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On the finite section method for computing exponentials of doubly-infinite skew-Hermitian matrices

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A B S T R A C T

Computing the exponential of large-scale skew-Hermitian matrices or parts thereof is frequently required in applications. In this work, we consider the task of extracting finite diagonal blocks from a doubly-infinite skew-Hermitian matrix. These matrices usually have unbounded entries which impede the application of many classical techniques from approximation theory. We analyze the decay property of matrix exponentials for several classes of banded skew-Hermitian matrices. Then finite section methods based on the decay property are presented. We use several examples to demonstrate the effectiveness of these methods.

1. Introduction

In a number of scientific applications, especially in quantum mechanics, it is desirable to compute $\exp(\mathrm{i}A)$ where A is a self-adjoint operator. For example, $\exp(\mathrm{i}A)$ naturally appears in the solution of the time-dependent Schrödinger equation [7]. We refer to, e.g., [9] for applications from other domains. In practice, the operator A is often given in

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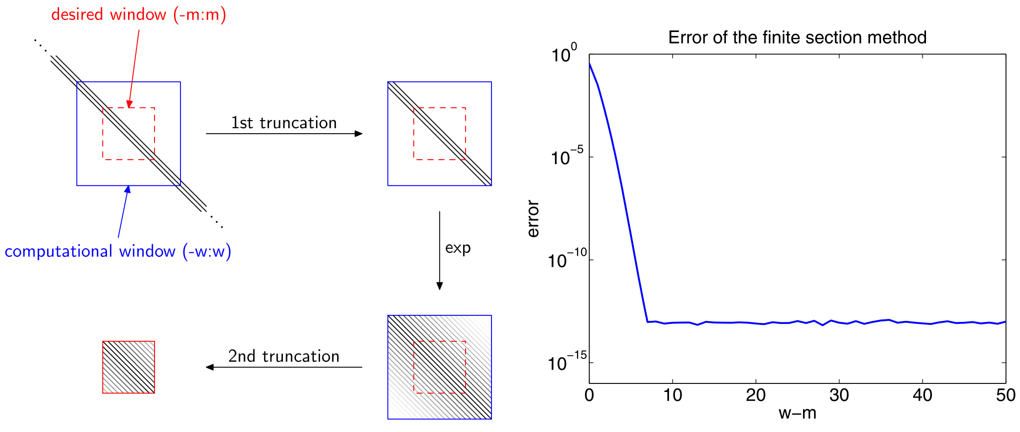

Fig. 1. A pictorial illustration of the finite section method. In this case A is the Wilkinson-type matrix $W^-(1)$.

discretized form, i.e., a doubly-infinite Hermitian matrix under a certain basis, and a finite diagonal block of $\exp(\mathrm{i}A)$ is of interest. Suppose the $(-m : m, -m : m)$ block[1] of $\exp(\mathrm{i}A)$ is desired. A simple way to solve this problem is illustrated in Fig. 1. We first compute the exponential of the $(-w : w, -w : w)$ block of A, where w is chosen somewhat larger than m, and then use its central $(2m+1)\times(2m+1)$ block to approximate the desired solution. In reference to similar methods for solving linear systems [15,20], we call this approach *finite section method*. The diagonal blocks $(-m : m, -m : m)$ and $(-w : w, -w : w)$ are called the *desired window* and the *computational window*, respectively.

To our knowledge, much of the existing literature on infinite matrices is concerned with solving infinite dimensional linear systems, see e.g., [5,6,27] and the references therein. The matrix exponential problem for infinite matrices has also been studied [14,16]. Despite the simplicity of the finite section method, it is crucial to ask how large the computational window needs to be, and whether this truncation produces sufficiently accurate approximation to the true solution. These questions are relatively easy to answer for bounded matrices, where standard polynomial approximation technique can be applied. But it turns out that the finite section method can also be applied to certain unbounded matrices, and still produces reliable solutions. For example, Fig. 1 illustrates this for an unbounded Wilkinson-type matrix $W^-(1)$, see Section 3.2, for which the error decays quickly when the size of the computational window increases. In this paper we will explain this phenomenon and establish the finite section method with error estimates for several classes of doubly-infinite Hermitian matrices.

The rest of this paper is organized as follows. In Section 2, we discuss the decay property of $\exp(\mathrm{i}A)$ for a bounded matrix A and show how this can be used to analyze the finite section method. In Section 3, we first analyze decay of entries for Wilkinson-type

[1] The MATLAB colon notation $i : j$ represents a set of consecutive integers $\{i, i+1, \ldots, j\}$.