Jacobi's ideas on eigenvalue computation in a modern context

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Matrix notation was unknown in 1846. This did not prevent Jacobi from inventing an algorithm for the computation of eigenvalues [3]. He did this in the context of linear systems related to the stabi- lity of the orbits of the then known 7 planets. Part of his method was reinvented 100 years later by Von Neumann and his colleagues, and part of Jacobi's method became popular for linear eigenproblems $Ax = cx$. The full Jacobi method was known to, for instance, Ostrowski and Bodewig, but for some reason discarded as a practical computer method. The (partial) method was some thirty years later over- taken by more successfull methods: QR and the methods of Lanczos and Arnoldi.

In 1975, the chemist Davidson proposed a new method that became very popular, specially for applications in Chemistry [2]. Numeri- cal analysts all over the world largely ignored his method, mainly because of lack of understanding. An important paper with insightful analysis of the Davidson method was published in 1994 by Crouzeix and co-workers [1]. They showed in fact that the Davidson method could converge with more general preconditioning, provided that the preconditioning was not too good, which is a intriguing result, indeed. Much more, apart from a discussion on the method by Saad, was not available from the numerical analysis community, but it contributed in a very meaningful way to the understanding of the Davidson method and it helped to keep interest in the method by the numerical analysts. Meanwhile, the Davidson method, and many variants, was heavily and successfully used, in particular in Chemistry. Part of the success seemed to be that the matrices in these applications were fairly diagonally dominant. The method was very sensitive to transformations, in particular, even an orthogonal transformation could destroy the convergence. Meanwhile, the methodd of Lanczos and Arnoldi were available. These were quite well understand and the common believe among numerical analysts was that they had to be preferred over the Davidson method. However, the Crouzeix paper hinted at more usefulness of the method.

In 1993 our numerical pride was triggered by chemists from Utrecht, who impressed us with the apparant superiority of the Davidson method for their problems. At the same time, a student at our institute did her Master thesis on the old publications of Jacobi. This led to some remarkable observations and eventually it led to a happy marriage between parts of the methods of Jacobi and Davidson [4].

References

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