An Outline of a Symmetric Spectrum Algorithm

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1 Reduction

Given a symmetric $n \times n$ matrix A define the generalized "ratio" of the $n \times k$ matrix X with respect to A as the $k \times k$ matrix $(X^t AX) \cdot (X^t X)^{-1}$. In what follows we assume that the columns of X are independent so that the inverse (rather than generalized inverse) of $X^t X$ exists. If the columns of X are orthonormal, i.e. $X^t X = I$ where I denotes an identity matrix, the ratio is $X^t AX$. If the columns of L are an *arbitrary* subset of the eigenvectors of A, then $D = L^t AL$ is diagonal, displaying the corresponding eigenvalues of A.

If the columns of L are a *proper* subset of orthonormal eigenvectors of A and T is an orthonormal basis of the null space of L, then $L^t L = I$, $L^t T = 0$, $T^t T = I$ and the size of the matrix $B = T^t AT$ is smaller than the size of A. Computing the spectrum of A is reduced to computing the spectrum of B as follows. Denote the subset of the orthonormal eigenvectors of A complementary to L by V. Then $AV = VD$ where D is diagonal, d_i is the eigenvalue that corresponds to the eigenvector v_i and $V^t V = I$. Since T and V are both orthonormal bases of the null space of L, there exists an orthonormal M such that $V = T \cdot M$ and we have $A(TM) = (TM)D$. This implies $(T^t AT)M = (T^t T)MD$ and $BM = MD$. Since M is orthogonal and D is diagonal, the columns of M are the eigenvectors of B and D displays their corresponding eigenvalues. Finally, the eigenvectors V of A are related to those of B by $V = T \cdot M$.

2 Algorithm

2.1 General Outline

Start with an empty set L of computed eigenvectors, an identity matrix as an orthonormal basis T for the null space of L, and $B = A$. Compute an eigenvector/eigenvalue pair of B. Update the set of computed eigenvalues and the set L of computed eigenvectors. Update the orthonormal basis T for the null space of L. Update B and repeat.

2.2 Implementation

Rayleigh Quotient Iteration (RQI, Algorithm 27.3 in [3]) can be used to compute an eigenvector/eigenvalue pair for the B matrix. The Conjugate Gradient algorithm (CG, Algorithm 38.1 in [3]) can be used to solve RQI's linear system.

Denote RQI's B-eigenvector by m. Then Tm is an eigenvector of A and L is updated. Finally, T and B can be updated using a finite, small, number of vector-matrix multiplications.

2.3 Notes

For detailed treatments of the spectrum problem see [1–4]. If α is not an eigenvalue of A, then $A - \alpha I = 0$ is non-singular and the only solution of the equation $(A - \alpha I)x = 0$ is $x = 0$ which is not an eigenvector since an eigenvector must be a non-zero vector. While the terms "not an eigenvalue" and "a non-zero vector" are meaningful as infinite precision concepts, the finite precision spectrum computation problem is closely related to singularity (if α is an eigenvalue of A) and ill-conditioning (if α is close to an eigenvalue of A) of $A - \alpha I$. A new algorithm (Algorithm B67 by this author) is stable, fast, and applicable on singular linear systems, but like all such iterative algorithms that do not terminate in a finite number of steps, its convergence rate is linear. It is therefore preferable to employ the CG algorithm, which enjoys the finite termination property, as the RQI's linear solver.

Taking advantage of the fact that a symmetric matrix has a full set of orthogonal eigenvectors regardless of the structure of its eigenvalues, a single eigenvector is computed at each step. The algorithm terminates since the eigenvector computed at a given step is orthogonal to the ones computed in previous steps.

RQI's rate of convergence is cubic and the number of multiplications employed to update the T and B matrices and by the CG algorithm is of the order of n^3 since the updates can be executed using vector-matrix multiplications only. For comments concerning the QR algorithm see Parlett [2, p. 159] and Trefethen and Bau [3, p. 338].

References

[1] Gene H. Golub and Charles F. Van Loan, *Matrix Computations,* 4th ed., Johns Hopkins, 2013.

[2] Beresford N. Parlett, *The Symmetric Eigenvalue Problem,* SIAM, 1998.

[3] Lloyd Trefethen and David Bau, III, *Numerical Linear Algebra,* SIAM, 1997.

[4] James H. Wilkinson, *The Algebraic Eigenvalue Problem,* Oxford University Press, 1965.