterations and Error Bounds for Algorithm 3.1 on Random Matrices

Tests for the Stabilized Matrix Sign Iterations (Algorithm 3.3) 4.2Applied to Polynomials

We tested Algorithm 3.3 on various modified benchmark polynomials from the website of MPSolve (http://numpi.dm.unipi.it/mpsolve-2.2/). With the exception of the polynomials of Type IV below, we tested benchmark polynomials that had only trivial real roots 0 and ± 1 , and we multiplied them by Chebyshev polynomials of degree r, for r = 8, 12, and 16, which have only real roots.

Having generated such a polynomial p = p(x) and its companion matrix C_p , we computed the condition numbers of the matrices $N_k = C_p + 2^{7+k} I_n$ with $k = 1, 2, \ldots$ and selected an integer k such that $\kappa(N_k) < 10^5$. Clearly, this is ensured for sufficiently large integers k defining diagonally dominant matrices N_k , but in our tests k was less than five in most cases.

Having fixed k and N_k and following the description of Algorithm 3.3, we computed at first the matrices $Y_1 = \alpha I_n + N_k$ and $Y_2 = \alpha I_n - N_k$, for $\alpha = 0.0001\sqrt{-1}$, and then successively the matrices $Y_{i+1,j} = \frac{1}{2}(Y_{i,j} - Y_{i,j}^{-1})$ with $Y_{0,j} = Y_j$, for j = 1, 2 (cf. Algorithms 3.1 and 3.3).

We have observed that with our real shifts by $2^{7+k}I_n$ at the initial stage, non-real eigenvalues of Y_1 and Y_2 were never close to $\pm \sqrt{-1}$ at the first 7 + k iterations. So we began checking convergence only when we have performed these initial iterations, and since that moment we checked convergence in every five iterations. As soon as we observed that $\operatorname{nrank}(Y'_i) = r$, for $Y'_i = Y_{i,1} + Y_{i,2}$ and for r denoting the number of distinct real roots of p(x), r = 8, 12, 16, we stopped the iterations and moved to the final stage of the algorithm, that is, approximated the real eigenvalues of matrix C_p , equal to the real roots of the polynomial p(x).

We have run numerical tests on polynomials of five types having degree n = 64, 128, 256, 512, 1024, and we compared our results with the outputs of MATLAB function "roots()". We defined polynomial p(x) of Types I–III and V as the products $p(x) = p_1(x)p_2(x)$ where $p_1(x)$ is the r-th degree Chebyshev polynomial and $p_2(x)$ are the following polynomials:

I. $p_2(x) = x^{n-r} - 1$,

II. $p_2(x) = 1 + 2x + 3x^2 + \dots + (n - r + 1)x^{n-r}$, III. $p_2(x) = (x + 1)(x + a)(x + a^2) \cdots (x + a^{n-r-1})$, with $a = \frac{i}{100}$, and V. $p_2(x) = \sum_{k=0}^{n} a_k x^k$, with a_0, \dots, a_n being i.i.d. standard random variables.

We also tested the following polynomials of Type IV,

IV. $p(x) = x^{n-r} - (ax - 1)^3$, where a = 60, 80, 100.

Tables 4.3–4.6 display the number of iterations and the maximum error bounds, for the polynomials of Types I–IV (cf. our Remark 3.1). Table 4.7 shows the average error bounds and the average numbers of iterations in 50 tests with the polynomials of Type V.

n	r	Iterations	Errors
64	8	10	1.03E - 10
64	12	23	1.32E - 08
64	16	23	3.97E - 06
128	8	10	1.60E - 10
128	12	23	4.91E - 04
128	16	23	2.22E - 03
256	8	10	6.18E - 06
256	12	28	1.75E - 09
256	16	28	3.54E - 06
512	8	15	8.05E - 13
512	12	28	1.71E - 08
512	16	28	2.78E - 05
1024	8	15	2.33E - 12
1024	12	28	1.27E - 09
1024	16	28	2.19E - 05

Table 4.3: Number of Iterations and Error Bounds for Algorithm 3.3 on Type I Polynomials

Table 4.4: Number of Iterations and Error Bounds for Algorithm 3.3 on Type II Polynomials

n	r	Iterations	Errors
64	8	10	1.53E - 11
64	12	23	1.30E - 07
64	16	23	1.40E - 05
128	8	28	9.42E - 11
128	12	10	7.51E - 08
128	16	28	2.27E - 04
256	8	28	1.92E - 11
256	12	28	2.21E - 07
256	16	28	1.69E - 03
512	8	28	3.68E - 12
512	12	28	2.17E - 06
512	16	33	1.53E - 02
1024	8	28	2.96E - 11
1024	12	33	$5.00 \dot{E} - 07$
1024	16	33	3.58E - 03

n	\mathbf{r}	Iterations	Errors
64	8	28	4.63E - 11
64	12	23	1.69E - 07
64	16	28	7.36E - 06
128	8	28	3.83E - 12
128	12	23	1.45E - 08
128	16	28	1.68E - 05
256	8	28	1.58E - 12
256	12	23	1.02E - 04
256	16	28	6.50E - 04
512	8	28	7.69E - 13
512	12	23	5.00E - 09
512	16	28	8.60E - 06
1024	8	28	9.90E - 14
1024	12	23	1.45E - 09
1024	16	28	2.64E - 05

Table 4.5: Number of Iterations and Error Bounds for Algorithm 3.3 on Type III Polynomials

Table 4.6: Number of Iterations and Error Bounds Algorithm 3.3 on Type IV Polynomials

n	a	Iterations	Errors
64	60	41	2.43E - 04
64	80	42	7.98E - 04
64	100	43	1.72E - 05
128	60	41	1.12E - 03
128	80	42	4.43E - 04
128	100	43	1.31E - 04
256	60	41	2.10E - 04
256	80	42	1.91E - 04
256	100	43	1.34E - 04
512	60	41	3.37E - 04
512	80	42	1.80E - 04
512	100	43	8.33E - 05
1024	60	36	1.10E - 01
1024	80	42	1.16E - 04
1024	100	43	1.76E - 04

n	r	Iterations	Errors
128	8	22.3	5.33E - 06
128	12	24.6	4.85E - 05
128	16	24.94	3.59E - 03
256	8	26.02	1.11E - 06
256	12	27.01	2.37E - 05
256	16	30.18	1.80E - 03
512	8	27.54	2.73E - 08
512	12	28.00	2.27E - 06
512	16	38.18	2.39E - 03

Table 4.7: Number of Iterations and Error Bounds for Algorithm 3.3 on Type V Polynomials

4.3 Tests for the Stabilized Matrix Sign Iterations (Algorithm 3.3) on Gaussian Random Matrices

We tested Algorithm 3.3 on randomly generated matrices of two types:

Type I: Gaussian random tridiagonal matrices of dimension n = 64, 128, 256, 512, 1024. We generated each entry in the tridiagonal part independently by using standard Gaussian distribution and set the other entries to 0. Our tables show the error bounds equal to the maximal difference of the outputs of our algorithm and MATLAB function "eig()". We generated 100 matrices, for each n, and recorded the mean and standard deviation of the error bounds and of the numbers of iterations.

Type II: Random matrices A with a fixed number of real eigenvalues. At first we generated a diagonal matrix Σ with r diagonal entries under the standard real Gaussian distribution and n - r diagonal entries under the standard complex Gaussian distribution, for n = 64, 128, 256, 512, 1024 and r = 8, 12, 16. Then we generated a standard Gaussian random orthogonal matrix Q. Finally we computed the matrices $A = Q^T \Sigma Q$. We generated 100 such matrices A, for each pair of n and r, and recorded the mean and standard deviation of the error bounds and of the numbers of iterations.

The following two tables summarize the performance data, showing a low number of iterations required for ensuring the approximation of the eigenvalues with a reasonable precision.

n	Iteration-mean	Iteration-std	Error-mean	Error-std
64	10.70	2.36	1.78E - 06	1.14E - 05
128	12.16	3.34	5.68E - 07	4.49E - 06
256	12,97	3.97	3.26E - 06	1.35E - 05
512	15.46	9.82	8.80E - 04	8.44E - 03
1024	16.52	10.26	2.43E - 03	2.25E - 02

Table 4.8: Number of Iterations and Error Bounds for Root-finding Algorithm 3.3 on Type I matrices

n	r	Iteration-mean	Iteration-std	Error-mean	Error-std
64	8	11.65	2.47	3.69E - 08	2.29E - 07
64	12	11.75	2.50	3.98E - 10	2.71E - 09
64	16	11.60	2.45	4.10E - 09	3.88E - 08
128	8	13.75	2.79	1.17E - 08	7.56E - 08
128	12	13.70	2.90	4.41E - 09	2.73E - 08
128	16	13.65	2.55	1.23E - 07	1.34E - 06
256	8	14.55	3.26	5.59E - 09	5.58E - 08
256	12	14.15	3.70	1.38E - 07	1.38E - 06
256	16	14.70	2.54	3.06E - 11	1.93E - 10
512	8	13.65	5.59	5.08E - 10	4.88E - 09
512	12	15.65	9.47	7.46E - 04	7.46E - 03
512	16	16.55	10.26	2.78E - 03	5.47E - 03
1024	8	18.20	15.35	2.33E - 10	1.22E - 09
1024	12	20.85	17.60	1.27E - 07	3.36E - 07
1024	16	24.35	19.56	2.19E - 03	4.33E - 03

Table 4.9: Number of Iterations and Error Bounds for Algorithm 3.3 on Type II matrices

4.4 Tests for the Hybrid Matrix Algorithm (Algorithm 3.2) on Benchmark Polynomials

We performed numerical tests of a hybrid algorithm. We began with Algorithm 3.1 and after sufficiently many iterations continued with its variation avoiding matrix inversion.

Namely, we first applied a real shift βI to the companion matrix C_p , such that the matrix $M = C_p + \beta I$ had condition number less than 10⁵. Based on our previous tests, we expected that, for such inputs, at least $T = \log_2 \beta$ iterations $M_{i+1} = \frac{1}{2}(M_i - M_i^{-1})$ would be required in order to move the complex nonreal eigenvalues close enough to $\pm \sqrt{-1}$. After the first T iterations, we periodically (in every 5 iterations) applied two iterations $M_{i+1} = \frac{1}{2}(M_i^3 + 3M_i)$, which converged with cubic rate provided that all complex eigenvalues have distance less than $\frac{1}{2}$ from $\sqrt{-1}$ or $-\sqrt{-1}$. Before switching to the iterations of the second type, we performed the following transformation in order to avoid problems of numerical stability:

Step 1: Compute $P = \frac{0.5M + \sqrt{-1} I}{0.5M + \sqrt{-1} I}$, which maps the real line into the unit circle. Step 2: Compute $Y = \frac{2\sqrt{-1}}{3}(P - P^{-1})$, mapping the unit circle onto the interval [-2/3, 2/3].

Note that these two maps together keep the values $\pm \sqrt{-1}$ unmoved.

We tested polynomials of Types II and IV of the previous section. For polynomials of Types I, III, and V, the test results were similar to those for polynomials of Type II, apparently due to the shared Chebyshev factors. The test results on Type IV polynomials indicate the strength of this algorithm in the case of clustered roots.

The number of iterations required and the error bound are displayed in the tables below.

Table 4.10: Number of Iterations and Error Bounds for Hybrid Algorithm on Type II Polynomials

n	r	Iterations	Errors
64	8	10	3.69E - 10
64	12	23	4.96E - 08
64	16	23	4.97E - 03
128	8	10	2.28E - 11
128	12	28	1.97E - 07
128	16	23	8.68E - 02
256	8	28	6.56E - 12
256	12	28	3.64E - 07
256	16	28	3.82E - 04
512	8	15	8.05E - 13
512	12	28	1.71E - 08
512	16	28	2.78E - 05
1024	8	28	3.72E - 11
1024	12	28	1.09E - 08
1024	16	33	2.19E - 05

Table 4.11: Number of Iterations and Error Bounds for Hybrid Algorithm on Type IV Polynomials

n	Iterations	Errors
64	33	7.32E - 05
128	33	6.12E - 06
256	38	1.60E - 05
512	38	1.08E - 04
1024	38	9.19E - 01

4.5 Tests for the Modular Square Root Iterations (Algorithm 3.4)

Table 4.12 displays our test results for Algorithm 3.4, that is, for the iterations $f_{i+1}(x) \equiv \frac{1}{2}(f_i(x) - f_i(x)^{-1}) \mod p(x)$, which computed polynomial inverses modulo p(x) by solving the associated Sylvester linear systems of equations. We applied the tests to polynomials of Types I and II.

Already after a small number of iterations, that is, for small integers i, the tests have consistently produced polynomials $f_i(x)$ whose roots approximated the complex roots of the polynomial p(x) of (1.1) within the fixed tolerance bound $\epsilon = 10^{-5}$. At this stage of our tests we applied the MATLAB function "roots()" in order to avoid actual computation of agcds. Namely, as soon as we observed that the polynomial p(x) shared all its complex roots with the polynomial $f_i(x)$, we stopped the iterations.

n	r	Type I	Type II
64	8	9	14
64	12	4	16
64	16	2	17
128	8	9	14
128	12	12	16
128	16	2	17
256	8	9	14
256	12	12	16
256	16	8	17
512	8	9	14
512	12	12	16
512	16	8	17
1024	8	10	14
1024	12	12	16
1024	16	11	17

Table 4.12: Number of Iterations for Algorithm 3.4 on Polynomials of Types I and II

Acknowledgements: This work has been supported by NSF Grant CCF-1116736 and PSC CUNY Award 67699-00 45. We are also grateful to Dario A. Bini and two anonymous reviewers, for thoughtful and helpful comments and to Ioannis Z. Emiris and Bernard Mourrain for pointing us out the bibliography on the distribution of real roots of a polynomial.

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Appendix

A Some Maps of the Variables and the Roots

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

Theorem A.1. (Root Inversion, Shift and Scaling, cf. [36].)

(i) Given a polynomial p(x) of (1.1) and two scalars a and b, one can compute the coefficients of the polynomial q(x) = p(ax + b) by using $O(n \log(n))$ arithmetic operations. This bound decreases to 2n - 1 multiplications if b = 0.

(ii) Reversing a polynomial inverts all its roots by involving no flops, that is,

$$p_{\text{rev}}(x) = x^n p(1/x) = \sum_{i=0}^n p_i x^{n-i} = p_n \prod_{j=1}^n (1 - xx_j).$$

Note that by shifting and scaling the variable, we can move all roots of p(x) into a fixed disc, e.g., $D(0,1) = \{x : |x| \le 1\}$.

Theorem A.2. (Dandelin's Root Squaring, cf. [25].)

(i) Let a polynomial p(x) of (1.1) be monic. Then $q(x) = (-1)^n p(\sqrt{x}) p(-\sqrt{x}) = \prod_{j=1}^n (x - x_j^2)$.

(ii) One can evaluate p(x) at the k-th roots of unity, for k > 2n, and then interpolate to q(x) by using $O(k \log(k))$ arithmetic operations overall.

Remark A.1. Recursive root-squaring is prone to numerical stability problems because the coefficients of the iterated polynomials very quickly span many orders of magnitude. It is somewhat surprising, but the Boolean complexity of the recursive root-squaring process is relatively reasonable if high output precision is required [34], [39]. Moreover, one can avoid numerical stability problems and perform all iterations with double precision by applying a special tangential representation of the coefficients and of the intermediate results proposed in [30]. In this case the computations involve more general operations than flops; in terms of the CPU time the computational cost per iteration has the same order as n^2 flops, performed with double precision.

Theorem A.3. (The Cayley Maps.)

(i) The map $y = (x - a\sqrt{-1})/(x + a\sqrt{-1})$, for any real nonzero scalar *a*, sends the real axis $\{x : x \text{ is real}\}$ onto the unit circle $C(0,1) = \{y : |y| = 1\}$.

(ii) The converse map $x = a\sqrt{-1} (1-y)/(y+1)$ sends the unit circle C(0,1) onto the real axis.

B Some Functional Iterations for Polynomial Root-finding

Newton's and Ehrlich–Aberth's are two celebrated functional iteration processes for the approximation of a single root of a polynomial p(x) of (1.1) and all its roots, respectively. They are highly efficient and popular, but not specialized to our task of approximating real roots, and we only use them as auxiliary root-refiners.

Hereafter a disc D(X, r) is said to be γ -isolated for a polynomial p(x) and $\gamma > 1$ if it contains all roots of the polynomial lying in the disc $D(X, \gamma r)$. In this case we say that the disc has isolation ratio at least γ .

Newton's iterations refine an approximation $y^{(0)}$ to a single root of a polynomial p(x) of (1.1),

$$y_0 = c, \ y^{(h+1)} = y^{(h)} - p(y^{(h)})/p'(y^{(h)}), \ h = 0, 1, \dots$$
 (B.1)

Ehrlich-Aberth's iterations refine n simultaneous approximations $z_1^{(0)}, \ldots, z_1^{(n)}$ to all n roots x_1, \ldots, x_n of such a polynomial,

$$z_i^{(h+1)} = z_i^{(h)} - 1/e_i^{(h)}, \text{ for } e_i^{(h)} = p(z_i^{(h)})/p(z_i^{(h)}) - \sum_{j \neq i} \frac{1}{z_i^{(h)} - z_j^{(h)}}, i = 1, \dots, n,$$
(B.2)

See [31], [32] for various other functional iterations.

As we can see next, both iterative algorithms refine very fast the crude initial approximations to simple isolated roots of a polynomial.

Theorem B.1. Assume a polynomial p = p(x) of (1.1) and let $0 < 3(n-1)|y_0 - x_1| < |y_0 - x_j|$, for j = 2, ..., n. Then Newton's iterations (B.1) converge to the root x_1 quadratically right from the start, namely, $|y_k - x_1| \le 2|y_0 - x_1|/2^{2^k}$, for k = 0, 1, ...

Proof. See [56, Theorem 2.4], which strengthens [51, Corollary 4.5].

Theorem B.2. (See [56, Theorem 3.3].) Assume a polynomial p = p(x) of (1.1) and crude initial approximations $y_j^{(0)}$ to the roots x_j such that $0 < 3\sqrt{n-1} |y_j^{(0)} - x_j| < |y_j^{(0)} - y_i^{(0)}|$, for $i \neq j$, $j = 1, \ldots, n$. Then Ehrlich–Aberth's iterations converge to the roots x_j with the cubic rate right from the start, namely, $|y_j^{(k)} - x_j| \leq |y_j^{(0)} - x_j|/(2^{3^k}\sqrt{(n-1)})$, for $j = 1, \ldots, n$ and $k = 0, 1, \ldots$.

The paper [56] also proves quadratic convergence of the WDK iterations to all n roots, lying in some given discs with an isolation ratios at least 3(n-1)/8. These iterations are due to Weierstrass [59], but are frequently attributed to its later re-discoveries by Durand in 1960 and Kerner in 1966.

By exploiting the correlations between the coefficients of a polynomial and the power sums of its roots, the paper [48] had weakened the above assumptions on the initial isolation. More precisely, assuming that a simple root lies in the disc D(0,1) and that the disc has an isolation ratio at least $s \ge 1 + 1/\log_2(n)$, the paper [48] increases it to cn^d , for any fixed pair of constants c and d, at the arithmetic cost O(n), and similarly increased the isolation ratio of the n discs covering all the n roots at the arithmetic cost $O(n \log^2(n))$.

In the case of a single disc, one can assume even an isolation ratio $s \ge 1 + c'/n^{d'}$, for any pair of constants c' and d', and then increase it to $s \ge cn^d$, for any other pair of constants c and d, at the arithmetic cost $O(n \log^2(n))$. Indeed one can achieve this by performing h root-squaring iterations of Theorem A.2, for h of order $\log(n)$ because each squaring of the roots also squares the isolation ratio. This lifting process ensures the desired isolation for the lifted roots of the new lifted polynomial, but the descending back to the original roots can be also achieved by using $O(n \log^2(n))$ arithmetic

operations [34], [39]. We refer the reader to Remark A.1 on the precision growth in these iterations and their Boolean complexity.

Can we completely relax the assumption of the initial isolation? Empirically fast global convergence (that is, convergence right from the start) is very strong over all inputs for the WDK, Ehrlich–Aberth, and some other iterations that approximate simultaneously all n roots of a polynomial p(x) of (1.1). The papers [41], [49], and [42] have challenged the researchers to support this observation with a formal proof, which is still missing, however.

C Fast Root-finding Where All Roots Are Real

Theorem C.1. Assume that all roots of a polynomial p(x) of (1.1) are real.

(i) Then the modified Laguerre algorithm of [15] converges to all of them right from the start, uses O(n) flops per iteration, and therefore approximates all the n roots within $\epsilon = 1/2^b$ by using $O(\log(b))$ iterations and performing $O(n\log(b))$ flops.

(ii) The latter asymptotic arithmetic cost bound is optimal and is supported by the alternative algorithms of [1] and [8] as well.

(iii) All these algorithms reach the optimal Boolean cost bound up to polylogarithmic factors.

D Counting the Roots in a Disc. Root Radii, Distances to the Roots, and the Proximity Tests

In this subsection we estimate the distances to the roots of p(x) from a complex point and the number of the roots in an isolated disc.

The latter task can be solved by using the following result from [51, Lemma 7.1] (cf. also [26], [52, Theorem 14.1] and [9]).

Theorem D.1. [51, Lemma 7.1] It is sufficient to perform FFT at $n' = 16\lceil \log_2 n \rceil$ points (using $1.5n' \log(n')$ flops) and O(n) additional flops and comparisons of real numbers with 0 in order to compute the number of roots of a polynomial p(x) of (1.1) in a 9-isolated disc D(0,r).

Remark D.1. The algorithm of [51] supporting Theorem D.1 only uses the signs of the real and imaginary parts of the n output values of FFT. For some groups of the values, the pairs of the signs stay invariant and can be represented by a single pair of signs. Can this observation be exploited in order to decrease the computational cost of performing the algorithm?

Corollary D.1. It is sufficient to perform $O(hn \log(n))$ flops and O(n) comparisons of real numbers with 0 in order to compute the number of roots of a polynomial p(x) of (1.1) in an s-isolated disc D(0,1), for $s = 9^{1/2^h}$ and any positive integer h.

Proof. Every root-squaring of Theorem A.2 squares all root-radii and the isolation ratios of all discs D(0,r), for all positive r. Suppose h repeated squaring iterations map a polynomial p(x) into $p_h(x)$, for which the disc D(0,1) is 9-isolated. Then, by applying Theorem D.1, we can compute the number of roots of $p_h(x)$ in this disc, equal to the number of roots of p(x).

In view of Remark A.1, one must apply the slower operations of [30] or high precision computations in order to support even a moderately long sequence of root-squaring iterations, but in some cases it is sufficient to apply Corollary D.1, for small positive integers h. Note that $9^{1/2^h}$ is equal to 1.3160..., for h = 2, to 1.1472..., for h = 3, to 1.0710..., for h = 4, and to 1.0349..., for h = 5.

We can use the following result if we agree to perform computations with extended precision.

Theorem D.2. (The Root Radii Approximation.)

Assume a polynomial p(x) of (1.1) and two real scalars c > 0 and d. Define the n root radii $r_j = |x_{k_j}|$, for j = 1, ..., n, distinct $k_1, ..., k_n$, and $r_1 \ge r_2 \ge \cdots \ge r_n$. Then, by using $O(n \log^2(n))$ arithmetic operations, one can compute n approximations \tilde{r}_j to the root radii r_j such that $\tilde{r}_j \le r_j \le (1 + c/n^d)\tilde{r}_j$, for j = 1, ..., n.

Proof. (Cf. [52], [35, Section 4].) At first fix a sufficiently large integer k and apply k times the root-squaring of Theorem A.2, which involves $O(kn \log(n))$ arithmetic operations. Then apply the algorithm of [52] (which uses O(n) arithmetic operations) in order to approximate within a factor of 2n all root radii $r_j^{(k)} = r_j^{2^k}$, j = 1, ..., n, of the output polynomial $p_k(x)$. By taking the 2^k -th roots, approximate the root radii $r_1, ..., r_n$ within a factor of $(2n)^{1/2^k}$, which is $1 + c/n^d$, for k of order $\log(n)$.

Alternatively we can approximate the root radii by applying the semi-heuristic method of [2], used in the packages MPSolve 2000 and 2012 (cf. [5] and [10]) or by recursively applying Theorem D.1, although neither of these techniques support competitive complexity estimates.

The following two theorems define the largest root radius r_1 of the polynomial p(x).

Theorem D.3. (See [57].) Assume a polynomial p(x) of (1.1). 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 $\gamma^+/n \le r_1 \le 2\gamma^+$.

Theorem D.4. (See [37].) 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 largest root radius r_1 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).

Both theorems can be immediately extended to the approximation of the smallest root radius r_n because it is the reciprocal of the largest root radius of the reverse polynomial $p_{rev}(x) = x^n p(1/x)$ (cf. Theorem A.1). Moreover, by shifting a complex point c into the origin (cf. Theorem A.1), we can turn our estimates for the root radii into the estimates for the *distances to the roots* from the point c. Approximation of the smallest distance from a complex point c to a root of p(x) is called the *proximity test* at the point. One can perform such a test by applying Theorems D.1, D.3, or D.4.

Alternatively, for heuristic proximity tests by action at a point c or at n points, one can apply Newton's iterations (B.1) or an appropriate functional iterations, such as the Ehrlich–Aberth iterations (B.2), and estimate the distance to the roots by observing convergence or divergence of the iterations.

Theorem D.4 and all these iterations, including Newton's, Ehrlich–Aberth's and WDK's, can be applied even where a polynomial p(x) is defined by a black box subroutine for its evaluation rather than by its coefficients.