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A fixed-point method for approximate projection onto the positive semidefinite cone

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ABSTRACT

The projection of a symmetric matrix onto the positive semidefinite cone is an important problem with application in many different areas such as economy, physics and, directly, semidefinite programming. This problem has analytical solution, but it relies on the eigendecomposition of a given symmetric matrix which clearly becomes prohibitive for larger dimension and dense matrices. We present a fixed-point iterative method for computing an approximation of such projection. Each iteration requires matrix–matrix products whose costs may be much less than $O(n^3)$ for certain structured matrices. Numerical experiments showcase the attractiveness of the proposed approach for sparse symmetric banded matrices.

Given a $n \times n$ symmetric matrix A, we address the problem of computing the projection of A onto $\mathcal{S}_+^n$, the set of symmetric positive semidefinite matrices, according to the Frobenius norm. It is a relevant problem with application in many different areas such as economy, physics and, directly, semidefinite programming [23,22,11]. This problem can be cast as a quadratic semidefinite programming problem:

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$$\min_{X \in \mathcal{S}^n} \frac{1}{2}\|A - X\|_F^2 \quad \text{s.t } X \succeq 0, \tag{1}$$

where $\mathcal{S}^n$ stands for the set of symmetric matrices of order n, $\|\cdot\|_F$ denotes the Frobenius norm and $X \succeq 0$ means that

$$X \in \mathcal{S}^n_+ = \{Y \in \mathcal{S}^n \,|\, \forall i:\ \lambda_i(Y) \geq 0\},$$

$\lambda_i(Y)$ denoting the i-th eigenvalue of Y.

For the reader interested in projecting a nonsymmetric matrix $A \in \mathbb{R}^{n\times n}$, we underline that

$$\|A - X\|_F^2 = \text{Trace}((A-X)^T(A-X)) = \|\frac{A+A^T}{2} - X\|_F^2 + \|\frac{A-A^T}{2}\|_F^2,$$

for any symmetric matrix X. Hence, in such a case, the objective function of problem (1) should be replaced by $1/2\|(A^T + A)/2 - X\|_F^2$.

It is well-known [21,14] that problem (1) has an analytical solution. Let $A = Q\Lambda Q^\top$ be the spectral decomposition of A. Then, the projection of A onto $\mathcal{S}^n_+$, with respect to the Frobenius norm, is given by

$$A_+ = Q\Lambda_+Q^\top = Q\,\text{diag}(\max\{0,\lambda_1\},\ldots,\max\{0,\lambda_n\})\,Q^\top, \tag{2}$$

where $\text{diag}(\cdot)$ represents a diagonal matrix.

However, the projection obtained from Eq. (2) requires the eigendecomposition of the symmetric matrix A whose cost is $O(n^3)$ – approximately $9n^3$ if a QR algorithm is applied after reducing A to tridiagonal form [9]; or approximately $4n^3$ if a divide-and-conquer approach is employed [10].

Certainly, the $O(n^3)$ cost turns prohibitive for larger values of n. In that case, in order to conceive affordable algorithms for computing the projection onto the positive semidefinite cone it is necessary to exploit the particular structure of the matrix A and/or sought properties of the projection.

The aim of the paper is to discuss an alternative method for approximately solving (1), as well as its particular usefulness for some sort of matrices, specifically, symmetric banded ones. We proposed a class of fixed-point methods based on polynomial filtering, which present quadratic convergence in the simplest case (a polynomial of degree three). In such a case, this polynomial has already appeared in computational quantum chemistry for purifying the density matrix, by giving rise to the so-called McWeeny purification [17,19]. In addition, it is not hard to show that there is a straight relation between this polynomial of degree three and the one given by the Newton–Schulz iteration for computing the sign function of a matrix [7,15].

This paper is organized as follows. Section 1 introduces the notation and some basic properties of the projection. The polynomial fixed-point iteration is proposed in Section 2