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Top Eigenpairs of Large Scale Matrices

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Abstract. This paper is devoted to the study of an extended global algorithm on computing the top eigenpairs of a large class of matrices. Three versions of the algorithm are presented that includes a preliminary version for real matrices, one for complex matrices, and one for large scale sparse real matrix. Some examples are illustrated as powerful applications of the algorithms. The main contributions of the paper are two localized estimation techniques, plus the use of a machine learning inspired approach in terms of a modified power iteration. Based on these new tools, the proposed algorithm successfully employs the inverse iteration with varying shifts (a very fast "cubic algorithm") to achieve a superior estimation accuracy and computation efficiency to existing approaches under the general setup considered in this work.

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Key words: Matrix eigenpair, extended global algorithm, localized estimation technique, top eigenpair, large sparse matrix.

1 Introduction: Extended global algorithm

The top eigenpairs of matrix play an important role in many fields. In particular, for the maximal eigenpair for instance, there are well-known algorithms in several different fields. For web-search, it is called PageRank. For economic optimization, there is so called left-positive eigenvector method (cf. [1; Chapter 10]). For statistics, there is principal component analysis (abbrev. PCA) which is also used in quantum mechanics computation (quantum chemistry in particular) and AI. In the last case, one needs not only the maximal one, but also a couple of the subsequent eigenpairs. Certainly, for such a well-developed field, there are some powerful algorithms in common use, the "singular value decomposition" (abbrev. SVD) for PCA for example. However, as mentioned at

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the beginning of [9; p.65, §2.6]: "In some cases, SVD will not only diagnose the problem, it will also solve it, in the sense of giving you a useful numerical answer, although, as we shall see, *not necessarily 'the' answer that you thought you should get*." This happens for a number of known algorithms (see [7; Example 1] for instance) and so more careful study is valuable.

This paper is motivated by the study on the global algorithms given in [3, 7], where some effective algorithms were presented for computing the maximal eigenpair of a rather larger class of matrices. Roughly speaking, two approaches are adopted there: the power iteration (abbrev. PI) and the inverse power iteration with varying/fixed shifts (abbrev. $\mathrm{IPI}_v/\mathrm{IPI}_f$). The PI has only a little restriction on the initial vector and so has a wide range of applications. It is also economical (having lower computational complexity), but has a quite slow convergence speed, especially near the target eigenvalue. The fast convergence speed of the algorithms given in [3, 7] is mainly due to the use of IPI_v (having higher computational complexity). It is however quite dangerous if the initial is not close enough (from above) to the target eigenvalue. The last problem was avoided in [3, 7] mainly due to the assumption: the off-diagonal elements of the matrix are all nonnegative. This is essential: it implies the existence of the maximal eigenpair (as an application of the Perron–Frobenius theorem, by a shift if necessary). Then we have some important variational formulas for the upper/lower bounds of the maximal eigenvalue, i.e., the Collatz–Wielandt (abbrev. C-W) formula (cf. [2; §1 and Corollary 12]). For nonnegative matrix, the formula takes the following form:

$$\sup_{x>0}\min_k \frac{(Ax)(k)}{x(k)} = \lambda = \inf_{x>0}\max_k \frac{(Ax)(k)}{x(k)},$$

where λ is the maximal eigenvalue of the matrix A and $x(k)$ is the kth component of the vector x. The upper bound in the formula is very important in using IPI_v for avoiding the pitfalls (cf. [4; §4]). Now, a challenge appears:

Question: What can we do without the assumption of the nonnegative property of the off-diagonal elements?

A typical model led to the question is PCA, for which some of the off-diagonal elements can be negative. The question is quite serious since almost each advantage introduced in the previous paragraph is lost. We do not have the Perron–Frobenius theorem; more seriously, we do not have the C-W formula; and furthermore, the IPI_v is not practical.

Certainly, the answer to the above question is not obvious. If you have luckily produced enough courage, you may look for a way to find a substitute of the C-W formula. Assume that the given matrix A is real. Assume also for a moment that the maximal eigenvalue λ we are working is positive. Of course, at the present case, the corresponding eigenvector g is not necessarily positive, and it may have negative or zero components. Because we are now bare-handed, to find an exit from the darkness, we have to go back