A fixed point iteration for computing the matrix logarithm

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In various areas of applied numerics, the problem of calculating the logarithm of a matrix $A$ emerges. Since series expansions of the logarithm usually do not converge well for matrices far away from the identity, the standard numerical method calculates successive square roots. In this article, a new algorithm is presented that relies on the computation of successive matrix exponentials. Convergence of the method is demonstrated for a large class of initial matrices and favorable choices of the initial matrix are discussed.

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I. INTRODUCTION

Calculating the logarithm of a quadratic matrix $A$ may be a difficult problem. Of course, for problems of moderate size it is usually not prohibitive to calculate its logarithm (if existent) by complete diagonalization. However, there may exist several arguments against this method: In some cases, $A$ might not be diagonalizable. Also, if $A(t)$ and $\ln A(t)$ are known for some given time $t$, one might want to have an efficient solution for $\ln A(t + dt)$ where $dt$ is small. The approximate calculation of eigenvalues and eigenvectors of $A$ with Arnoldi methods would enable one to follow a time-dependent spectrum efficiently. Unfortunately, these methods only yield a part of the spectrum. In such cases, direct diagonalization is probably not the best method to compute $\ln A$.

If the matrix $A$ is near the identity matrix, one may truncate the Taylor series expansion of the logarithm

$$\ln[1 - (1 - A)] = -\sum_{n=1}^{\infty} \frac{(1 - A)^n}{n}.$$  

However, if this is not the case, convergence may become extremely slow or even fail, such that such a series expansion is of little practical use. The standard resolution to this problem is to bring $A$ near the identity by repeatedly computing its square root

$$\ln A = 2^k \ln A^{1/2^k}.$$  

If the square-roots are only approximated, this can be adapted to an efficient method.

The present work undertakes a different step to decrease the computational burden. Instead of calculating successive square roots, a fixed-point iteration is presented that requires the calculation of successive exponentials. The article is organized as follows: After discussing the fixed point iteration scheme in section II, in section III further improvements are discussed. In section IV a numerical implementation is discussed, and its performance is analyzed in V.

II. FIXED POINT ITERATION SCHEME

Consider the iteration formula

$$X_{n+1} = g(X_n) = A e^{-X_n} - 1 + X_n.$$  

If one regards $X_i$ as real numbers, it is quite straightforward to see that for any $X_0 > 0$ the above iteration formula converges to

$$\lim_{n \to \infty} X_n = \ln A.$$  

For example, it is immediately evident that $X_\infty = \ln A$ is the only fixed point of $g(x)$ in $\mathbb{R}$. In addition, by investigating that $|g'(X_\infty)| = |x| < 1$ one can conclude that this fixed point is stable and thus that one has a contractive map which converges to $\ln x$ for all positive numbers.

Evidently, one can also consider the iteration for matrices $X_n$ and $A$ (assumed to have a well-defined logarithm). Clearly, one still has fixed points at the logarithm $g[\ln(A) + 2k\pi i] = \ln(A) + 2k\pi i$. The question is under which conditions these fixed points are attractive, i.e., for which matrices $X_i$ the difference (with respect to some norm) to $\ln A$ becomes smaller with each iteration.

For simplicity I will restrict myself to an initial matrix $X_0$ that commutes with $A$. It is straightforward to show that

$$[X_0, A] = 0 \implies [X_{i+1}, A] = 0,$$  

and therefore if $[X_0, A] = 0$ the iteration defines a series of mutually commuting matrices.

With inserting $X_i = \ln(A) + \Delta_i$ one has (using $[A, \Delta_i] = 0$)

$$\Delta_{i+1} = e^{-\Delta_i} + \Delta_i - 1.$$  

From now on I will assume that $\Delta_i$ is a normal matrix, i.e., $[\Delta_i, \Delta_i^\dagger] = 0$. The spectral theorem implies the existence of an orthonormal basis, within which $\Delta_i$ has diagonal form (with possibly complex eigenvalues $\lambda_j^{(i)}$). Therefore, the iteration transforms the eigenvalues of the deviation matrix $\Delta_i$ according to

$$e^{-\lambda + \lambda - 1} \geq 0 \quad : \quad -\infty < \lambda < \infty.$$  

If the eigenvalues of $\Delta_i$ are real, one can deduce from

$$e^{-\lambda} + \lambda - 1 \geq 0 \quad : \quad -\infty < \lambda < \infty.$$
that the next deviation matrix $\Delta_{i+1}$ will be positive semidefinite. Also, one obtains for the operator norm (for a positive semidefinite matrix this is simply its largest eigenvalue)

$$\|\Delta_{i+1}\| = \max_j \left[e^{-\lambda_j} + \lambda_j - 1\right]. \quad (8)$$

Then, one can deduce from

$$e^{-\lambda} + \lambda - 1 \leq |\lambda| : \quad \lambda \geq -1.256 \ldots \quad (9)$$

that the norm of $\Delta_{i+1}$ will be smaller than the norm of $\Delta_i$ if $\Delta_i$ is positive semidefinite. In other words, for any matrix $X_0 = \ln A + \Delta_0$ with a self-adjoint initial deviation matrix $\Delta_0$ and $[\Delta_0, A] = 0$ the iteration (3) is contractive and will converge to $\ln A$. Note that (under the precondition that $[A, \Delta_0] = 0$) $\Delta_0 = \Delta_0^\dagger$ does not imply that $A = A^\dagger$, but $A = A^\dagger$ implies $\Delta_0 = \Delta_0^\dagger$. Complex eigenvalues $\lambda = x + iy$ (in case of $\Delta$, being normal) are also transformed according to (6). Demanding that the modulus of all eigenvalues of $\Delta$ should become smaller with each iteration, one obtains a region of convergence $V$. If all eigenvalues of the $\Delta$-matrix are contained within

$$V = \{\lambda = x + iy \in C : |e^{-\lambda} + \lambda - 1|^2 \leq |\lambda|^2\} \quad (10)$$

convergence is assured, see also figure 1. Note that the ambiguity of the logarithm function does not pose a major problem here, since the $\Delta$-matrix can be chosen to represent the difference to any specific branch of the logarithm without any difference.

With the Banach fixed point theorem one can then show that the iteration (3) will converge towards $\ln A$. In the following, some suitable choices for an initial matrix to the algorithm will be discussed.

### III. ALGORITHMIC OPTIMIZATIONS

Beyond performing scaling transformations $\ln A = \ln (A/\sigma) + \ln (\sigma) 1$, one has further options to improve the algorithmic performance.

It is evident from (9) and figure 1 that a good initial guess for the matrix logarithm may save a lot of computation time. Such a guess can be made if some bounds on the eigenvalues of $A$ (and hence also to those of $\ln A$) are known. Such bounds can for example be cheaply extracted from Gershgorins circle theorem (which is especially useful if the matrix $A$ is diagonally dominant) or they may be already known from the definition of the problem. Then an initial matrix with eigenvalues close to $\ln A$ can be constructed from the linear Taylor approximation that could be optimized for the regime $[\ln(\lambda_{\min}), \ln(\lambda_{\max})]$. Assuming an approximately uniform distribution of eigenvalues, one could for example consider

$$X_0 = \left[\ln \left(\frac{\lambda_{\min} + \lambda_{\max}}{2}\right) - 1\right]1 + \frac{2}{\lambda_{\min} + \lambda_{\max}} A. \quad (11)$$

Other choices could include some adapted polynomials of $A$.

In addition to a good guess for an initial matrix one may also think of optimizations of the algorithm itself. For example, the iteration

$$X_{n+1} = X_n - \frac{1}{2} [Ae^{-X_n} - A^{-1}e^{X_n}] \quad (12)$$

has in the 1-dimensional case near its fixed point $X_\infty = \ln A$ better convergence properties than (3). However, the iteration does not converge far away from the solution. Therefore, it could be used as an optional last refinement step after the conventional iteration (3) has converged with sufficient accuracy.

### IV. A NUMERICAL ALGORITHM

The fixed-point iteration (3) requires the calculation of the exponential of the iterates. The associated computational burden can be reduced by exploiting that the proposed fixed-point iteration produces a series of mutually commuting matrices, if initialized properly. Therefore, two successive exponentials can also be computed iteratively, which has the advantage that the norm of the matrix to be exponentiated in each step does not become
too large. In this case, the inverse scaling and squaring method, which is based on
\[
e^B = [\exp(B/2^j)]^{2j}
\]
(13)
is known to produce good results with a modest number of matrix multiplications \[3,6\]. For example using a \(k\)-th order Taylor approximant the exponential (13) can be calculated with just \(k+j-1\) matrix multiplications. The algorithm can be summarized as follows

- Determine an initial matrix \(X_0\)
  - with eigenvalues close to those of \(\ln A\)
  - with \([X_0,A]=0\)
- set \(Y_0 = \exp(-X_0)\)
- iterate
  \[
  X_{n+1} = AY_n - 1 + X_n
  \]
  \[
  Y_{n+1} = Y_n \exp\{- (AY_n - 1)\}
  \]
until convergence is reached
- or a maximum number of iterations has been exceeded

- refinement step [optional]:
  \[
  X_{\text{fin}} = X_n - \frac{1}{2} [A^{-1} e^{X_n} - A e^{-X_n}]
  \]

Note that \(Y_n\) will converge to the inverse of \(A\) (although there exist by far more efficient methods to achieve this).

V. PERFORMANCE ANALYSIS

In order to estimate the performance of the algorithm, some sample matrices have been generated. For different matrix dimensions, 1000 matrices have been randomly generated. Some test matrices had a uniform eigenvalue distribution in the interval \([1 \cdot 10^{-8}, 1]\), others were exponentially distributed according to \(\rho_A(x) = \lambda e^{-\lambda x}\) also in the interval \([1 \cdot 10^{-8}, 1]\). The diagonal matrix generated by these eigenvalues has been transformed into a non-diagonal test matrix by applying random orthogonal transformations \(A = Q^\dagger A p Q\) with \(Q_{ij} = \delta_{ij} - 2 \cos \theta_{iv} v_j\) and \(\sum_i v_i^2 = 1\). All iterations were initialized with \(X_0 = 2A - (1 + \ln(2))1\), which is not necessarily the optimum choice. For all norm calculations, the Frobenius matrix norm has been used. The iteration for the logarithm used as a stopping criterion \(|X_n|, |X_{n+1} - X_n| \leq \varepsilon\), and the calculation of the exponential of a matrix \(B\) used \(\|B\|^p \leq \varepsilon\). To calculate the matrix exponential, the scaling and squaring method was used in combination with truncated Taylor approximants \[3\]. Note that the efficiency of the scaling and squaring method can in principle be increased by approximately 50% if instead of Taylor approximants, Padé approximants are used \[3\]. The number of matrix multiplications to obtain convergence was therefore counted with and without including those required by computing the Taylor approximants to the matrix exponential, see figure 2. Whereas the number of total required matrix multiplications increases approximately linearly with \(\varepsilon\), it is visible that the algorithm shifts the computational burden towards matrix exponentiation, and the total number of matrix multiplications increases approximately linearly with the required precision. Around \(\varepsilon \approx 1 \cdot 10^{-10}\) the scaling breaks down due to numerical roundoff errors (error bars omitted), compare also figure 3. It is also visible that the dependence on the dimension of the matrix is rather weak.

In order to get an estimate on the error of \(\ln A\) one can perform the inverse operation, i.e., exponentiate the result (with a much better precision) and compare it with the original test matrix. Thus, from \(|\exp(\ln A + \Delta) - A| / |A|\) one has an estimate for the actual error \(|\Delta|\), see figure 4. It becomes visible that for \(\varepsilon \geq 10^{-10}\) the accuracy of the computed logarithm is much better than one might have expected. In addition, with a single application of (12), the final error of the algorithm can be reduced by orders of magnitude.
VI. SUMMARY

The fixed-point iteration presented here has some advantages in comparison to standard algorithms \[3, 4\]. One of the most important advantages is the ease of implementation. Given the simplicity of the inverse-scaling and squaring algorithm for computing the matrix exponential, the user basically has to implement matrix-matrix multiplication. As has been demonstrated, the fixed point iteration guarantees fast convergence if a good initial guess is given. For some special test problems, the convergence is competitive with state of the art algorithms. With some knowledge on the spectrum of the matrix of which the logarithm should be taken, the convergence can be tuned to the specific problem. In any case, the presented iteration can be used as a final step with a low-precision result produced with established methods \[3, 4\].

In the future, it would be interesting whether the iteration algorithm can be adapted to increase convergence for a bad initial guess.

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