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Efficient mixed rational and polynomial approximation of matrix functions

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ABSTRACT

This paper presents an efficient method for computing approximations for general matrix functions based on mixed rational and polynomial approximations. A method to obtain this kind of approximation from rational approximations is given, reaching the highest efficiency when transforming nondiagonal rational approximations with a higher numerator degree than the denominator degree. Then, the proposed mixed rational and polynomial approximation can be successfully applied for matrix functions which have any type of rational approximation, such as Padé, Chebyshev, etc., with maximum efficiency for higher numerator degrees than the denominator degrees. The efficiency of the mixed rational and polynomial approximation is compared with the best existing evaluating schemes for general polynomial and rational approximations, providing greater theoretical accuracy with the same cost in terms of matrix multiplications. It is well known that diagonal rational approximants are generally more accurate than the corresponding nondiagonal rational approximants which have the same computational cost. Using the proposed mixed approximation we show that the above statement is no longer true, and nondiagonal rational approximants are in fact generally more accurate than the corresponding diagonal rational approximants with the same cost.

1. Introduction

Matrix functions play a fundamental role in many areas of science and engineering and are an important subject of study in pure and applied mathematics [1,2]. Evaluating a function $f(A)$ of an n-by-n matrix A is a frequently occurring problem and many techniques for its computation have been proposed. The main methods for general functions are those based on polynomial approximations, rational approximations, similarity transformations and matrix iterations [1].

In this paper we propose the use of mixed rational and polynomial approximations to compute matrix functions. We show that this kind of approximation can be more efficient than polynomial and rational approximations which provide similar theoretical accuracy. Moreover, we show their relation with rational approximations, and provide a method to obtain the mixed approximations from rational approximations whenever they exist for the considered matrix function, showing that the mixed rational and polynomial approximation can be applied to matrix functions which have any type of rational approximation, such as Padé, Chebyshev, etc., reaching maximum efficiency for nondiagonal rational approximations.

Throughout this paper $\mathbb{R}^{n\times n}$ and $\mathbb{C}^{n\times n}$ denote the sets of real and complex matrices of size $n \times n$, respectively, and I denotes the identity matrix for both sets. $\mathbb{Z}$ denotes the set of integers, $\lceil x \rceil$ denotes the lowest integer not less than x and $\lfloor x \rfloor$ denotes the highest integer not exceeding x.

We will describe the cost of the computations counting the number of matrix operations, denoting by M the cost of a matrix multiplication, and by D the cost of the solution of a multiple right-hand side linear system $AX = B$, where matrices A and B are $n \times n$.

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This paper is organized as follows. Section 2 summarizes results for efficient polynomial and rational approximations for general matrix functions. Section 3 deals with the proposed mixed rational and polynomial approximation. Section 4 gives a method to obtain the mixed approximations from nondiagonal rational approximations, and discusses some rounding error issues in the evaluation of the mixed approximation. Section 5 studies the cost of the new technique comparing it with efficient schemes for rational and polynomial approximations. Finally, conclusions are given in Section 6.

2. Polynomial and rational approximations

Many methods for the computation of matrix functions based on polynomial and rational approximations have been proposed [2,1]. Among them, the most widely used techniques are those based on Taylor, Padé and Chebyshev approximations. In the following subsections we summarize results for the cost of evaluating polynomial and rational approximations, and some basic properties for Taylor, Padé and Chebyshev approximations.

2.1. Polynomial approximations of matrix functions

Among the different polynomial approximations, Taylor series is a basic tool for computing matrix functions, see Section 4.3 of [1, pp. 76–78]. Let $f(A)$ be a matrix function defined by a Taylor series that converges for the square matrix A. Then, we denote $T_m(A)$ the matrix polynomial of degree m that defines the truncated Taylor series of $f(A)$. For $x \in \mathbb{C}$ the truncated Taylor series $T_m(x)$ of a scalar function $f(x)$ about the origin satisfies

$$f(x) - T_m(x) = O(x^{m+1}), \tag{1}$$

and, from now on, we will refer to m as the order of the Taylor approximation.

Below we retrieve some results for the cost of evaluating a matrix polynomial in terms of matrix multiplications M. From (4.3) of [1, p. 74] it follows that the cost of evaluating a matrix polynomial of degree m

$$P_m(A) = \sum_{k=0}^{m} b_k A^k, \tag{2}$$

using Horner and Paterson-Stockmeyer's methods [3] is

$$(s + r - 1 - g(s,m))M, \quad \text{with } r = \lfloor m/s \rfloor, \; g(s,m) = \begin{cases} 1 & \text{if } s \text{ divides } m, \\ 0 & \text{otherwise}, \end{cases} \tag{3}$$

and this quantity is approximately minimized by $s = \sqrt{m}$, so we can take $s = \lceil \sqrt{m} \rceil$ or $s = \lfloor \sqrt{m} \rfloor$, giving both values the same cost [1, p. 74].

From [4, pp. 6454–6455], see Table 4.1 of [1, p. 74], using Horner and Paterson-Stockmeyer's methods the maximum degrees of the matrix polynomial (2) that can be evaluated for a given number of matrix products are

$$m^* = \{1, 2, 4, 6, 9, 12, 16, 20, 25, 30, 36, \ldots\}, \tag{4}$$

i.e. for $m = s^2$ (odd positioned elements in m^*) and $m = s(s+1)$ (even positioned elements in m^*), both with $s = 1, 2, 3, \ldots$ The evaluation of matrix polynomial (2) for the degrees in m^* can be performed with minimum cost using evaluation formula (23) of [4, p. 6455]

$$\begin{aligned} P_m(A) = \Big\{\Big\{ \cdots \Big\{ & b_m A^s + b_{m-1} A^{s-1} + \cdots + b_{m-s+1} A + b_{m-s} I \Big\} \\ & \times A^s + b_{m-s-1} A^{s-1} + b_{m-s-2} A^{s-2} + \cdots + b_{m-2s+1} A + b_{m-2s} I \Big\} \\ & \times A^s + b_{m-2s-1} A^{s-1} + b_{m-2s-2} A^{s-2} + \cdots + b_{m-3s+1} A + b_{m-3s} I \Big\} \\ & \quad \cdots \\ & \times A^s + b_{s-1} A^{s-1} + b_{s-2} A^{s-2} + \cdots + b_1 A + I b_0, \end{aligned} \tag{5}$$

after computing and saving matrix powers $A^2, A^3, \ldots, A^s$, where one can take $s = \lceil \sqrt{m} \rceil$ or $s = \lfloor \sqrt{m} \rfloor$. Both selections of s divide m and give the same total cost. Hence, the cost of evaluating (5), denoted by C_P, is $(s-1)M$ to compute the matrix powers, plus $(m/s - 1)M$ for evaluating the remaining matrix products in (5), to give

$$C_P = (r + s - 2)M, \quad \text{with } r = \lfloor m/s \rfloor = m/s, \tag{6}$$

Table 1
Cost C_P in terms of matrix multiplications for the evaluation of polynomial $P_m(A)$ with the first 10 values of m^*.

m^*	1	2	4	6	9	12	16	20	25	30
C_P	0	1	2	3	4	5	6	7	8	9