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A General Algorithm to Calculate the Inverse Principal p-th Root of Symmetric Positive Definite Matrices

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Abstract. We address the general mathematical problem of computing the inverse p-th root of a given matrix in an efficient way. A new method to construct iteration functions that allow calculating arbitrary p-th roots and their inverses of symmetric positive definite matrices is presented. We show that the order of convergence is at least quadratic and that adjusting a parameter q leads to an even faster convergence. In this way, a better performance than with previously known iteration schemes is achieved. The efficiency of the iterative functions is demonstrated for various matrices with different densities, condition numbers and spectral radii.

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1 Introduction

The first attempts to calculate the inverse of a matrix by the help of an iterative scheme were amongst others made by Schulz in the early thirties of the last century [1]. This

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resulted in the well-known Newton-Schulz iteration scheme that is widely used to approximate the inverse of a given matrix [2]. One of the advantages of this method is that for a particular start matrix as an initial guess, convergence is guaranteed [3]. The convergence is of order two, which is already quite satisfying, nevertheless there have been a lot of attempts to speed up this iteration scheme and to extend it to not only to calculate the inverse, but also the inverse p-th root of a given matrix [4–8]. This is an important task which has many applications in applied mathematics, computational physics and theoretical chemistry, where efficient methods to compute the inverse or inverse square root of a matrix are indispensable. An important example are linear-scaling electronic structure methods, which in many cases require to invert rather large sparse matrices in order to approximately solve the Schrödinger equation [9–30]. A related example is Löwdin's method of symmetric orthogonalization [31–38], which transforms the generalized eigenvalue problem for overlapping orbitals into an equivalent problem with orthogonal orbitals, whereby the inverse square root of the overlap matrix has to be calculated.

Common problems in the applications alluded to above, are the stability of the iteration function and its convergence. For $p \neq 1$, most of the iteration schemes have quadratic order of convergence, with for instance Halley's method being a rare exception [7, 39, 40], whose convergence is of order three. Altman, however, generalized the Newton-Schulz iteration to an iterative method of inverting a linear bounded operator in a Hilbert space [41]. He constructed the so-called *hyperpower method of any order of convergence* and proved that the method of degree three is the optimum one, as it gives the best accuracy for a given number of multiplications.

In this article, we describe a new general algorithm for the construction of iteration functions for the calculation of the inverse principal p-th root of a given matrix A. In this method, we have two variables, the natural number p and another natural number $q \geq 2$ that represents the *order of expansion*. We show that two special cases of this algorithm are Newton's method for matrices [5–8, 40, 42, 43] and Altman's hyperpower method [41].

The remainder of this article is organized as follows. In Section 2, we give a short summary of the work presented in the above mentioned papers and show how we can combine this to a general expression in Section 3. In Section 4, we study the introduced iteration functions for both, the scalar case and for symmetric positive definite random matrices. We investigate the optimal order of expansion q for matrices with different densities, condition numbers and spectral radii.

2 Previous work

Calculating the inverse p-th root, where p is a natural number, has been studied extensively in previous works. The characterization of the problem is quite simple. In general, for a given matrix $A \in \mathbb{C}^{n \times n}$ one wants to find a matrix B that fulfills $B^{-p} = A$. If A is invertible, one can always find such a matrix B, though B may not be unique. The problem