Read me: An efficient algorithm to compute the exponential of skew-Hermitian matrices for the time integration of the Schrödinger equation

Philipp Bader Sergio Blanes Fernando Casas
Muaz Seydaoğlu

April 9, 2021

Given a skew-Hermitian matrix, $X \in \mathbb{C}^{N\times N}$, $X^H = -X$, we propose in [1] an algorithm to evaluate e^X that is more efficient than the Matlab function `expm`. Computing this matrix exponential is often required in quantum mechanical problems. In that case one has to compute e^{-iA} with A a Hermitian matrix, but our algorithm is also able to solve this problem. So, given the skew-Hermitian matrix, X, to compute e^X the flow of the algorithms first takes $A = iX$ and next the algorithm computes e^{-iA}.

This algorithm uses the scaling-and-squaring technique in a similar way as the procedure in `expm`, but it approximates the scaled exponential by a truncated Chebyshev polynomial (instead of a diagonal Padé approximant) that is evaluated with a new technique to reduce the number of matrix-matrix products. The new algorithm has been written as a Matlab function called `expmC.m`, and available at the following link:

`http://www.gicas.uji.es/Research/ExpSkewHermitian.html`

One simply has to download the file and, given a skew-Hermitian matrix `X`, one just has to replace `expm(X)` by `expmC(X)`. The new algorithm provides a similar accuracy but, in general, with a reduced number of products (you can check it with your own selected examples!).

In the particular, but very important, case in which the matrix $A = iX$ is real and symmetric, $A^T = A \in \mathbb{R}^{N\times N}$, then

$$\mathrm{e}^{-iA} = \cos(A) - i\sin(A),$$

and we also provide an algorithm for computing $\cos(A)$ and $\sin(A)$ simultaneously that only involves products of real symmetric matrices. This new algorithm is more efficient than the previous ones since they usually require products of complex matrices. The squaring is replaced by the double angle formulae.

The new algorithm has also been written as a Matlab function called `cosmsinmC.m`, also available at the previous link.

One has to download the file and, given a skew-Hermitian matrix, X, such that $A = iX$ is a real and symmetric matrix `A`, one just has to replace `expm(X)` by `cosmsinmC(X)` (or `expm(-1i*A)` by `cosmsinmC(-1i*A)`). Similar accuracy is provided but, in general, with a reduced number of products of matrices that are real, symmetric and that they commute.

The speed of the algorithm can be considerably increased if one uses an optimized algorithm to compute the product of two real and symmetric matrices, A, B, that also commute, i.e. $AB = BA$.

We illustrate in a very simple example how the functions are used.

Example

We consider the real symmetric matrix $A \in \mathbb{R}^{N\times N}$ defined as

$$A = \frac{1}{4}\begin{pmatrix} 2 & -1 & & & 1 \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & -1 & 2 & -1 \\ 1 & & & -1 & 2 \end{pmatrix}$$

that has real eigenvalues distributed in the interval $(0,1)$ and $\|A\|_1 = 1$.

We now consider the matrix C whose elements are random numbers normally distributed generated with `C=randn(N)` then $B = \frac{1}{2}(C - C^T)$ is a skew-symmetric matrix and we build the Hermitian matrix $H = A + iB$.

The file `Example_0.m` define these matrices and compute the exponentials e^{-itH} with `expm` and `expmC`

```
E0=expm(-1i*t*H);
E1=expmC(-1i*t*H);
```

as well as e^{-itA} with `expm` and `cosmsinmC`

```
S0=expm(-1i*t*A);
S1=cosmsinmC(-1i*t*A);
```

It provides as the output the difference between these solutions and we can observe that similar accuracies (about roundoff accuracy) are obtained using our new schemes which are faster in terms of number of matrix-matrix products. The new algorithms do not involve the computation of the inverse of matrices being a further improvement when considering sparse matrices. The algorithm contains the parameters t and N that can be used to change the norm of the matrices or their dimensions.

References

[1] P. Bader, S. Blanes, F. Casas, and M. Seydaoğlu, *An efficient algorithm to compute the exponential of skew-Hermitian matrices for the time integration of the Schrödinger equation.* arXiv:2103.10132 [math.NA], 2021.