Global Convergence of Hessenberg Shifted QR I: Dynamics

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Abstract

Rapid convergence of the shifted QR algorithm on symmetric matrices was shown more than fifty years ago. Since then, despite significant interest and its practical relevance, an understanding of the dynamics of the shifted QR algorithm on nonsymmetric matrices has remained elusive.

We give a family of shifting strategies for the Hessenberg shifted QR algorithm with provably rapid global convergence on nonsymmetric matrices of bounded nonnormality, quantified in terms of the eigenvector condition number of the input matrix — the convergence is linear with a constant rate and the arithmetic cost of implementing each QR step scales roughly logarithmically in the eigenvector condition number. The key ideas in the analysis are: (1) to use certain higher degree shifts to dampen transient effects due to nonnormality (2) to characterize and detect slowly converging trajectories with respect to such shifts in terms of certain symmetry considerations, and to break this symmetry explicitly in the shifting strategy.

We perform our analysis in exact arithmetic. In the companion papers [BGVS22a, BGVS22b], we show that our shifting strategies can be implemented efficiently in finite arithmetic.

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1 Introduction

The Hessenberg Shifted QR Algorithm, discovered in the late 1950’s independently by Francis [Fra61, Fra62] and Kublanovskaya [Kub62], has been for several decades the most widely used method for approximately computing all of the eigenvalues of a dense matrix. It is implemented in all of the major software packages for numerical linear algebra and was listed as one of the “Top 10 algorithms of the twentieth century,” along with the Metropolis algorithm and the Simplex algorithm [DS00, Par00]. The algorithm is specified by a shifting strategy, which is an efficiently computable function

\[ \text{Sh} : \mathbb{H}^{n \times n} \to \mathbb{P}_k, \]

where \( \mathbb{H}^{n \times n} \) is the set of \( n \times n \) complex Hessenberg matrices and \( \mathbb{P}_k \) is the set of monic complex univariate polynomials of degree \( k \), for some \( k = k(n) \) typically much smaller than \( n \). The word “shift” comes from the fact that when \( k = 1 \) we have \( p_t(H_t) = H_t - s_tI \) for some \( s_t \in \mathbb{C} \). The algorithm then consists of the following discrete-time isospectral nonlinear dynamical system on \( \mathbb{H}^{n \times n} \), given an initial condition \( H_0 \):

\[
\begin{align*}
Q_tR_t &= p_t(H_t) \quad \text{where } p_t = \text{Sh}(H_t) \quad \text{whenever } p_t(H_t) \text{ is invertible}, \\
H_{t+1} &= Q_t^*H_tQ_t, \quad t = 0, 1, 2, \ldots.
\end{align*}
\]

The first step in (1) is a QR decomposition so that \( Q_t \) is unitary. It is not hard to see that each iteration preserves the Hessenberg structure; we ignore the case when \( p_t(H_t) \) is singular in this introduction (see Section 1.3 for a discussion).

The relevance of this iteration to the eigenvalue problem stems from two facts. First, every matrix \( A \in \mathbb{C}^{n \times n} \) is unitarily similar to a Hessenberg matrix \( H_0 \), and in exact arithmetic such a similarity can be computed exactly in \( O(n^3) \) operations. Second, it was shown in [Fra61, Kub62] that for the trivial “unshifted” strategy \( p(z) = z \), the iterates \( H_t \) under some mild genericity conditions always converge to an upper triangular matrix \( H_\infty \); this is because the unshifted QR iteration can be precisely related to the (inverse) power iteration (see e.g. [TBI97]). Combining the unitary similarities accumulated during the iteration, these two facts yield a Schur factorization \( A = Q^*H_\infty Q \) of the original matrix, from which the eigenvalues of \( A \) can be read off. The unshifted QR iteration does not give an efficient algorithm, however, as it is easy to see that convergence can be arbitrarily slow if the ratios of the magnitudes of the eigenvalues of \( H_0 \) are close to 1. The role of the shifting strategy is to adaptively improve these ratios and thereby accelerate convergence. The challenge is that this must be done efficiently without prior knowledge of the eigenvalues.

We quantify the rate of convergence of a sequence of iterates of (1) in terms of its \( \delta \)-decoupling time \( \text{dec}_\delta(H_0) \), which is defined as the smallest \( t \) at which some subdiagonal entry of \( H_t \) satisfies

\[ |H_t(i+1, i)| \leq \delta \|H_t\|. \]

In this context, “rapid” convergence means that \( \text{dec}_\delta(H_0) \) is a very slowly growing function of \( n \) and \( 1/\delta \), ideally logarithmic or polylogarithmic.

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1 In the sense of backward error, i.e., exactly computing the eigenvalues of a nearby matrix.

2 In this paper, we assume exact arithmetic with complex numbers and count arithmetic operations as a measure of complexity.

3 A matrix \( H \) is (upper) Hessenberg if \( H(i,j) = 0 \) whenever \( i > j + 1 \). Such matrices are “almost” upper triangular.
In a celebrated work, Wilkinson [Wil68] proved global convergence of shifted QR on all real symmetric tridiagonal matrices using the shifting strategy that now carries his name. The linear convergence bound $\text{dec}_\delta(H_0) \leq O(\log(1/\delta))$ for this shifting strategy was then obtained by Dekker and Traub [DT71] (in the more general setting of Hermitian matrices), and reproven by Hoffman and Parlett [HP78] using different arguments. Other than these results for Hermitian matrices, there is no known bound on the worst-case decoupling time of shifted QR for any large class of matrices or any other shifting strategy. Shifted QR is nonetheless the most commonly used algorithm in practice for the nonsymmetric eigenproblem on dense matrices. The strategies implemented in standard software libraries heuristically converge very rapidly on “typical” inputs, but occasionally examples of nonconvergence are found [Day96, Mol14] and dealt with in ad hoc ways.

Accordingly, the main theoretical question concerning shifted QR, which has remained open since the 1960s, is:

**Question D.** Is there a shifting strategy for which the Hessenberg shifted QR iteration provably and rapidly decouples on nonsymmetric matrices?

Question D was asked in various forms e.g. by Parlett [Par73, Par74], Moler [Mol78, Mol14], Demmel [Dem97, Ch. 4], Higham [HDG15, IV.10], and Smale [Sma97] (who referred to it as a “great challenge”).

The main result of this article (Theorem 1.3) is a positive answer to Question D which is quantified in terms of the degree of nonnormality of the input matrix $H_0$. Let $\mathcal{H}_B^{n \times n}$ be the set of diagonalizable complex Hessenberg matrices $H_0$ with eigenvector condition number $\kappa_V(H_0) \leq B$. We exhibit a two parameter family of deterministic shifting strategies $S_{k,B}$ indexed by a degree parameter $k = 2, 4, 8 \ldots$ and a nonnormality parameter $B \geq 1$ such that:

(i) The strategy $S_{k,B}$ satisfies $\text{dec}_\delta(H_0) \leq O(\log(1/\delta))$ for every $H_0 \in \mathcal{H}_B^{n \times n}$ and $\delta > 0$.

(ii) $S_{k,B}$ has degree $k$ and can be computed in roughly $O((\log k + B^{1/k})kn^2)$ arithmetic operations, which is simply $O(n^2k\log k)$ for the judicious setting $k = \Omega(\log B \log \log B)$.

Thus, the computational cost of the shifting strategy required for convergence blows up as the input matrix becomes more and more nonnormal, but the dependence on nonnormality is very mild.

We remark that such a result was not previously known even in the case $B = 1$ of normal matrices. Further, as we discuss in Remark 1.4, a tiny random perturbation of any $H_0 \in \mathcal{H}_B^{n \times n}$ is likely to be an element of $\mathcal{H}_B^{n \times n}$ for small $B$ (not depending on $H_0$). Thus, while our theorem does not give a single shifting strategy which works for all matrices, it does give a strategy which works for a tiny random perturbation of every matrix (with high probability, where “tiny” and “small” must be quantified appropriately). This may be viewed as a smoothed analysis result in the sense of [ST04], with the notable feature that the running time of the algorithm depends very mildly on

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4i.e., from any initial condition $H_0$.

5i.e., arising as the Hessenberg form of symmetric matrices.

6For nonnormal matrices, it is not even known if there is a shifting strategy which yields global convergence regardless of an effective bound on the decoupling time. A thorough discussion of related work appears in Section 1.3.

7See Section 1.1 for a precise definition.
the size of the perturbation, or alternatively as a quantitative statement about the shifting strategy succeeding for “almost all” matrices.

Remark 1.1 (Arithmetic Complexity from Decoupling Time). The motivation for the particular measure of convergence above is that there is a procedure called deflation which zeroes out the smallest subdiagonal entry of a $\delta$-decoupled Hessenberg matrix and obtains a nearby block upper triangular matrix, which allows one to pass to subproblems of smaller size incurring a backward error of $\delta\|H_0\|$. Repeating this procedure $n$ times (and exploiting the special structure of Hessenberg matrices to compute the $Q_i$ efficiently) yields an algorithm for computing a triangular $T$ and unitary $Q$ such that $\|H_0 - Q^*TQ\| \leq n\delta\|H_0\|$ in a total of $O(n^3\dec(H_0))$ arithmetic operations [Wat07]. Thus, the interesting regime is to take $\delta \ll 1/n$.

1.1 Statement of Results

We need the following two notions to precisely state our main theorem.

Eigenvector Condition Number. The eigenvector condition number $\kappa_V(M)$ is defined for a diagonalizable matrix $M$ as

$$\kappa_V(M) := \inf_{V:M = VDV^{-1}} \| V \| \| V^{-1} \|.$$ 

Note that $\kappa_V(M) = 1$ for a normal matrix and that $\kappa_V(H_t) = \kappa_V(H_0)$ for all iterates of the QR algorithm due to unitarily similarity. It is not hard to see that the infimum is achieved.

$\theta$-Optimal Ritz Values. Like most previously studied shifting strategies, we define $\text{Sh}_{k,B}(H_t)$ in terms of the Ritz values of the current iterate $H_t$. Recall that the Ritz values of order $k$ of a Hessenberg matrix $H$ are the eigenvalues of its bottom right $k \times k$ corner $(H)_{(k)}$; they are also characterized variationally as the roots of the degree $k$ monic polynomial $p$ minimizing $\| e_n^* p(H) \|$, where $e_n$ is the last standard basis vector (see Lemma 2.2 for details). Since computing eigenvalues exactly is impossible when $k \geq 5$, we assume access to a method for computing approximate Ritz values, in the sense encapsulated in the following definition.

Definition 1.2 ($\theta$-Optimal Ritz values and Ritz value finders). Let $\theta \geq 1$. We call $\mathcal{R} = \{r_1, \ldots, r_k\} \subset \mathbb{C}$ a set of $\theta$-optimal Ritz values of a Hessenberg matrix $H$ if

$$\left\| e_n^* \prod_{i \leq k} (H - r_i) \right\|^{1/k} \leq \theta \min_{p \in \mathcal{P}_k} \| e_n^* p(H) \|^{1/k}. \tag{2}$$

A Ritz value finder is an algorithm OptRitz$(H,k,\theta)$ that takes as inputs a Hessenberg matrix $H \in \mathbb{C}^{n \times n}$, a positive integer $k$ and an accuracy parameter $\theta > 1$, and outputs a set $\mathcal{R} = \{r_1, \ldots, r_k\}$ of $\theta$-optimal Ritz values of $H$ whenever the right hand side of (2) is nonzero. Let $T_{\text{OptRitz}}(k,\theta,\delta)$ be the maximum number of arithmetic operations used by OptRitz$(H,k,\theta)$ over all inputs $H$ such that the right hand side of (2) satisfies\(^8\)

$$\min_{p \in \mathcal{P}_k} \| e_n^* p(H) \|^{1/k} \geq \delta \| H \|.$$ 

\(^8\)Such a lower bound is needed, since otherwise we could use OptRitz to compute the eigenvalues of $H_{(k)}$ to arbitrary accuracy in finite time.
A Ritz value finder satisfying Definition 1.2 can be efficiently instantiated using polynomial root finders (e.g. [Pan02]) or other provable eigenvalue computation algorithms (e.g. [BGVKS20b, BGVS22a]) with guarantees of type \( T_{\text{OptRitz}}(\theta, k, \delta) = O(k^2 \log(\frac{1}{\theta-1})) \). We defer a detailed discussion of numerical issues surrounding this implementation to our companion papers [BGVS22a, BGVS22b]. The subtlety of not being able to compute Ritz values exactly is secondary to the dynamical phenomena which are the focus of this paper, so on first reading it is recommended to assume \( \theta = 1 \) (i.e., Ritz values are computed exactly), even though this is unrealistic when \( k > 4 \). The theorem below is stated with \( \theta = 2 \), which is also the parameter setting used in [BGVS22a].

We now present our main theorem. All logarithms are base 2.

**Theorem 1.3.** There is a family of deterministic shifting strategies \( \text{Sh}_{k,B} \) (described in Section 2) parameterized by degree \( k = 2, 4, 8, \ldots \) and nonnormality bound \( B \geq 1 \) with the following properties.

1. **(Rapid Decoupling)** If \( H_0 \in \mathbb{H}_B^{n \times n} \), then for every \( \delta > 0 \), the QR iteration with strategy \( \text{Sh}_{k,B} \) satisfies
   \[
   \text{dec}_\delta(H_0) \leq 4 \log(1/\delta).
   \]  

2. **(Cost Per Iteration Before Decoupling)** Given a Ritz value finder \( \text{OptRitz}(H, k, \theta) \) with complexity \( T_{\text{OptRitz}}(k, \theta, \delta) \), an accuracy parameter \( \delta > 0 \), and a Hessenberg matrix \( H_t \in \mathbb{H}_B^{n \times n} \), computing \( H_{t+1} \) given \( H_t \) has a cost per iteration of at most
   \[
   \left( \log k + N_{\text{net}} \left( 0.002 B^{-\log^2 k + 4} \right) \right) \cdot T_{\text{iqr}}(k, n) + T_{\text{OptRitz}}(k, 2, \delta) + \log k
   \]  
   arithmetic operations for all iterations before (3) is satisfied, where \( N_{\text{net}}(\epsilon) = O(e^{-2}) \) is number of points in an efficiently computable \( \epsilon \)-net of the unit disk and \( T_{\text{iqr}}(k, n) \leq 7kn^2 \) is an upper bound on the arithmetic cost of a degree \( k \) implicit QR step (see Section 2).

The term involving \( N_{\text{net}} \) captures the cost of performing certain “exceptional shifts” (see Section 1.3) used in the strategy. The tradeoff between the nonnormality of the input matrix and the efficiency of the shifting strategy appears in the cost of the exceptional shift, where it is seen that setting
   \[
   k = \Omega(\log B \log \log B)
   \]  
yields a total running time of \( O(n^2 k \log k) \) operations per iteration. Note that the bound \( B \geq \kappa_V(H_0) \) must be known in advance in order to determine how large a \( k \) is needed to make the cost of the exceptional shift small. One may also take \( k \) to be a constant independent of \( B \), but this causes the arithmetic complexity of each iteration to depend polynomially on \( B \) rather than logarithmically. Note that for normal matrices one may take \( k = 2 \) and \( B = 1 \).

**Remark 1.4** (Regularization of \( \kappa_V \) by Random Perturbation). The pseudospectral regularization guarantees from [BKMS21] (verifying the conjecture of [Dav08]) imply that every matrix \( A \) is \( \delta \)-close in operator norm to matrices with \( \kappa_V = O(n^2/\delta) \). Such a nearby, well-conditioned matrix can be produced (with high probability) by perturbing each entry of \( A \) with an independent complex Gaussian of variance \( \delta^9 \). After perturbing we can thus (with high probability) take \( B = O(n^2/\delta) \) in Theorem 1.3 and set \( k = O(\log(n/\delta) \log \log (n/\delta)) \), incurring a backward error of \( \delta \) and yielding a

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\[^9\text{See also [BGVKS20a, JSS20] for more general perturbations which have a similar effect and [ABB}^{18}\text{] for similar results in the complex Gaussian case.}\]
per iteration arithmetic cost of \( O(n^2 \log(n/\delta) \log \log^2(n/\delta)) \) before \( \delta \)-decoupling. This approach embraces the fact that the shifted QR algorithm can only in the first place guarantee backward accuracy of the eigenvalues it computes, so there is no harm in using an initial small random perturbation as a “preconditioning” step.

**Remark 1.5 (Higher Degree Shifts).** A QR step with a degree \( k \) shift \( p(z) = (z - r_1) \ldots (z - r_k) \) is identical to a sequence of \( k \) steps with degree 1 shifts \((z - r_1), (z - r_2), \ldots, (z - r_k)\) (see e.g. [Wat07] for a proof), so any degree \( k \) strategy can be simulated by a degree 1 strategy while increasing the iteration count by a factor of \( k \).\(^{10}\) We choose to present our strategy as higher degree for conceptual clarity. The efficiency of using degrees as high as \( k = 180 \) has been tested in the past [BBM02, Section 3] and \( k = 50 \) is often used in practice [Kre21].

**Remark 1.6 (Numerical Stability, Deflation, and Bit Complexity).** The strategy in Theorem 1.3 can be implemented in floating point arithmetic using \( O(k \log(n/\delta)) \) bits of precision for the implicit QR steps\(^{11}\) and \( O(k^2 \log^2(n/\delta)) \) bits of precision for the Ritz value finder\(^{12}\), while preserving both correctness and rapid convergence, with the caveat that the numerical implementation requires using randomization in order to be efficient. This is proved in the companion papers [BGVS22a, BGVS22b], along with a detailed analysis of deflation, yielding a complete algorithm for computing the eigenvalues of a matrix with good bit complexity estimates.

### 1.2 Techniques

There are two distinct phenomena which make analyzing the dynamics of shifted QR challenging.

1. **Transient behavior due to nonnormality.** In the nonnormal case, the iterates \( H_t \) can behave chaotically on short time scales,\(^{13}\) lacking any kind of obvious algebraic or geometric monotonicity properties (which are present in the symmetric case). This lack of monotonicity makes it hard to reason about convergence.

2. **Fixed points and periodic orbits due to symmetry.** The most natural shifting strategies define \( p_t(z) \) as a simple function of the entries of \( H_t \), typically a function of the characteristic polynomial of the bottom right \( k \times k \) corner \( (H_t)_{(k)} \) of \( H_t \) (see Section 1.3 for more details). These strategies typically have attractive fixed points and cycles which are not upper triangular, leading to slow convergence or nonconvergence (e.g. see [Par66, Bat90, Day96]). The conceptual cause of these fixed points is symmetry — at a very high level, the dynamical system “cannot decide which invariant subspace to converge to.” This feature is seen even in normal matrices, and in fact its most severe manifestation occurs in the case of unitary matrices.

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\(^{10}\)This also has some important advantages with regards to numerical stability, which are discussed in [BGVS22a].

\(^{11}\)Hence, when a random perturbation is used as a preconditioner, in view of Remark 1.4 the number of bits of precision required becomes \( O(\log^2(n/\delta) \log\log(n/\delta)) \).

\(^{12}\)The Ritz value finder is invoked only on small \( k \times k \) matrices and incurs a subdominant cost.

\(^{13}\)We measure time not as the number of QR steps, but as the number of QR steps of degree 1, so for example a QR step with a degree \( k \) shift corresponds to \( k \) time steps.
Example 1.7. Both pathologies are seen in the instructive family of \( n \times n \) examples

\[
M = \begin{pmatrix}
\beta_1 & \beta_n \\
\beta_2 & \\
& \ddots \\
& & \ddots \\
& & & \beta_{n-1}
\end{pmatrix}
\]

where \( \beta_1, \ldots, \beta_n \in (0, 1) \). Observe that, for \( k \leq n - 1 \), the characteristic polynomial of \( M_{(k)} \) is just \( z^k \), so any naïve shifting strategy based on it will yield the trivial shift. One can verify that a QR step with the trivial strategy applied to \( M \) cyclically permutes the \( \beta_i \), while leaving the zero pattern of \( M \) intact. This means that for adversarially chosen \( \beta_1, \ldots, \beta_n \), the bottom few subdiagonal entries of \( M \) — the traditional place to look for monotonicity in order to prove convergence — exhibit arbitrary behavior over a small number of QR steps. At very long time scales of \( n \) steps, the behavior becomes periodic and predictable, but there is still no convergence.

Previous approaches to Question D have been essentially algebraic (relying on examining entries of the iterates, their resolvents, or characteristic polynomials of their submatrices) or geometric (viewing the iteration as a flow on a manifold), and have been unable to surmount these difficulties in the nonsymmetric case.

In contrast, we take an essentially analytic approach. The key idea is to associate a measure \( \mu_t \), similar in spirit to the notion of spectral measure of a normal matrix, with the not necessarily normal iterates \( H_t \). When the eigenvector condition number \( \kappa_V(H_0) \) is bounded, the dynamics of shifted QR can be understood in terms these measures: it turns out that while the \( \mu_t \) may evolve erratically on short time scales, they must behave in a predictable way over time scales of \( k \) degree 1 QR steps when \( k \gg \log \kappa_V(H_0) \) as in \((5)\) — essentially, this is enough to “damp” the transient behavior due to nonnormality (this is articulated precisely in Section 2.1). Specifically, the behavior of the \( \mu_t \) can be related to the geometric mean of the bottom \( k \) subdiagonal entries of \( H_t \), which we show satisfies an approximate monotonicity property and use as a potential function to track convergence.

To see this phenomenon in action, if we impose a bound on \( \kappa_V(M) \) in Example 1.7, it can be seen that the ratios of the \( \beta_i \) cannot be arbitrary and the geometric mean of the bottom \( \log \kappa_V(M) \) subdiagonal entries of \( M \) must remain almost-constant on intervals of \( k \) unshifted QR steps.

The above insights are sufficient to handle the transience issue but not the symmetry issue. For the latter, we carefully design a shifting strategy which satisfies the following dichotomy: either (i) a certain QR step of degree \( k \) significantly decreases the potential function defined above, or (ii) the measure \( \mu_t \) associated to the current iterate \( H_t \) must have a special structure (essentially, being well-supported on an annulus of a particular radius). In the second case (which corresponds to the symmetry case discussed above) we exploit the structure to design a simple exceptional shift which is guaranteed to significantly reduce the potential, yielding linear convergence in either case. Thus, our proof articulates that transients and symmetry are the only obstacles to rapid convergence of the shifted QR iteration on nonsymmetric matrices.
1.3 History and Related Work

The literature on shifted QR is vast, so we mention only the most relevant works — in particular, we omit the large body of experimental work and do not discuss the many works on local convergence of shifted QR (i.e., starting from an $H_0$ which is already very close to decoupling). The reader is directed to the excellent surveys [Bat95, Sma97, Chu08] or [Par00, Wat08, GU09] for a dynamical or numerical viewpoint, respectively, or to the books [GVL96, TBI97, Dem97, Wat07] for a comprehensive treatment.

Most of the shifting strategies studied in the literature are a combination of the following three types. The motivation for considering shifts depending on $H^{(k)}$ is closely related to Krylov subspace methods, see e.g. [Wat07]. Below $H$ denotes the current Hessenberg iterate.

1. **k-Francis Shift.** Take $p(z) = \det(z - H^{(k)})$ for some $k$. The case $k = 1$ is called Rayleigh shift.

2. **Wilkinson Shift.** Take $p(z) = (z - a)$ where $a$ is the root of $\det(z - H^{(2)})$ closer to $H^{(1)}$.

3. **Exceptional Shift.** Let $p(z) = (z - x)$ for some $x$ chosen randomly or arbitrarily, perhaps with a specified magnitude (e.g. $|x| = 1$ for unitary matrices in [EH75, Wan01, WG02, WG03]).

Shifting strategies which combine more than one of these through some kind of case analysis are called “mixed” strategies.

**Symmetric Matrices.** Jiang [Exr92] showed that the geometric mean of the bottom $k$ subdiagonal entries is monotone for the $k$-Francis strategy in the case of symmetric tridiagonal matrices. Aishima et al. [AMMS12] showed that this monotonicity continues to hold for a “Wilkinson-like” shift which chooses $k - 1$ out of $k$ Ritz values. Both of these results yield global convergence on symmetric tridiagonal matrices (without a rate).

**Rayleigh Quotient Iteration and Normal Matrices.** The behavior of shifted QR is well known to be related to shifted inverse iteration (see e.g. [TBI97]). In particular, the Rayleigh shifting strategy corresponds to a vector iteration process known as Rayleigh Quotient Iteration (RQI). Parlett [Par74] (building on [Ost57, Buu58, PK68]) showed that RQI converges globally (but without giving a rate) on almost every normal matrix and investigated how to generalize this to the nonnormal case.

Batterson [Bat90] studied the convergence of 2-Francis shifted QR on $3 \times 3$ normal matrices with a certain exceptional shift and showed that it always converges. The subsequent work [Bat94] showed that 2-Francis shifted QR converges globally on almost every real $n \times n$ normal matrix (without a rate). In Theorem 6 of that paper, it was shown that the same potential that we consider is monotone-decreasing when the $k$-Francis shift is run on normal matrices, which was an inspiration for our proof of almost-monotonicity for nonnormal matrices.

**Nonnormal Matrices.** Parlett [Par66] showed that an unshifted QR step applied to a singular matrix leads to immediate 0-decoupling, taking care of the singularity issue that was glossed over in the introduction, and further proved that all of the fixed points of an extension of the 2-Francis shifted QR step (for general matrices) are multiples of unitary matrices.

In a sequence of works, Batterson and coauthors investigated the behavior of RQI and 2-Francis on nonnormal matrices from a dynamical systems perspective. Batterson and Smillie
[BS89, BS90] showed that there are real matrices such that RQI fails to converge for an open set of real starting vectors. The latter paper also established that RQI exhibits chaotic behavior on some instances, in the sense of having periodic points of infinitely many periods. Batterson and Day [BD92] showed that 2-Francis shifted QR converges globally and linearly on a certain conjugacy class of $4 \times 4$ Hessenberg matrices.

In the realm of periodicity and symmetry breaking, Day [Day96], building on an example of Demmel, showed that there is an open set of $4 \times 4$ matrices on which certain mixed shifting strategies used in the EISPACK library fail to converge rapidly in exact arithmetic; such an example was independently discovered by Moler [Mol14] who described its behavior in finite arithmetic. These examples are almost normal in the sense that they satisfy $\kappa_V \leq 2$, so the reason for nonconvergence is symmetry, and our strategy $\text{Sh}_{k,B}$ with modest parameters $k = B = 2$ is guaranteed to converge rapidly on them (in exact arithmetic).

Using topological considerations, Leite et al. [LST13] proved that no continuous shifting strategy can decouple on every symmetric matrix. Accordingly (in retrospect), the most successful shifting strategy for symmetric matrices, the Wilkinson Shift, is discontinuous in the entries of the matrix and explicitly breaks symmetry when it occurs. Our strategy $\text{Sh}_{k,B}$ is also discontinuous in the entries of the matrix.

**Mixed and Exceptional Shifts.** Eberlein and Huang [EH75] showed global convergence (without a bound on the rate) of a certain mixed strategy for unitary Hessenberg matrices; more recently, the works [Wan01, WG02, WG03] exhibited mixed strategies which converge globally for unitary Hessenberg matrices with a bound on the rate, but this bound depends on the matrix in a complicated way and is not clearly bounded away from 1. Our strategy $\text{Sh}_{k,B}$ is also a mixed strategy which in a sense combines all three types above. Our choice of exceptional shift was in particular inspired by the work of [EH75, WG02] — the difference is that the size of the exceptional shift is naturally of order 1 in the unitary case, but in the general case it must be chosen carefully at the correct spectral scale.

**Higher Degree Shifts.** The idea of using higher degree shifts was already present in [Fra61, DT71], but was popularized in by Bai and Demmel in [BD89], who observed that higher order shifts can sometimes be implemented more efficiently than a sequence of lower order ones; see [BD89, Section 3] for a discussion of various higher order shifting strategies which were considered in the 1980s.

**Integrable Systems.** The unshifted QR algorithm on Hermitian matrices is known to correspond to evaluations of an integrable dynamical system called the Toda flow at integer times [DNT83]; such a correspondence is not known for any nontrivial shifting scheme or for nonnormal matrices. See [Chu08] for a detailed survey of this connection. More recently, the line of work [PDM13, DMOT14, DT19] studied the universality properties of the decoupling time of unshifted QR on random matrices, and used the connection to Toda flow to prove universality in the symmetric case; it was experimentally observed that such universality continues to hold for shifted QR.

We defer a detailed discussion of the extensive related work on numerical issues related to shifted QR as well as a comparison to other algorithms for computing eigenvalues (in particular, [ABB+18] and [BGVKS20b]) to our companion paper [BGVS22a].
Organization. The remainder of the paper, Section 2, contains the proof of Theorem 1.3. Section 2.1 contains some elementary but important lemmas, as well as the notion of approximate functional calculus (see Lemma 2.4) which will be used repeatedly in the sequel. The notion of a promising Ritz value, around which our shifting strategy revolves, appears in Section 2.2 along with a discussion of its key properties. We describe the shifting strategy $\text{Sh}_{k,B}$ and prove Theorem 1.3 in Section 2.3, deferring some lemmas and details to the final sections.

2 Main Result

Throughout the remainder of the paper, $H = (h_{i,j})_{i,j \in \mathbb{N}}$ will denote an $n \times n$ upper Hessenberg matrix, $B \geq \kappa_V(H)$ an upper bound on its eigenvector condition number and and $k \geq 2$ a power of two, which the reader may consider for concreteness to be on the order of $\log B \log \log B$; all logarithms will be taken base two for simplicity. As above, we use $H_k$ and $\chi_k(z)$ to denote the lower-right $k \times k$ corner of $H$ and its characteristic polynomial respectively. All matrix norms are operator norms, denoted by $\| \cdot \|$.

We will use the geometric mean of the last $k$ subdiagonal entries of the $H$ to track convergence of the Shifted QR iteration, since we are guaranteed $\delta$-decoupling once this quantity is smaller than $\delta \|H\|$. More explicitly, define the potential $\psi_k(H)$ of $H$ to be

$$\psi_k(H) := |h_{n-k,n-k-1} \cdots h_{n,n-1}|^{\frac{1}{k}}.$$  

Fixing some $\gamma \in (0,1)$, we will show that our shifting strategy guarantees potential reduction: the efficient computation of a Hessenberg matrix $\tilde{H}$, unitarily equivalent to $H$, with the property that

$$\psi_k(\tilde{H}) \leq \gamma \psi_k(H).$$  

(6)

Since $\psi_k(H) \leq \|H\|$, it follows immediately that we can achieve $\delta$-decoupling in $\frac{\log \delta}{\log \gamma}$ iterations. Note that the relationship (5) between $k$ and $B$ is not required for the proof of potential reduction, but impacts the cost of performing each iteration. The table below collates several constants which will appear throughout the paper.

| Symbol | Meaning | Typical Scale |
|--------|---------|---------------|
| $H$    | Upper Hessenberg matrix | | |
| $B$    | Eigenvector condition bound | $B \geq \kappa_V(H)$ |
| $k$    | Shift degree | $O(\log B \log \log B)$ |
| $\delta$ | Decoupling parameter | |
| $\gamma$ | Decoupling rate | 0.8 |
| $\theta$ | Approximation parameter for Ritz values | 2 |
| $\alpha$ | Promising Ritz value parameter | $B^{4k^{-1}} \log k = 1 + o(1)$ |

We assume black box access to a routine for efficiently performing a QR step in $O(kn^2)$ arithmetic operations rather than $O(kn^3)$. 

10
Definition 2.1 (Implicit QR Algorithm). For \( k \leq n \), an exact implicit QR algorithm \( \text{iqr}(H, p(z)) \) takes as inputs a Hessenberg matrix \( H \in \mathbb{C}^{n \times n} \) and a polynomial \( p(z) = (z - s_1) \cdots (z - s_k) \) and outputs a Hessenberg matrix \( \hat{H} \) satisfying
\[
\hat{H} = Q^* H Q,
\]
where \( Q \) is a unitary matrix such that \( p(H) = QR \) for some upper triangular matrix \( R \), as well as the number \( \| e_n^* p^{-1}(H) \| \) whenever \( p(H) \) is invertible. It runs in at most
\[
T_{\text{iqr}}(k, n) \leq 7kn^2
\]
operations.

See e.g. [Wat08, Section 3] for a proof in exact arithmetic of the existence of an efficient implicit QR algorithm.

2.1 Basic Lemmas and Approximate Functional Calculus

Before introducing and analyzing our shifting strategy, we pause to prove three simple and essential lemmas relating the potential \( \psi_k(H) \), the Hessenberg structure of \( H \), its eigenvector condition number \( \kappa_V(H) \), and certain measures associated with \( H \). The first is well known and gives a variational characterization of the potential (see [TBI97, Theorem 34.1]).

Lemma 2.2 (Variational Formula for \( \psi_k \)). Let \( H \in \mathbb{C}^{n \times n} \) be any Hessenberg matrix. Then, for any \( k \)
\[
\psi_k(H) = \min_{p \in \mathcal{P}_k} \| e_n^* p(H) \|^{\frac{1}{k}},
\]
with the minimum attained for \( p = \chi_k \).

Proof. Since \( H \) is upper Hessenberg, for any polynomial \( p \in \mathcal{P}_k \) we have
\[
p(H)_{n,n-j} = \begin{cases} 
p(H_{(k)})_{k,k-j+1} & j = 0, \ldots, k-1, \\
h_{n-k,n-k-1} \cdots h_{n,n-1} & j = k, \\
0 & j \geq k+1. \end{cases}
\]
Thus for every such \( p \),
\[
\min_{p \in \mathcal{P}_k} \| e_n^* p(H) \| \geq | h_{n-k,n-k-1} \cdots h_{n,n-1} | = \psi_k(H)^k,
\]
and the bound will be tight for any polynomial whose application to \( H_{(k)} \) zeroes out the last row; by Cayley-Hamilton, the matrix \( \chi_k(H_{(k)}) \) is identically zero. \( \square \)

It will be useful to have a mechanism for proving upper bounds on the potential of \( \hat{H} \) produced from \( H \) by an implicit QR step. To this end, let \( p \in \mathcal{P}_k \) and define
\[
\tau_p(H) := \| e_n^* p(H)^{-1} \|^{\frac{1}{k}},
\]
when \( p(H) \) is invertible, and \( \tau_p(H) = 0 \) otherwise. The special case \( k = 1 \) of this quantity has been used to great effect in previous work studying linear shifts (e.g. [HP78]), and our next lemma shows that it bounds the potential of \( \hat{H} = \text{iqr}(H, p(z)) \) for shift polynomials \( p \) of arbitrary degree.
Lemma 2.3 (Upper Bounds on $\psi_k(\hat{H})$). Let $H \in \mathbb{C}^{n \times n}$ be a Hessenberg matrix, $p(z)$ a monic polynomial of degree $k$ and $\hat{H} = \text{iqr}(H, p(z))$. Then

$$\psi_k(\hat{H}) \leq \tau_p(H).$$

*Proof.* Assume first that $p(H)$ is singular. In this case for any QR decomposition $p(H) = QR$, the entry $R_{n,n} = 0$, and because $p(\hat{H}) = Q^* p(H) Q = RQ$, the last row of $p(\hat{H})$ is zero as well. In particular $\psi_k(\hat{H}) = |p(\hat{H})_{1,k+1}|^\frac{1}{2} = 0 = \tau_p(H)$. When $p(H)$ is invertible, applying Lemma 2.2 and using repeatedly that $Q$ is unitary, $R$ is triangular, and $p(H) = QR$,

$$\psi_k(\hat{H})^k \leq \|e_n^* p(\hat{H})\| = \|e_n^* Q^* p(H)\| = \|e_n^* R\| = \|e_n^* R^{-1} Q^*\|^{-1} = \|e_n^* p(H)^{-1}\|^{-1} = \tau_p(H)^k.$$

Lemma 2.3 ensures that given $H$, we can reduce the potential with an implicit QR step by producing a polynomial $p$ with $\|e_n^* p(H)^{-1}\|^{-1} \leq \gamma \psi_k(H)$. To do so, we will require a final lemma relating quantities of this form to the moments of a certain measure associated to $H$ which quantifies the overlap of the vector $e_n^*$ with the left eigenvectors of $H$.

**Measures on Spec($H$).** The following construction will be used extensively throughout the paper. Assume that $H = VDV^{-1}$ is diagonalizable, with $V$ chosen\(^\dagger\) so that $\|V\| = \|V^{-1}\| = \sqrt{\kappa_V(H)}$ and $D$ a diagonal matrix with $D_{i,i} = \lambda_i$, the eigenvalues of $H$. Write $Z_H$ for the random variable\(^\ddagger\) supported on the eigenvalues of $H$, with distribution

$$\mathbb{P}[Z_H = \lambda_i] = \frac{|e_n^* V e_i|^2}{\|e_n^* V\|^2}$$

so that $\mathbb{P}[Z_H = \lambda_i] = 1$ exactly when $e_n^*$ is a left eigenvector with eigenvalue $\lambda_i$.

When $H$ is normal, the distribution of $Z_H$ is the spectral measure of $H$ associated to $e_n^*$, and by the functional calculus we have $\|e_n^* p(H)^{-1}\| = \mathbb{E}\|p(Z_H)^{-1}\|^{-1}$, meaning that the (inverse) moments of $Z_H$ are observable to us even without knowing the true eigenvectors and eigenvalues of $H$. The following lemma generalizes this fact to the nonnormal case, at a multiplicative cost of $\kappa_V(H)$.

**Lemma 2.4 (Approximate Functional Calculus).** For any upper Hessenberg $H$ and complex function $f$ whose domain includes the eigenvalues of $H$,

$$\|e_n^* f(H)\| \leq \mathbb{E}\|f(Z_H)^{-1}\|^\frac{1}{2} \leq \kappa_V(H) \|e_n^* f(H)\|.$$

*Proof.* By the definition of $Z_H$ above,

$$\mathbb{E}\|f(Z_H)^{-1}\|^\frac{1}{2} = \frac{\|e_n^* f(H)V\|}{\|e_n^* V\|} \leq \|e_n^* f(H)\| \|V\| \|V^{-1}\| = \|e_n^* f(H)\| \kappa_V(H),$$

and the left hand inequality is analogous. \(\square\)

---

\(^\dagger\)In the event that there are multiple such choices of $V$ it does not matter which we choose, only that it remains fixed throughout the analysis.

\(^\ddagger\)Our shifting strategy is deterministic, but we use random variables rather than measures for notational convenience.
Using this lemma with some carefully chosen rational functions $f$ of degree $k$, we are able to probe the distribution of $Z_H$ for each iterate $H$ of the algorithm by examining the observable quantities $\|e_n f(H)\|_1^2$ — for appropriately large $k$, these are related to $(\mathbb{E}|f(Z_H)|^2)^{1/2}$ by a multiplicative factor of $\kappa_V(H)^{1/2} \approx 1$, so we obtain accurate information about $Z_H$, which enables a precise understanding of convergence. Since the iterates are all unitarily similar, $\kappa_V$ is preserved with each iteration, so the $k$ required is an invariant of the algorithm. Thus the use of a sufficiently high-degree shifting strategy is both an essential feature and unavoidable cost of our approach.

### 2.2 Promising Ritz Values and Almost Monotonicity of the Potential

In the same spirit as Wilkinson’s shift, which chooses a particular Ritz value (out of two), but using a different criterion, our shifting strategy will begin by choosing a Ritz value (out of $k$) that has the following property for some $\alpha \geq 1$.

**Definition 2.5** ($\alpha$-promising Ritz value). Let $\alpha \geq 1$, $R = \{r_1, \ldots, r_k\}$ be a set of $\theta$-approximate Ritz values for $H$, and $p(z) = \prod_{i=1}^{k} (z - r_i)$. We say that $r \in R$ is $\alpha$-promising if

$$
\mathbb{E} \frac{1}{|Z_H - r|^{2k}} \geq \frac{1}{\alpha^k} \mathbb{E} \frac{1}{|p(Z_H)|}.
$$

(9)

Note that there is at least one 1-promising Ritz value in every set of approximate Ritz values, since

$$
\frac{1}{k} \sum_{i=1}^{k} \mathbb{E} \frac{1}{|Z_H - r_i|^{2k}} = \mathbb{E} \frac{1}{k} \sum_{i=1}^{k} \mathbb{E} \frac{1}{|Z_H - r_i|^{2k}} \geq \mathbb{E} \frac{1}{|p(Z_H)|}
$$

(10)

by linearity of expectation and AM/GM. The notion of $\alpha$-promising Ritz value is a relaxation which can be computed efficiently from the entries of $H$ (in fact, as we will explain in Section 2.4, using a small number of implicit QR steps with Francis-like shifts of degree $k/2$).

As a warm-up for the analysis of the shifting strategy, we will first show that if $k \gg \log \kappa_V(H)$ and $r$ is a promising Ritz value, the potential is almost monotone under the shift $(z - r)^k$. This justifies the intuition from Section 1.2 and suggests that promising Ritz values should give rise to good polynomial shifts, but is not actually used in the proof of our main theorem. Subsequent proofs will instead use the stronger property (11) established below.

**Lemma 2.6** (Almost-monotonicity and Moment Comparison). Let $R = \{r_1, \ldots, r_k\}$ be a set of $\theta$-optimal Ritz values and assume that $r \in R$ is $\alpha$-promising. If $\hat{H} = iqr(H, (z - r)^k)$ then

$$
\psi_k(\hat{H}) \leq \kappa_V(H)^{1/2} \alpha \theta \psi_k(H),
$$

and moreover

$$
\mathbb{E} \left[ |Z_H - r|^{-2k} \right] \geq \mathbb{E} \left[ |Z_H - r|^{-k} \right]^2 \geq \frac{1}{\kappa_V(H)^2 (\alpha \theta \psi_k(H))^{2k}}.
$$

(11)

**Proof.** Let $p(z) = \prod_{i=1}^{k} (z - r_i)$. The claim follows from the following chain of inequalities:

$$
\sqrt{\mathbb{E} \left[ |Z_H - r|^{-2k} \right]} \geq \mathbb{E} \left[ |Z_H - r|^{-k} \right] \quad \text{Jensen, } x \mapsto x^2
$$

$$
\geq \frac{1}{\alpha^k} \mathbb{E} \left[ |p(Z_H)|^{-1} \right] \quad r \text{ is } \alpha\text{-promising}
$$
\[ \geq \frac{1}{\alpha^k} \sqrt{E[|p(Z_H)|^2]} \quad \text{Jensen, } x \mapsto x^2 \]
\[ \geq \frac{1}{\alpha^k \|e^*_n p(H)\| \kappa_V(H)} \quad \text{Lemma 2.4} \]
\[ \geq \frac{1}{\alpha^k \theta^k \|e^*_n \chi_k(H)\| \kappa_V(H)} \quad \text{Definition 1.2 of } \theta \text{-optimal} \]
\[ = \frac{1}{\alpha^k \theta^k \psi_k(H) / \kappa_V(H)} \quad \text{Lemma 2.2}. \]

This already shows (11). For the other claim, rearrange both extremes of the above inequality to get
\[ a \theta \kappa_V(H)^{1/2} \psi_k(H) \geq \mathbb{E} \left[ |Z_H - r|^{-2k} \right]^{-1/2} \]
\[ \geq \frac{\tau(z-r)^k(H)}{\kappa_V(H)^{1/2}} \quad \text{Lemma 2.4} \]
\[ \geq \frac{\psi_k(H)}{\kappa_V(H)^{1/2}} \quad \text{Lemma 2.3} \]

which concludes the proof. \(\square\)

In Section 2.3, we will see that when the shift associated with a promising Ritz value does not reduce the potential, Lemma 2.6 can be used to provide a two-sided bound on the quantities \(\mathbb{E}[|Z_H - r|^{-2k}]\) and \(\mathbb{E}[|Z_H - r|^{-k}]^2\). This is the main ingredient needed to obtain information about the distribution of \(Z_H\) when potential reduction is not achieved.

### 2.3 The Shifting Strategy

An important component of our shifting scheme, discussed in detail in Section 2.4, is a simple subroutine, “Find,” guaranteed to produce a \(\alpha\)-promising Ritz value with \(\alpha = \kappa_V(H)^{4k^{-1} \log k}\). Guarantees for this subroutine are stated in the lemma below and proved in Section 2.4.

**Lemma 2.7 (Guarantees for Find).** The subroutine Find specified in Section 2.4 produces a \(\kappa_V(H)^{4k^{-1} \log k}\)-promising Ritz value, using at most \(12k \log k n^2 + \log k\) arithmetic operations.

Our strategy is then built around the following dichotomy, which crucially uses the \(\alpha\)-promising property: in the event that a degree \(k\) implicit QR step with the \(\alpha\)-promising Ritz value output by Find does not achieve potential reduction, we show that there is a modestly sized set of exceptional shifts, one of which is guaranteed to achieve potential reduction. These exceptional shifts are constructed by the procedure “Exc” described in Section 2.5. The overall strategy is specified below.
The failure of line (2) of $\text{Sh}_{k,B}$ to reduce the potential gives useful quantitative information about the distribution of $Z_H$, articulated in the following lemma. This will then be used to design the set $S$ of exceptional shifts produced by $\text{Exc}$ in line (3) and prove that at least one of them makes progress in line (4).

**Lemma 2.8 (Stagnation Implies Support).** Let $\gamma \in (0, 1)$ and $\theta \geq 1$, and let $\mathcal{R} = \{r_1, \ldots, r_k\}$ be a set of $\theta$-approximate Ritz values of $H$. Suppose $r \in \mathcal{R}$ is $\alpha$-promising and assume

$$\psi_k\left(\text{iqr}(H, (z - r)^k)\right) \geq \gamma \psi_k(H) > 0. \quad (12)$$

Then $Z_H$ is well-supported on an disk of radius approximately $\alpha \psi_k(H)$ centered at $r$ in the following sense: for every $t \in (0, 1)$:

$$\mathbb{P}\left[|Z_H - r| \leq \theta \alpha \left(\frac{\kappa_V(H)}{t}\right)^{1/k} \psi_k(H)\right] \geq (1 - t)^2 \frac{\gamma^{2k}}{\alpha^2 \theta^{2k} \kappa_V(H)^4}. \quad (13)$$

**Proof.** Observe that $H - r$ is invertible since otherwise, for $\hat{H} = \text{iqr}(H, (z - r)^k)$, we would have $\psi_k(\hat{H}) = 0$ by Lemma 2.3. Our assumption implies that that:

$$\gamma \psi_k(H) \leq \psi_k(\hat{H}) \leq \tau_{(z-r)^k}(H) = \|e^*_n(H-r)^{-k}\|^{-\frac{1}{k}} \leq \left(\frac{\kappa_V(H)}{\mathbb{E}[|Z_H - r|^{-2k}]^{\frac{1}{2}}}\right)^{1/k}$$

hypothesis \quad \text{Lemma 2.3} \\
\text{definition} \quad \text{Lemma 2.4.}

Rearranging and using (11) from Lemma 2.6 we get

$$\frac{\kappa_V(H)^2}{(1 - \gamma)^{2k} \psi_k(H)^{2k}} \geq \mathbb{E}\left[|Z_H - r|^{-2k}\right] \geq \mathbb{E}\left[|Z_H - r|^{-k}\right]^2 \geq \frac{1}{\alpha^2 \theta^{2k} \psi_k(H)^{2k} \kappa_V(H)^2}, \quad (14)$$

which upon further rearrangement yields the “reverse Jensen” type bound:

$$\frac{\mathbb{E}[|Z_H - r|^{-2k}]}{\mathbb{E}[|Z_H - r|^{-k}]^2} \leq \left(\frac{\alpha \theta}{\gamma}\right)^{2k} \kappa_V(H)^4. \quad (15)$$
We now have
\[
\mathbb{P} \left[ |Z_H - r| \leq \frac{\alpha}{\theta^2 \theta \psi_k(H) k^2 v} \right] = \mathbb{P} \left[ |Z_H - r|^{-k} \geq \frac{1}{\theta^2 \theta \psi_k(H) k^2 v} \right]
\]
\[
\geq \mathbb{P} \left[ |Z_H - r|^{-k} \geq t \mathbb{E}[|Z_H - r|^{-k}] \right] \quad \text{by (14)}
\]
\[
\geq (1 - t)^2 \frac{\mathbb{E}[|Z_H - r|^{-k}]^2}{\mathbb{E}[|Z_H - r|^{-2k}]} \quad \text{Paley-Zygmund}
\]
\[
\geq (1 - t)^2 \frac{\gamma^{2k}}{\alpha^{2k} \theta^{2k} \psi_k^2(H) k^4} \quad \text{by (15)},
\]
establishing (13), as desired.

In Section 2.5, we will use Lemma 2.8 to prove the following guarantee on Exc.

**Lemma 2.9** (Guarantees for Exc). The subroutine Exc specified in Section 2.5 produces a set S of exceptional shifts, one of which achieves potential reduction. If \( \theta \leq 2, \gamma = 0.8, \) and \( \alpha = B^4 \log \frac{k}{k} \), then both the arithmetic operations required for Exc, and the size of S, are at most
\[
N_{\text{net}} \left( 0.002B^{-\frac{8 \log \kappa V}{k}} \right),
\]
where \( N_{\text{net}}(\epsilon) = O(\epsilon^{-2}) \) denotes number of points in an efficiently computable \( \epsilon \)-net of the unit disk. In the normal case, taking \( B = \alpha = \theta = 1, k = 4, \gamma = 0.8, \) the arithmetic operations required and the size of \( |S| \) are both bounded by 50.

**Remark 2.10** (Improving the Disk to an Annulus). Control on the other tail of \( |Z_H - r| \) can be achieved by using Markov’s inequality and the upper bound (15) on the inverse moment \( \mathbb{E}[|Z_H - r|^{-2k}] \). Then, for \( k \gg \log \kappa V(H) \), the control on both tails yields that the distribution of \( Z_H \) has significant mass on a thin annulus (the inner and outer radii are almost the same).\(^\text{16}\) In this scenario one can take a net S with fewer elements when calling the exceptional shift, which would reduce the running time of \( T_{\text{exc}}(k, B) \). However, following this path would complicate the analysis and for the sake of exposition we do not pursue it any further in this paper.

We are now ready to prove Theorem 1.3.

**Proof of Theorem 1.3.** Rapid convergence. In the event that we choose a \( \alpha \)-promising Ritz value in step (1) that does not achieve potential reduction in step (2), Lemma 2.9 then guarantees we achieve potential reduction in (3). Thus each iteration decreases the potential by a factor of at least \( \gamma \), and since \( \psi_k(H_0) \leq \|H\| \) we need at most
\[
\frac{\log(1/\delta)}{\log(1/\gamma)} \leq 4 \log(1/\delta)
\]
iterations before \( \psi_k(H_t) \leq \delta \|H_0\| \), which in particular implies \( \delta \)-decoupling.

\(^\text{16}\)We note in passing (cf. [Par66]) that when \( H \) is normal, \( \alpha = 1, \theta = \gamma = 0, \) and \( k = 1 \), the above arguments can be modified to show that, under the assumption of Lemma 2.8, \( Z_H \) is fully supported on a circle with center \( r \) and radius \( \psi_k(H) \), and hence \( \frac{1}{\psi_k(H)}(H - r) \) is a unitary matrix.
**Arithmetic Complexity.** Computing a full set $\mathcal{R}$ of $\theta$-approximate Ritz values of $H$ has a cost $T_{\text{OptRitz}}(k, \theta, \delta)$. Then, using an efficient implicit QR algorithm (cf. Definition 2.1) each computation of $\text{iqr}(H, (z - r_j)^k)$ has a cost of $7kn^2$. By Lemma 2.7, we can produce a promising Ritz value in at most $12k \log kn^2 + \log k$ arithmetic operations. Then, in the event that the promising shift fails to reduce the potential the algorithm calls $\text{Exc}$, which takes $N_{\text{net}}(0.002B^{-\frac{4\log k+4}{k-1}})$ arithmetic operations to specify the set $S$ of exceptional shifts. Some exceptional shift achieves potential reduction, and we pay $7kn^2$ operations for each one that we check. 

\[\square\]

### 2.4 Efficiently Finding a Promising Ritz Value

In this section we show how to efficiently find a promising Ritz value, in $O(n^2k\log k)$ arithmetic operations. Note that it is trivial to find a $\kappa_V(H)^{2/k}$-promising Ritz value in $O(n^2k^2)$ arithmetic operations simply by computing $\|e_n^*(H - r_i)^{-k/2}\|$ for $i = 1, \ldots, k$ with $k$ calls to $\text{iqr}(H, (z - r_i)^{k/2})$, choosing the maximizing index $i$, and appealing to Lemma 2.4. The content of Lemma 2.7 below that this can be done considerably more efficiently if we use a binary search type procedure. This improvement has nothing to do with the dynamical properties of our shifting strategy so readers uninterested in computational efficiency may skip this section.

**Find**

**Input:** Hessenberg $H$, a set $\mathcal{R} = \{r_1, \ldots, r_k\}$ of $\theta$-optimal Ritz values of $H$.

**Output:** A complex number $r \in \mathcal{R}$

**Requires:** $\psi_k(H) > 0$

**Ensures:** $r$ is $\alpha$-promising for $\alpha = \kappa_V(H)^{-\frac{4\log k}{k-1}}$.

1. For $j = 1, \ldots, \log k$
   
   (a) Evenly partition $\mathcal{R} = \mathcal{R}_0 \cup \mathcal{R}_1$, and for $b = 0, 1$ set $p_{j,b} = \prod_{r \in \mathcal{R}_b} (z - r)$
   
   (b) $\mathcal{R} \leftarrow \mathcal{R}_b$, where $b$ maximizes $\|e_n^*p_{j,b}(H)^{-2^{j-1}}\|

2. Output $\mathcal{R} = \{r\}$

**Proof of Lemma 2.7 (Guarantees for Find).** First, observe that $\|e_n^*q(H)\| \neq 0$ for every polynomial appearing in the definition of Find, since otherwise we would have $\psi_k(H) = 0$.

On the first step of the subroutine $p_{1,0}p_{1,1} = p$, the polynomial whose roots are the full set of approximate Ritz values, so

\[
\max_b \|e_n^*p_{1,b}(H)^{-1}\| \geq \frac{1}{\kappa_V(H)^2} \mathbb{E}\left[\frac{1}{2} (|p_{1,0}(Z_H)|^{-2} + |p_{1,1}(Z_H)|^{-2})\right]
\]

\[\text{Lemma 2.4}\]

\[
\geq \frac{1}{\kappa_V(H)^2} \mathbb{E}[|p(Z_H)|^{-1}]
\]

AM/GM.

On each subsequent step, we’ve arranged things so that $p_{j+1,0}p_{j+1,1} = p_{j,b}$, where $b$ maximizes $\|e_n^*p_{j,b}(H)^{-2^{j-1}}\|$, and so by the same argument

\[
\max_b \|e_n^*p_{j+1,b}(H)^{-2^{j-1}}\| \geq \frac{1}{\kappa_V(H)^2} \mathbb{E}\left[\frac{1}{2} (|p_{j+1,0}(Z_H)|^{-2^{j+1}} + |p_{j+1,1}(Z_H)|^{-2^{j+1}})\right]
\]

\[\text{Lemma 2.4}\]
\[
\begin{align*}
\geq & \frac{1}{\kappa_V(H)^2} \mathbb{E} \left[ |p_{j+1,0}(Z_H)p_{j+1,1}(Z_H)|^{-2/1} \right] \\ 
\geq & \frac{1}{\kappa_V(H)^4} \|e_n^*(p_{j+1,0}(H)p_{j+1,1}(H))^{-2/1}\| \\ 
= & \frac{1}{\kappa_V(H)^4} \max_b \|e_n^*p_{j,b}(H)^{-2/1}\|.
\end{align*}
\]

Paying a further \(\kappa_V(H)^2\) on the final step to convert the norm into an expectation, we get
\[
\mathbb{E} \left[ |Z_H - r|^{-k} \right] \geq \frac{1}{\kappa_V(H)^4 \log k} \mathbb{E} \left[ |p(Z_H)|^{-1} \right]
\]
as promised.

For the runtime, we can compute every \(\|e_n^*p_{j,b}(H)^{-2/1}\|\) by running an implicit QR step with the polynomials \(p_{j,b}^{-1}\), all of which have degree \(k/2\). There are \(2\log k\) such computations throughout the subroutine, and each one requires \(6kn^2\) arithmetic operations. Beyond that we need only compare the two norms on each of the log \(k\) steps.

\[\square\]

**Remark 2.11** (Opportunism and Judicious Partitioning). In practice, it may be beneficial to implement Find *opportunistically*, meaning that in each iteration one should check if the new set of Ritz values gives potential reduction (this can be combined with the computation of \(\|e_n^*p_{j,b}(H)^{-2/1}\|\) and implemented with no extra cost). Moreover, note that Find does not specify a way to partition the set of Ritz values obtained after each iteration, and as can be seen from the above proof, the algorithm works regardless of the partitioning choices. It is conceivable that a judicious choice of the partitioning could be used to obtain further improvements.

### 2.5 Analysis of the Exceptional Shift

To conclude our analysis, it remains only to define the subroutine “Exc,” which produces a set \(S\) of possible exceptional shifts in the event that an \(\alpha\)-promising Ritz value does not achieve potential reduction. The main geometric intuition is captured in the case when \(H\) is normal and \(\kappa_V(H) = 1\). Here, Find gives us a 1-promising Ritz value \(r\) and Lemma 2.8 with \(t = 1/2\) tells us that if \(r\) does not achieve potential reduction, then \(Z_H\) has measure at least \(\frac{1}{4}(\gamma/\theta)^{2k}\) on a disk of radius \(R := 2^{1/k}\theta\psi_k(H)\).

For any \(\epsilon > 0\), we can easily construct an \(\text{Re-net} S\) contained in this disk — i.e., a set with the property that every point in the disk is at least \(\text{Re-close}\) to a point in \(S\) — with \(O(1/\epsilon)^2\) points. One can then find a point \(s \in S\) satisfying
\[
\tau_{(z-s)^2}(H)^{-2k} = \|e_n^*(H-s)^{-k}\|^2 = \mathbb{E}[|Z_H - s|^{-2k}] \geq \frac{P[Z_H - s | \leq \psi_k(H)]}{|S|(|\text{Re}|)^{2k}} \approx \frac{1}{4} \left(\frac{\gamma}{\theta}\right)^{2k} \frac{1}{R^{2k} \epsilon^{2k-2}}.
\]
where the first equality is by normality of \(H\), and second inequality comes from choosing \(s \in S\) to maximize \(|Z_H - s|^{-2k}\). Since \(\psi_k(\text{qrf}(H, (z-s)^k)) \leq \tau_{(z-s)^2}(H)\), we can ensure potential reduction by setting \(\epsilon \approx \Re_k(H) \approx (\gamma/\theta)^2\).

When \(H\) is nonnormal, the chain of inequalities above hold only up to factors of \(\kappa_V(H)\), and Find is only guaranteed to produce a \(\kappa_V(H)^{4\log k/k}\)-promising Ritz value. The necessary adjustments are addressed below in the implementation of Exc and the subsequent proof of its guarantees.
Input: Hessenberg $H$, a $\theta$-approximate Ritz value $r$, a condition number bound $B$, promising parameter $\alpha$

Output: A set $S \subset \mathbb{C}$

Requires: $\kappa_V(H) \leq B$, $r$ is $\alpha$-promising, and $\psi_k(iqr(H, (z - r)^k)) \geq \gamma \psi_k(H)$

Ensures: For some $s \in S$, $\psi_k(iqr(H, (z - s)^k)) \leq \gamma \psi_k(H)$

1. $R \leftarrow 2^{1/k} \theta \alpha B^{1/k} \psi_k(H)$
2. $\epsilon \leftarrow \left(\frac{\gamma^2}{(12B^4)^{1/4} \alpha^2 \theta^2}\right)^{\frac{1}{k-1}}$
3. $S \leftarrow \epsilon R$-net of $R \psi_k(H)$.

Proof of Lemma 2.9: Guarantees for Exc. Instantiating $t = 1/2$ in equation (13), we find that for the setting of $R$ in line (1) of Exc,

$$P \left[ |Z_H - r| \leq D(r, R) \right] \geq \frac{1}{4B^4} \left( \frac{\gamma}{\alpha \theta} \right)^{2k}.$$ 

Let $S$ be an $\epsilon R$-net of $D(r, R)$; it is routine that such a net has at most $(1 + 2/\epsilon)^2 \leq 9/\epsilon^2$ points. By Lemma 2.3, to show that some $s \in S$ achieves potential reduction, it suffices to find one for which

$$\|e^*_n(H - s)^{-k}\|^2 \geq \frac{1}{\gamma^{2k} \psi_k(H)^{2k}}.$$ 

We thus compute

$$\max_{s \in S} \|e^*_n(H - s)^{-k}\|^2 \geq \frac{1}{\kappa_V(H)^2 |S|} \sum_{s \in S} \mathbb{E} \left[ |Z_H - s|^{-2k} \right]$$ 

Fubini and $\kappa_V(H) \leq B$

$$\geq \frac{\epsilon^2}{9B^2} \mathbb{E} \left[ \sum_{s \in S} |Z_H - s|^{-2k} \cdot 1_{Z_H \in D(r, R)} \right]$$ 

$S$ is an $\epsilon R$-net

$$\geq \frac{\epsilon^2}{9B^2} \mathbb{E} \left[ \max_{s \in S} |Z_H - s|^{-2k} \cdot 1_{Z_H \in D(r, R)} \right]$$

$$\geq \frac{\epsilon^2}{9B^2} \mathbb{E} \left[ \frac{1_{Z_H \in D(r, R)}}{(\epsilon R)^{2k}} \right]$$

with the second to last line following from the fact that some $s \in S$ is at least $\epsilon R$-close to $Z_H$ whenever the latter is in $D(r, R)$, and the final inequality holding provided that

$$\epsilon \leq \left( \frac{P[|Z_H - r| \leq R \psi_k(H)] \gamma^{2k} \psi_k(H)^{2k}}{9B^2 R^{2k}} \right)^{\frac{1}{k-1}}.$$
Expanding the probability and using the definition of $R$ in line 1, it suffices to set $\epsilon$ smaller than
\[
\left( \frac{\gamma^{2k} \psi_k(H)^{2k}}{4B^4} \right) \left( \frac{1}{\epsilon B^2} \right) \gamma^2 (H) \frac{\alpha^2 k^4}{\epsilon} \theta^2 \cdot \frac{\gamma^2}{\psi_k(H)^{2k}} \right)^{\frac{1}{2-k}} = \left( \frac{\gamma^2 (12B^4)^{1/8} \alpha^2 k^4 \theta^2}{\epsilon} \right)^{\frac{1}{2-k}},
\]
which is the quantity appearing in line 2. Setting $\theta = 2, \gamma = 0.8$, and $\alpha = B^4 \log k$, and using $k \geq 2$, we obtain the expression appearing in $N_{\text{net}}(\cdot)$ in the statement of Lemma 2.9.

However, a more practical choice (and the one that we will use in the companion paper [BGVS22a]) is an equilateral triangular lattice with spacing $\sqrt{3} \epsilon$, intersected with the $D(r, (1 + \epsilon) R)$. Such a construction is optimal as $\epsilon \to 0$, and can be used to give a better bound on $N_{\text{net}}(\epsilon)$ when $\epsilon$ is small. For instance, by adapting an argument of [ABB+18, Lemma 2.6] one can show that this choice of $S$ satisfies
\[
N_{\text{net}}(\epsilon) \leq \frac{2\pi}{3\sqrt{3}} (1 + 1/\epsilon)^2 + \frac{4\sqrt{2}}{\sqrt{3}} (1 + 1/\epsilon) + 1.
\]
In the normal case, when $B = \alpha = \theta = 1, k = 4, \gamma = 0.8$, the above bound gives
\[
|S| \leq N_{\text{net}} \left( \frac{0.8^2}{121/4} \right)^{4/3} \leq 49.9.
\]
\[\square\]

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