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NEUTRALLY STABLE FIXED POINTS OF THE QR ALGORITHM

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Abstract. Practical QR algorithm for the real unsymmetric algebraic eigenvalue problem is considered. The global convergence of shifted QR algorithm in finite precision arithmetic is addressed based on a model of the dynamics of QR algorithm in a neighborhood of an unreduced Hessenberg fixed point. The QR algorithm fails at a "stable" unreduced fixed point. Prior analyses have either determined some unstable unreduced Hessenberg fixed points or have addressed stability to perturbations of the reduced Hessenberg fixed points. The model states that sufficient criteria for stability (e.g. failure) in finite precision arithmetic are that a fixed point be neutrally stable both with respect to perturbations that are constrained to the orthogonal similarity class and to general perturbations from the full matrix space. The theoretical analysis presented herein shows that at an arbitrary unreduced fixed point "most" of the eigenvalues of the Jacobian(s) are of unit modulus. A framework for the analysis of special cases is developed that also sheds some light on the robustness of the QR algorithm.

Key Words. Unsymmetric eigenvalue problem, QR algorithm, unreduced fixed point

1. Background

QR iteration is the standard method for computing the eigenvalues of an unsymmetric matrix [13, 16, 9, 2]. The global convergence properties of *un*shifted QR iteration are well established [14, 5]. For the shifted QR iteration there is no proof of convergence, and yet in practice failure is extremely rare.

A brief review of QR iteration follows. Please see [9] for a comprehensive discussion. The matrix $A = [a_{i,j}]$ has lower bandwidth k if $i > j + k$ implies that $a_{i,j} = 0$. A matrix with unit lower bandwidth is called an (*upper*) *Hessenberg* matrix. Any square matrix is orthogonally similar to a Hessenberg matrix.

In the eigenvalue problem, a given matrix is first reduced by orthogonal similarity transformations to Hessenberg form. A Hessenberg matrix is unreduced if no entry on the first subdiagonal vanishes. QR iteration is applied to the irreducible diagonal blocks consecutively.

Shifted QR iteration from H_0 with shift function $p(\cdot)$ is defined by

$$p(B_m) = Q_m R_m \qquad \text{and} \quad p(B_{m+1}) = R_m Q_m.$$

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The matrices Q_m and R_m are orthogonal and upper triangular respectively. In the unshifted iteration, $p(x) = x$. QR iteration preserves the lower bandwidth of B.

The goal of QR iteration is to reduce a matrix by a sequence of orthogonal similarity transformations to a block upper triangular matrix, with one by one and two by two diagonal blocks. The decomposition is called a real Schur form.

QR iteration defines a matrix valued function whose singularities are the reduced Hessenberg matrices. In [3, 1]. the unshifted QR algorithm is viewed as a fixed-point iteration on the flag manifold, and the stability properties of the *reduced* fixed points are studied. Unreduced Hessenberg fixed points are always degenerate critical points (not obvious, see for example Theorem E), and are not structurally stable.

Though QR iteration has unreduced fixed points, in the cases considered for example in [4], convergence at an unreduced fixed point is nice in floating point arithmetic because the unreduced fixed points are strongly repelling. The observed robustness of the shifted iteration in finite precision arithmetic is due in part to the scarcity of "stable" fixed points.

Consider for example $f(x) = x + x^2 - x^3$. The fixed point zero is not strongly repelling and $f^k(x) = x + kx^2 + O(x^3)$. If x is slightly larger than the square root of the machine precision, then the number of iterations required for convergence (to $x = 1$) is inversely proportional to the machine precision.

QR iteration fails if the number of iterations to decouple a given matrix exceeds a maximum value. Herein the dynamics of QR iteration near *un*reduced Hessenberg fixed points in finite precision arithmetic are studied. The use of finite precision arithmetic introduces perturbations. At "unstable" fixed points, iteration amplifies the perturbations and the iterates escape the fixed point.

The convergence properties of the shifted QR iteration depend on the shift strategy (the map from the Hessenberg matrix and the iteration number to the shift polynomial). The implementations [13, 16, 2] all have evolved subtly different shift strategies in the attempt to enhance the convergence properties. The present study develops general results that apply to any shift strategy.

The current work relies on the first author's study of the 4×4 Hamiltonian fixed points of shifted QR iteration as implemented in [16] or [2]. The connection between integrable flows and the QR algorithm is well known (see [12], page 59 or [17, 7]). The elementary explanations in [8] are inherently lengthy and provide only a relatively limited insight into the problem at hand.

The basis for our analysis is an **empirical model** of the dynamics of the QR algorithm implemented in finite precision arithmetic and applied to matrices near to a fixed point. The dynamics of the QR algorithm in exact arithmetic is much more complicated. For instance, the stability on center manifolds must be addressed. The empirical model was derived in [8], and is the simplest model whose predictions coincide with all the observations known to the first author.

In finite precision arithmetic, QR iteration is backward stable [9] but forward unstable [11]. Consecutive QR iterates are nearly orthogonally similar, to within machine precision, but the computed iterate is not necessarily near to the iterate determined in exact arithmetic. The term orthogonal similarity class refers to the set of Hessenberg matrices orthogonally similar to a given matrix. The derivative along the orthogonal similarity class (which is low dimensional and tractable) predicts the dynamics in many situations, but not near to the unreduced fixed points [8]. Suppose that QR iteration is applied to a n by n matrix. There the difference between consecutive iterates is transverse to the orthogonal similarity