A HISTORY OF INVERSE ITERATION*

ILSE C. F. IPSEN†

1. The Method. Inverse iteration is a method for computing eigenfunctions of linear operators. Here we consider inverse iteration for the solution of the algebraic eigenvalue problem

$$Ax = \lambda x,$$

where A is a real or complex square matrix, the scalar λ is an eigenvalue, and the non-zero vector x is an eigenvector. Inverse iteration is the method of choice when one has at one's disposal approximations to a specified subset of eigenvalues of A, for which one wants to compute associated eigenvectors. The method is frequently used in structural mechanics, for instance, when the extreme eigenvalues and corresponding eigenvectors of Hermitian positive-(semi)definite eigenproblems are sought [2, 3, 12, 13, 18, 30].

Given an approximation $\bar{\lambda}$ to an eigenvalue of A, inverse iteration generates a sequence of vectors x_k from a given starting vector x_0 by solving the linear systems[1]

$$(A - \bar{\lambda} I)x_k = s_k x_{k-1}, \qquad k \geq 1.$$

The scalar s_k is responsible for normalising x_k. Usually one choses s_k so that $\|x_k\| = 1$ in some norm. If everything goes well, the sequence of iterates x_k converges to an eigenvector associated with an eigenvalue closest to $\bar{\lambda}$. In particular when there is only a single eigenvalue λ closest to $\bar{\lambda}$, then the x_k converge to an eigenvector associated with λ, provided the starting vector x_0 contains a contribution of this eigenvector. Since x_k is a multiple of the vector $(A - \bar{\lambda}I)^{-k}y_0$ and since $1/(\lambda - \bar{\lambda})$ is the largest eigenvalue of $(A - \bar{\lambda}I)^{-1}$, the contribution in x_k of the eigendirection associated with λ increases faster as $k \to \infty$ than the contributions associated with the other eigenvalues. Inverse iteration is mathematically identical[2] to the power method applied to $(A - \bar{\lambda}I)^{-1}$.

In 1979 Wilkinson remarked: 'Inverse iteration is now the most widely used method for computing eigenvectors corresponding to selected eigenvalues which have already been computed more or less accurately' [26, p 339]. A look at software in the public domain shows that this is still true today [1, 25, 28].

Yet, after so many years, the behaviour of the method is still not completely understood – neither in exact nor in floating point arithmetic [4]. As a consequence, even highly sophisticated, state of the art software like LAPACK still comes across matrices for which it cannot compute eigenvectors to high accuracy without a drastic sacrifice in efficiency.

This article describes the efforts undertaken on behalf of inverse iteration[3] from its

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† Department of Mathematics, North Carolina State University, P. O. Box 8205, Raleigh, NC 27695-8205, USA (ipsen@math.ncsu.edu). This work was supported in part by NSF grant CCR-9102853.

[1] Here I denotes the identity matrix.

[2] Mathematical identity means that equality holds in exact arithmetic but not necessarily in finite precision arithmetic because the two methods determine their iterates by means of different operations.

[3] We concentrate on the solution of the ordinary eigenvalue problem rather than the generalised eigenvalue problem $Ax = \lambda Bx$; and we do not discuss techniques for convergence acceleration such as Rayleigh quotient iteration where the shift changes with each iteration.

inception to the present day (October 1994). Here are a few of the issues that prompted these efforts: The iterates may not converge to an eigenvector because the starting vector x_0 does not have a contribution in the desired eigenvector, or because there may be several different eigenvalues of A at the same distance from $\bar{\lambda}$. The eigenvalue closest to λ may be a multiple eigenvalue, and inverse iteration may have to compute a basis for the corresponding invariant subspace. Unless linear independence is enforced explicitly, inverse iteration usually fails to compute the desired basis. When the matrix is Hermitian, linear independence is enforced by orthogonalising an iterate against the already computed eigenvectors. But, depending on the shift $\bar{\lambda}$ and the starting vector x_0, iterates may still fail to converge. The problem becomes even more pronounced when $\bar{\lambda}$ happens to approximate a cluster of close but not identical eigenvalues. Should one treat the cluster like a collection of separate eigenvalues, or like a single multiple eigenvalue, or like several multiple eigenvalues? How close together must eigenvalues be to qualify as a cluster? Should an iterate be orthogonalised against all eigenvectors in the cluster or against just a few?

2. Wielandt Started It. Inverse iteration was introduced by Wielandt in 1944 [37]. Although Peters and Wilkinson remark [26, p 339], without further elaboration, that 'a number of people seem to have had the idea independently', Wielandt is usually the one credited with the introduction of inverse iteration [11, 15, 31, 32, 39]. He refers to inverse iteration as *fractional iteration* ('gebrochene Iteration' in German) because the matrix $(A - \bar{\lambda}I)^{-1}$ is a fractional linear function of A [37, p 3]. He points out the benefit of inverse iteration in the stability analysis of vibrating systems that are small perturbations of systems whose behaviour is known [37, §I]. In this case good approximations to the eigenvalues of the perturbed system are available. The computational aspects of Wielandt's work leading to the development of inverse iteration are described in the companion paper [16].

Adapted to the algebraic eigenvalue problem, Wielandt's justification for inverse iteration looks as follows [36, §III(c)]: Choose ϵ so that $\lambda = \bar{\lambda} + \epsilon$. Then $Ax = \lambda x$ becomes

$$(A - \bar{\lambda}I)x = \epsilon x.$$

Replacing x on the left by x_k and on the right by x_{k-1}, and writing s_k instead of ϵ gives inverse iteration.

In 1951, Crandall [7] presents inverse iteration for real symmetric matrices as an instance of a particular relaxation method[4]. He does not reference Wielandt's paper.

3. Wilkinson's Idea. The person most closely associated with inverse iteration for the algebraic eigenvalue problem is Jim Wilkinson. Although Wilkinson gives the credit for inverse iteration to Wielandt [26, 39, 41], he himself came up with it independently in 1958 [38] as a result of trying to improve Givens's method for computing a single eigenvector of a symmetric tridiagonal matrix.

We modify Wilkinson's idea slightly and present it for a general matrix A rather than just a symmetric tridiagonal matrix. Suppose A has order n, and the shift $\bar{\lambda}$ is

[4] Crandall [7, page 416] gives the following characterisation of relaxation methods: 'A unique feature of relaxation methods is that they are approximate procedures which are not rigidly prescribed in advance. The precise procedure to be followed is not dictated but is left to the intuition and accumulated experience of the computer. The computer's intelligence is thus an active or dynamic link in the computational chain. It is this fact which has made relaxation so attractive to many computers.' Thus, at the time Crandall wrote his paper, a computer was (still) a human being; and 'for exploratory purposes' the relaxation methods were carried out with a slide rule [8, p 141].

closer to the simple eigenvalue λ than to any other eigenvalue of A. Wilkinson's idea is the following: Since an eigenvector x is determined up to a multiple by $n-1$ of the n equations $(A-\lambda I)x=0$, approximate x by a non-zero vector z that solves $n-1$ equations of $(A-\bar{\lambda}I)z=0$.

Why should such a z be a good approximation to x? Partition A so as to distinguish its leading principal submatrix $\tilde{A}$ of order $n-1$, and partition z conformally,

$$A \equiv \begin{pmatrix} \tilde{A} & a_1 \\ a_2 & \alpha \end{pmatrix}, \qquad z \equiv \begin{pmatrix} \tilde{z} \\ \zeta \end{pmatrix}.$$

Suppose $\bar{\lambda}$ is also not an eigenvalue of $\tilde{A}$, so $\tilde{A}-\bar{\lambda}I$ is non-singular. If we fix ζ to a non-zero value then there exists a solution $\tilde{z}$ to the smaller system

$$(\tilde{A}-\bar{\lambda}I)\tilde{z} = -\zeta a_1.$$

This implies that z is a non-zero solution to the larger system[5]

$$(A-\bar{\lambda}I)z = \beta e_n, \qquad \text{where} \quad \beta \equiv a_2\tilde{z}+\alpha\zeta.$$

If βe_n contains a contribution of an eigenvector x then this contribution is amplified in z by $1/(\lambda-\bar{\lambda})$. Since λ is the single closest eigenvalue to $\bar{\lambda}$, the contributions of all other eigenvectors in z are amplified by smaller amounts. Thus, z is closer to x than is βe_n.

Instead of solving the first $n-1$ equations one could solve any set of $n-1$ equations. If the ith equation is the one that is omitted then the right-hand side is a multiple of e_i. In general, the right-hand side can be any vector x_0, as long as it contains a contribution of a desired eigenvector x. Then the solution x_1 of $(A-\bar{\lambda}I)x_1 = x_0$ is closer to x than is x_0. Hence, as inverse iteration progresses the iterates x_k converge to an eigenvector x, provided the associated eigenvalue λ is simple.

4. Wilkinson Takes Charge. The foremost issues on Wilkinson's mind were the choice of appropriate starting vectors, and the misfortune of having to solve a linear system that is highly ill-conditioned when $\bar{\lambda}$ is an accurate approximation to an eigenvalue of A.

From 1958 to 1965 Wilkinson analysed the computation of a single eigenvector of a symmetric tridiagonal matrix: determination of the convergence rate in exact arithmetic; choice of a good starting vector in exact arithmetic; and effect of the backward error due to the solution of the linear system by Gaussian elimination with partial pivoting on the size of the iterate and the convergence rate [38], [39, pp 142-7], [40, pp 321-30]. Regarding the computation of eigenvectors associated with almost coincident eigenvalues, he recommends a different perturbation of the shift $\bar{\lambda}$ for each eigenvalue, and the use of the Gram-Schmidt algorithm to orthogonalise the current iterate against previously computed eigenvectors [40, p 329].

Wilkinson applies a similar treatment to computing a single eigenvector when the eigenvalue is semisimple and the matrix is real and nonsymmetric [40, pp 619-35]. As Wielandt had already observed in the context of the power method, Wilkinson realises that the iterates do not necessarily improve in successive iterations when the desired eigenvalue is almost defective. In particular, Wilkinson analyses the effect of the backward error due to the solution of the linear system on the size of the iterate and the residual. He also gives a roundoff error analysis for the computation of complex eigenvectors of real Hessenberg matrices in real arithmetic. In the same spirit, Varah

[5] The vector e_i denotes the ith column of the identity matrix.

[34] analyses the computation of a single eigenvector for a complex Hessenberg matrix, and presents perturbation and roundoff error analyses for well-separated eigenvalues in [34].

5. Software on the Horizon. About six years later, in 1971, Peters and Wilkinson [25] publish ALGOL subroutines that perform inverse iteration on three classes of matrices: real, symmetric tridiagonal; real upper Hessenberg; and complex upper Hessenberg. They recommend that these subroutines be used only if no more than twenty-five percent of the eigenvectors are desired.

Shortly thereafter appears EISPACK [29, 28] a collection of FORTRAN subroutines for the computation of eigenvalues and eigenvectors that is based upon the ALGOL subroutines in [43] (the EISPACK story is told in [23], along with some of the difficulties in translating the subroutines from ALGOL to FORTRAN). EISPACK contains essentially the same subroutines for inverse iteration as its ALGOL predecessor.

On the mathematical side, Wilkinson shows that it is not too difficult to find good starting vectors. If the shift $\bar{\lambda}$ is a good approximation[6] to an eigenvalue of A then, inspite of a backward error from linear system solution, one can always find a x_0 for which x_1 is a good approximation[7] to an eigenvector of A [41, §4]. In particular, among the vectors of any orthogonal basis there is at least one that constitutes a good starting vector [41, p 373].

Wilkinson also considers the computation in exact arithmetic of a single eigenvector when the eigenvalue is ill-conditioned[8] [41, 42] and when the eigenvalue is defective [25]. He remarks with regard to a single iteration [41, p 376] that, even in the case of an ill-conditioned eigenvalue, 'the extraordinary ability of inverse iteration to produce an exact eigenvector of a neighbouring matrix corresponding to a given eigenvalue is immensely valuable and reassuring in practice'.

In 1973, Parlett and Poole [22, 24] present a geometric theory of inverse iteration without orthogonalisation. This theory applies to general complex matrices and provides conditions for the convergence of starting subspaces to invariant subspaces. Watkins resumes this geometric point of view nearly twenty years later [35].

In his last paper on inverse iteration [26], considered by many to be *the* definitive treatment, Wilkinson argues that there is no danger in solving an ill-conditioned system. He demonstrates that even though the computed solution may be totally wrong, it is still likely to have the right direction – and that is all we need. He also shows that, to first order, inverse iteration is related to Newton's method for solving non-linear systems.

At last, there is a block version of inverse iteration, called subspace iteration or simultaneous iteration, that iterates on several vectors simultaneously and enforces linear independence of the vectors from time to time [6, 5, 22, 27]. Chatelin shows that subspace iteration is unstable when used to compute a basis of an invariant subspace associated with a defective eigenvalue, because the basis consists of principal vectors in addition to eigenvectors [6, §5.9], [5]. She presents a numerically stable modified Newton's method to compute the basis of such defective invariant subspaces.

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[6] Wilkinson means 'good' in the backward sense: $\bar{\lambda}$ is an eigenvalue of a matrix close to A [41, p 371].

[7] As before this means 'good' in the backward sense: x_1 is an eigenvector corresponding to the eigenvalue $\bar{\lambda}$ of a matrix close to A.

[8] A simple eigenvalue is called ill-conditioned if the acute angle between its left and right eigenvectors is large [27, §III.3.1], [40, §§2.8ff].

6. The New Age. After several years of relative calm there is renewed interest in inverse iteration. Jessup and Ipsen [20] take up the case of starting vectors. They perform a statistical analysis to justify the choice of random vectors as starting vectors. In order to improve the accuracy of TINVIT, the EISPACK implementation of inverse iteration for real symmetric tridiagonal matrices, they modify three features of TINVIT: choice of starting vectors, convergence criterion, and the decision of when and which iterates to orthogonalise. The desire for improving the accuracy came as a result of comparing parallel implementations of Cuppen's divide and conquer method [9] and inverse iteration [17]. While the parallel implementation of TINVIT with bisection in [17] turned out to be the fastest method on an INTEL iPSC hypercube, it was not as accurate as Cuppen's method. The changes in [20] increase the numerical accuracy of TINVIT to that of Cuppen's method for matrices of order up to 525.

A more recent parallel implementation of inverse iteration for real, symmetric tridiagonal matrices on the MasPar SP-1/2 [14] solves the linear system first by a fast parallel method such as cyclic reduction. If the solution is not accurate enough, the system is subsequently solved by a more accurate, possibly slower method such as Gaussian elimination with partial pivoting.

The collection of FORTRAN subroutines in LAPACK [1] for solving eigenvalue problems is designed to replace the EISPACK routines. LAPACK contains subroutines for inverse iteration on symmetric tridiagonal matrices, and real and complex upper Hessenberg matrices.

Demmel and Veselic [10] derive *relative* error bounds, as opposed to the traditional absolute error bounds, for eigenvalues and eigenvectors of symmetric positive-definite matrices for the case of componentwise relative perturbations. They conclude that inverse iteration with bisection, when applied to the original matrix, gives better error bounds than a method that requires a preliminary transformation of the matrix to tridiagonal form.

Combinations of Rayleigh quotient and inverse iteration are explored in [19, 18, 21, 33].

7. Not All Is Well. In spite of all the efforts devoted to the development of inverse iteration, the method still has its pitfalls. In corroboration we give two quotes from *The Algebraic Eigenvalue Problem* [40] which, thirty years after its first publication, is still the 'bible' for eigenvalue problems.

With regard to the loss of orthogonality in the computation of eigenvectors associated with nearly coincident eigenvalues of symmetric tridiagonal matrices, and the necessity to orthogonalise iterates against previously computed eigenvectors, Wilkinson says [40, p 329]: 'Of course we cannot expect the computed vectors to be orthogonal, but remember that deterioration of orthogonality sets in well before we reach pathologically close eigenvalues. It must be admitted though, that this solution to the problem is somewhat inelegant. It has the disadvantage that if we require orthogonal vectors we must apply the Schmidt orthogonalization process to the computed vectors. Also, unless the process can be put on a sounder footing, there remains the danger that we shall not have full digital information about the subspace'.

Later on he concludes [40, p 344]: 'Inverse iteration gives a very satisfactory solution to the problem as far as reasonably well-separated eigenvalues are concerned. The problem of determining reliably full digital information in the subspace spanned by eigenvectors corresponding to coincident or pathologically close eigenvalues has never been satisfactorily solved.'

Unfortunately, this is still true today. Compared to other methods, current implementations of inverse iteration sometimes give a lower accuracy or require more work to attain the same accuracy when eigenvalues are not well separated or when they occur in large clusters. Because the criteria are heuristic for deciding when eigenvalues are sufficiently close to warrant orthogonalisation, an iterate may be orthogonalised against too many or too few previously computed eigenvectors.

Part of the problem is that inverse iteration is not as easy to analyse as the power method, due to the nonlinear occurrence of the shift [16, §9]. Most existing analyses concentrate on the finite precision behaviour of inverse iteration. But lots of things can wrong in exact arithmetic. Even when the matrix is Hermitian and the number of iterations is allowed to be infinite, an unwisely chosen shift can result in a failure to compute all desired eigenvectors or in the pairing up of eigenvectors with the wrong eigenvalues [4]. The choice of an appropriate shift becomes even more delicate when the number of iterations is finite, even though the arithmetic is still exact. Therefore it is most important to carefully separate the properties of inverse iteration in exact arithmetic from those in floating point arithmetic. Chandrasekaran and Ipsen [4] pursue this approach rigorously and derive criteria for shift selection, orthogonalisation of iterates and against previously computed eigenvectors and convergence criteria. The goal is a numerically robust and provably accurate inverse iteration algorithm.

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