On development of accurate eigensolvers

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April 5, 2000

Abstract

We study the development of accurate algorithms for matrix (generalized) symmetric eigenvalue problems. A desirable property of such an algorithm is that it approximates the well determined eigenvalues (and singular values) with high relative accuracy independent of their magnitudes. This is an important issue because the smallest eigenvalues are in applications usually the most interesting ones and, unfortunately, the most sensitive ones in presence of numerical errors. To design such an algorithm, we need detailed knowledge of the structure of errors produced by finite precision implementation of the algorithm, as well as deep understanding of the sensitivity to perturbations of the original problem. We are interested in methods based on orthogonal similarities (so–called direct methods) as well as in methods based on spectral approximations from subspaces (so–called iterative methods).

Consider for simplicity the ordinary symmetric eigenvalue problem $Hx = \lambda x$. The matrix H is diagonalized by an infinite number of orthogonal similarity transformations, $\cdots U_2^T(U_1^T H U_1)U_2 \cdots \longrightarrow \Lambda$, and in the limit $U^T H U = \Lambda$, where $U = U_1 U_2 \cdots$ and Λ is the diagonal matrix of H's eigenvalues. In finite precision computation, each transformation U_i is approximated by some $\tilde{U}_i$, and applied with some error E_i. Moreover only a finite number of transformations is used:

$$\tilde{H}_k = \tilde{U}_k^T(\cdots(\tilde{U}_2^T(\tilde{U}_1^T H \tilde{U}_1 + E_1)\tilde{U}_2 + E_2)\cdots)\tilde{U}_k + E_k.$$

The index k is chosen so that $\tilde{H}_k$ is sufficiently close to diagonal matrix and its diagonals are taken as approximative eigenvalues $\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n$ of H. Let $\hat{U} = \tilde{U}_1 \cdots \tilde{U}_k$, and let $\tilde{U}$ denote the computed matrix $\hat{U}$. The columns of $\tilde{U}$ are the computed approximations of the eigenvectors of H. To assess the error in the computed values, we prove the existence of symmetric perturbation δH such that $\hat{U}^T(H + \delta H)\hat{U} = \tilde{H}_k$ exactly. The matrix δH is called backward

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error. Different algorithms produce backward errors of different structures and different sizes. For example, if the backward error δH in positive definite H is such that[1], for all i, j, $|\delta H_{ij}| \leq \epsilon \sqrt{H_{ii} H_{jj}}$ (as in the Jacobi method), we expect optimal accuracy. If we can only claim small $\|\delta H\|/\|H\|$ (as in the methods based on tridiagonalization and bidiagonalization, which are faster than the Jacobi method), the results are less satisfactory.

Many questions arise. How many digits in the computed eigenvalues are correct? How small are the angles between the computed and the exact eigenspaces? Can we compute accurate approximations of the eigenvectors a posteriori (from linear systems)? How to design numerical algorithm with minimal (numerical) complexity to get optimal accuracy? Can we fix bidiagonalization (tridiagonalization) to get backward error comparable to the one in Jacobi methods? What are the best algorithms for the generalized problems?

If the matrix is large (and sparse), and if only a few eigenpairs are needed, one usually constructs a sequence of low–dimensional subspaces and hopes to approximate the target eigenpairs from these subspaces.

To be successful in designing efficient algorithms, one needs to know *(i)* how good is the current subspace, e.g. how accurate are the Ritz pairs obtained from that subspace; *(ii)* how to enrich the current subspace with directions close to the target vectors, thus ensuring fast convergence; *(iii)* how to compute accurate Rayleigh quotient matrix and the Ritz pairs in finite precision (floating–point) arithmetic.

So, for instance, if the task is to approximate the lowest eigenvalue λ of positive definite matrix, we wish to know how many correct digits are in our current (floating–point) approximation $\lambda + \delta\lambda$. Sharp computable error bound assures good stopping criterion and accurate approximations.

We analyze the Ritz and the harmonic Ritz values and present computable bounds for $|\delta\lambda/\lambda|$ and show how perturbation theory sheds a new light on some well–known eigensolvers. We also discuss how to use these results to construct better subspaces, which could lead to substantial improvement of some well–known algorithms.

Our presentation will be a tutorial spiced with some new results.

[1] Here ϵ denotes small quantity proportional to the round–off.