The computation of the exponential and logarithmic mappings and their first and second linearizations

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SUMMARY
We describe two simple methods for the evaluation of the exponential and logarithmic mappings and their first and second linearizations based on the Taylor expansion and the spectral representation. We also provide guidelines for switching between those representations on the basis of the size of the argument. The first and second linearizations of the exponential and logarithmic mappings provided here are based directly on the exponential formula for the solutions of systems of linear ordinary differential equations. This representation does not require the use of perturbation formulae for eigenvalues and eigenvectors. Our approach leads to workable and straightforward expressions for the first and second linearizations of the exponential and logarithmic mappings regardless of degeneracies in the spectral decomposition of the argument. Copyright © 2001 John Wiley & Sons, Ltd.

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1. INTRODUCTION

The need to evaluate the exponential and logarithmic mappings of square matrices, and their first and second linearizations, arises in a number of applications. For instance, some models of finite-deformation material behaviour are formulated in terms of Hencky’s logarithmic strain (see [1, 2] and references therein; see also [3–13]). In addition, several update algorithms for finite deformation plasticity have been proposed which make explicit use of the exponential and logarithmic mappings [14–16]. In these examples, the computation of the stress tensor requires the evaluation of the exponential and logarithmic mappings as well as their first linearizations. If, in addition, a Newton–Raphson solution procedure is used, the computation of the tangent moduli requires a second linearization of the exponential and logarithmic mappings.

The exponential and logarithmic mappings may be evaluated by a variety of means, including the direct summation of their corresponding Taylor expansions, or by recourse to an eigenvalue or spectral decomposition of the argument and the use of the spectral function.
theorem. A standard starting point for studies in this area is the work of Moler et al. [17], who discuss 19 different ways of computing the exponential of a matrix and argue on the computational stability and efficiency of each method. It sometimes happens that the argument of the exponential mapping is close to the null matrix or that the argument of the logarithmic mapping is close to the identity. For instance, this situation may arise during constitutive updates when the incremental deformations are small. Under these conditions, the Taylor series converge in a small number of iterations and is advantageous in comparison to the spectral decompositions. Conversely, when the argument of the exponential mapping is large or the argument of the logarithmic mapping differs greatly from the identity, the Taylor series may be expected to converge slowly or not at all, and the spectral decomposition becomes advantageous. We present numerical tests which provide an indication of where the optimal cross-over point between the Taylor and spectral representations lies.

The first and second derivatives of the exponential and logarithmic mappings may be evaluated differentiating the Taylor expansion term by term, or from the spectral decomposition by recourse to perturbation formulae for the eigenvalues and eigenvectors (see, e.g., [18] and references therein). However, this latter approach is cumbersome and fraught with difficulties, especially in the presence of repeated eigenvalues. Here we present a simpler approach based on the well-known exponential representation of the solutions of systems of linear ordinary differential equations which does not require the linearization of the spectral decomposition. Our approach leads to workable and straightforward expressions for the first and second linearizations of the exponential and logarithmic mappings regardless of degeneracies in the spectral decomposition of the argument. In the case of symmetric argument, our results are consistent with those of Ogden [19], who treated explicitly the computation of first and second derivatives; see also [20, 21].

2. EVALUATION OF THE EXPONENTIAL AND LOGARITHMIC MAPPING AND THEIR DERIVATIVES

Let $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times n}$ be square real matrices, not necessarily symmetric. The exponential of $A$ is defined as

$$\exp(A) = \sum_{k=0}^{\infty} \frac{1}{k!} A^k$$

(1)

This series is absolutely convergent [22]. The logarithm of $B$ is defined as

$$\log(B) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} (B - I)^k$$

(2)

This series is absolutely convergent if $\|B - I\| < 1$ [22]. The problem now is to derive computationally convenient and straightforward formulae for the evaluation of the mappings $\exp(A)$ and $\log(B)$, as well as their first and second derivatives, $D\exp(A)$, $D^2\exp(A)$, and $D\log(B)$, $D^2\log(B)$. 

2.1. Spectral representation

Let $\mathbf{A}$ have eigenvalues $\{\lambda_z, \ z = 1, \ldots, n\}$, right eigenvectors $\{\mathbf{u}_z, \ z = 1, \ldots, n\}$, and left eigenvectors $\{\mathbf{v}_z, \ z = 1, \ldots, n\}$. Then,

$$
\mathbf{A}\mathbf{u}_z = \lambda_z \mathbf{u}_z, \quad z = 1, \ldots, n \tag{3}
$$

and

$$
\mathbf{A}^T\mathbf{v}_z = \lambda_z \mathbf{v}_z, \quad z = 1, \ldots, n \tag{4}
$$

and

$$
\mathbf{A} = \sum_{z=1}^{n} \lambda_z \mathbf{u}_z \otimes \mathbf{v}_z \tag{5}
$$

The exponential of $\mathbf{A}$ then admits the spectral representation

$$
\exp(\mathbf{A}) = \sum_{z=1}^{n} \exp(\lambda_z) \mathbf{u}_z \otimes \mathbf{v}_z \tag{6}
$$

Next, we wish to linearize the exponential mapping twice. To this end, we begin by recalling that the solution to the problem

$$
\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) + \mathbf{f}(t), \quad t \geq 0 \tag{7}
$$

$$
\mathbf{x}(0) = \mathbf{x}_0 \tag{8}
$$

in $\mathbb{R}^n$ is

$$
\mathbf{x}(t) = \exp(t\mathbf{A})\mathbf{x}_0 + \int_0^t \exp((t - \tau)\mathbf{A})\mathbf{f}(\tau) \, d\tau, \quad t \geq 0 \tag{9}
$$

It therefore follows that $\exp(\mathbf{A})\mathbf{x}_0$ is the $i$th component of the solution of the initial-value problem (7) and (8) at $t = 1$ with $\mathbf{f}(t) = 0$ and $\mathbf{x}_0 = \mathbf{e}_j \equiv j$th standard basis vector in $\mathbb{R}^n$.

Imagine now perturbing the matrix $\mathbf{A}$ to $\mathbf{A} + \delta\mathbf{A}$ in (7) and (8), resulting in a perturbed solution $\mathbf{x}(t) + \delta\mathbf{x}(t)$. To first order, $\delta\mathbf{x}(t)$ is the solution of the problem

$$
\delta\dot{\mathbf{x}}(t) = \mathbf{A}\delta\mathbf{x}(t) + \delta\mathbf{A}\mathbf{x}(t), \quad t \geq 0 \tag{10}
$$

$$
\delta\mathbf{x}(0) = \mathbf{0} \tag{11}
$$

From (9),

$$
\delta\mathbf{x}(t) = \int_0^t \exp((t - \tau)\mathbf{A})\delta\mathbf{A} \exp(\tau\mathbf{A})\mathbf{x}_0 \, d\tau \tag{12}
$$

But we also have

$$
\mathbf{x}(t) + \delta\mathbf{x}(t) = \exp(t(\mathbf{A} + \delta\mathbf{A}))\mathbf{x}_0 = [\exp(t\mathbf{A}) + D \exp(t\mathbf{A})\delta\mathbf{A}]\mathbf{x}_0 + \text{hot} \tag{13}
$$
Comparison of (12) and (13) yields

$$D \exp(A) \delta A = \int_0^1 \exp((1 - \tau)A) \delta A \exp(\tau A) \, d\tau$$  \hspace{1cm} (14)

or, in components

$$D \exp(A)_{ijkl} = \int_0^1 \exp((1 - \tau)A)_{ik} \exp(\tau A)_{lj} \, d\tau$$  \hspace{1cm} (15)

We may further make use of representation (5) to write (15) in the form

$$D \exp(A)_{ijkl} = \sum_{x=1}^n \sum_{\beta=1}^n \left[ \int_0^1 e^{(\hat{\lambda}_x - \hat{\lambda}_\beta) \tau} \, d\tau \right] u_{xj} v_{xk} u_{i\beta} v_{l\beta}$$  \hspace{1cm} (16)

which evaluates to

$$D \exp(A)_{ijkl} = \sum_{x=1}^n \sum_{\beta=1}^n f(\hat{\lambda}_x, \hat{\lambda}_\beta) u_{xj} v_{xk} u_{i\beta} v_{l\beta}$$  \hspace{1cm} (17)

or, in invariant notation,

$$D \exp(A) = \sum_{x=1}^n \sum_{\beta=1}^n f(\hat{\lambda}_x, \hat{\lambda}_\beta) u_x \otimes v_\beta \otimes v_x \otimes u_\beta$$  \hspace{1cm} (18)

In these expressions we have written

$$f(\hat{\lambda}_x, \hat{\lambda}_\beta) = \frac{e^{\hat{\lambda}_\beta} - e^{\hat{\lambda}_x}}{\hat{\lambda}_\beta - \hat{\lambda}_x} \quad \text{if} \quad \hat{\lambda}_\beta \neq \hat{\lambda}_x$$  \hspace{1cm} (19)

$$f(\hat{\lambda}_x, \hat{\lambda}_\beta) = e^{\hat{\lambda}_x} \quad \text{otherwise}$$  \hspace{1cm} (20)

Note that the above expressions are valid in the presence of repeated eigenvalues.

In order to determine the second derivative of the exponential mapping we may differentiate (15) to obtain

$$D^2 \exp(A)_{ijklmn} = \int_0^1 (1 - \tau)D \exp((1 - \tau)A)_{ikmn} \exp(\tau A)_{lj} \, d\tau$$

$$+ \int_0^1 \tau \exp((1 - \tau)A)_{ik} D \exp(\tau A)_{ljmn} \, d\tau$$  \hspace{1cm} (21)
Inserting (5) and (17) into this expression gives

\[
D^2 \exp(A)_{ijklmn} = \sum_{x=1}^{n} \sum_{\beta=1}^{n} \sum_{\gamma=1}^{n} \left[ \int_0^1 (1 - \tau) f((1 - \tau)\lambda_x, (1 - \tau)\lambda_\beta)e^{\tau \lambda_\gamma} \, d\tau \right] u_{x1} v_{2m} u_{j\alpha} v_{i\delta} v_{j\ell} v_{i\delta} \\
+ \sum_{x=1}^{n} \sum_{\beta=1}^{n} \sum_{\gamma=1}^{n} \left[ \int_0^1 \tau f(\tau \lambda_x, \tau \lambda_\beta) e^{(1 - \tau) \lambda_\gamma} \, d\tau \right] u_{x2} v_{2m} u_{j\beta} v_{i\delta} v_{j\ell} v_{i\delta} (22)
\]

Defining

\[
F(\lambda_x, \lambda_\beta, \lambda_\gamma) = \int_0^1 \tau f(\tau \lambda_x, \tau \lambda_\beta) e^{(1 - \tau) \lambda_\gamma} \, d\tau 
\]

Equation (22) simplifies to

\[
D^2 \exp(A)_{ijklmn} = \sum_{x=1}^{n} \sum_{\beta=1}^{n} \sum_{\gamma=1}^{n} F(\lambda_x, \lambda_\beta, \lambda_\gamma) v_{2m} u_{j\alpha} v_{i\delta} v_{j\ell} v_{i\delta} + u_{x2} v_{2m} u_{j\beta} v_{i\delta} v_{j\ell} v_{i\delta} (24)
\]

which is the sought expression. Finally, a straightforward evaluation of (23) leads to the result:

\[
F(\lambda_x, \lambda_\beta, \lambda_\gamma) = \begin{cases} 
\frac{\lambda_x e^{\lambda_x} - \lambda_x e^{\lambda_\beta} + \lambda_\beta e^{\lambda_x} + \lambda_x e^{\lambda_\gamma} - \lambda_\beta e^{\lambda_\gamma}}{(\lambda_x - \lambda_\beta)(\lambda_x - \lambda_\gamma)(\lambda_\beta - \lambda_\gamma)} & \text{if } \lambda_x \neq \lambda_\beta, \lambda_x \neq \lambda_\gamma, \lambda_\beta \neq \lambda_\gamma \\
\frac{-e^{\lambda_x} + \lambda_x e^{\lambda_x} - \lambda_\gamma e^{\lambda_x} + e^{\lambda_\gamma}}{(\lambda_x - \lambda_\gamma)(\lambda_x - \lambda_\gamma)} & \text{if } \lambda_x = \lambda_\beta, \lambda_x \neq \lambda_\gamma, \lambda_\beta \neq \lambda_\gamma \\
\frac{1}{2} e^{\lambda_x} & \text{if } \lambda_x = \lambda_\beta, \lambda_x = \lambda_\gamma, \lambda_\beta = \lambda_\gamma
\end{cases} (25)
\]

where the remaining cases follow by a cyclic permutation of the labels \(\{x, \beta, \gamma\}\).

The derivatives of the logarithmic mapping can be obtained directly from the previous expressions by recognizing that \(\log = \exp^{-1}\) and using the properties of inverse functions [22]. This leads to [22]

\[
D \log(B)_{ijkl} = D \exp(A)^{-1}_{ijkl} \\
D^2 \log(B)_{ijklmn} = -D \exp(A)^{-1}_{ijpq} D \exp(A)^{-1}_{rkl} D \exp(A)^{-1}_{iunm} D^2 \exp(A)_{pqstu} (27)
\]

where \(B = \exp(A)\). The first of these expressions evaluates to

\[
D \log(B)_{ijkl} = \sum_{\mu=1}^{n} \sum_{\alpha=1}^{n} g(\mu, \alpha) u_{x\mu} v_{2\mu} u_{j\alpha} v_{i\delta} v_{j\ell} v_{i\delta} (28)
\]

where \(\{\mu, \ x = 1, \ldots, n\}\) are the eigenvalues of \(B\), \(\{u_x, \ x = 1, \ldots, n\}\) are its right eigenvectors, and \(\{v_x, \ x = 1, \ldots, n\}\) its left eigenvectors. In invariant notation

\[
D \log(B) = \sum_{\mu=1}^{n} \sum_{\beta=1}^{n} g(\mu, \beta) u_\mu \otimes v_\beta \otimes v_\mu \otimes u_\beta (29)
\]

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where we write

\[ g(\mu_z, \mu_y) = \frac{\log \mu_y - \log \mu_z}{\mu_y - \mu_z} \quad \text{if} \quad \mu_y \neq \mu_z \]  

\[ g(\mu_z, \mu_y) = \frac{1}{\mu_z} \quad \text{otherwise} \]  

Note again that the above expressions are valid in the presence of repeated eigenvalues. Using (26) and (29), (27) may be rewritten explicitly in the form

\[ D^2 \log(B)_{ijklmn} = -D \log(B)_{ijpq} D \log(B)_{rskl} D \log(B)_{tumn} D^2 \exp(A)_{pqrstu} \]  

which does not require matrix inversion.

2.2. Taylor series expansion

The evaluation of the formulae in the preceding section requires the computation of eigenvalues and eigenvectors, which entails a non-negligible computational overhead. Therefore, for small \( \mathbf{A} \) it may be cheaper to evaluate the exponential mapping and its derivatives directly from its Taylor series expansion (1). Likewise, for \( \mathbf{B} \) close to the identity it may be cost-effective to use (2) directly. To this end, it proves convenient to express (1) in the form

\[ \exp(\mathbf{A}) = \sum_{k=0}^{\infty} \exp^{(k)}(\mathbf{A}) \]  

where the terms \( \exp^{(k)}(\mathbf{A}) \) in the expansion follow from the recurrence relation

\[ \exp^{(0)}(\mathbf{A}) = \mathbf{I} \]  

\[ \exp^{(k+1)}(\mathbf{A}) = \frac{1}{k+1} \exp^{(k)}(\mathbf{A})A, \quad k = 0, \ldots \]  

Here \( \mathbf{I} \) is the identity matrix. It follows from this representation that

\[ D \exp(\mathbf{A}) = \sum_{k=1}^{\infty} D \exp^{(k)}(\mathbf{A}) \]  

where

\[ D \exp^{(1)}(\mathbf{A}) = DA \]  

\[ D \exp^{(k+1)}(\mathbf{A}) = \frac{1}{k+1} [D \exp^{(k)}(\mathbf{A})A + \exp^{(k)}(\mathbf{A})DA], \quad k = 1, \ldots \]
In components

\[ D \exp^{(1)}(A)_{ijkl} = \delta_ik \delta_jl \]  

(39)

\[ D \exp^{(k+1)}(A)_{ijkl} = \frac{1}{k+1} [D \exp^{(k)}(A)_{ijkl} + \exp^{(k)}(A)_{ik} \delta_jl], \quad k = 1, \ldots \]  

(40)

Likewise

\[ D^2 \exp(A) = \sum_{k=2}^{\infty} D^2 \exp^{(k)}(A) \]  

(41)

where

\[ D^2 \exp^{(2)}(A) = \frac{1}{2} D^2 A^2 \]  

(42)

\[ D^2 \exp^{(k+1)}(A) = \frac{1}{k+1} \{D^2 \exp^{(k)}(A)A + 2\text{sym}[D \exp^{(k)}(A)DA]\}, \quad k = 2, \ldots \]  

(43)

where sym denotes the symmetrization algorithm. In components

\[ D^2 \exp^{(2)}(A)_{ijklmn} = \frac{1}{2} (\delta_ik \delta_m \delta_jn + \delta_in \delta_km \delta_jl) \]  

(44)

\[ D^2 \exp^{(k+1)}(A)_{ijklmn} = \frac{1}{k+1} [D^2 \exp^{(k)}(A)_{ijklmn} + \exp^{(k)}(A)_{ik} \delta_jlm + \exp^{(k)}(A)_{im} \delta_kjn + \exp^{(k)}(A)_{kn} \delta_jlm], \quad k = 2, \ldots \]  

(45)

The logarithmic mapping can be given a similar treatment. Begin by expressing (2) in the form

\[ \log(B) = \sum_{k=1}^{\infty} \log^{(k)}(B) \]  

(46)

where the terms \( \log^{(k)}(B) \) in the expansion follow from the recurrence relation

\[ \log^{(1)}(B) = B - 1 \]  

(47)

\[ \log^{(k+1)}(B) = -\frac{k}{k+1} \log^{(k)}(B)(B - 1), \quad k = 1, \ldots \]  

(48)

It follows from this representation that

\[ D \log(B) = \sum_{k=1}^{\infty} D \log^{(k)}(B) \]  

(49)
where

\[ D \log^{(1)}(B) = DB \]  \hspace{1cm} (50)

\[ D \log^{(k+1)}(B) = -\frac{k}{k+1} [D \log^{(k)}(B)(B - I) + \log^{(k)}(B)\partial B], \quad k = 1, \ldots \]  \hspace{1cm} (51)

In components

\[ D \log^{(1)}(B)_{ijkl} = \delta_{ik} \delta_{jl} \]  \hspace{1cm} (52)

\[ D \log^{(k+1)}(B)_{ijkl} = -\frac{k}{k+1} [D \log^{(k)}(B)_{ipkl}(B_{pj} - \delta_{pj}) + \log^{(k)}(B)_{jk} \delta_{jl}], \quad k = 1, \ldots \]  \hspace{1cm} (53)

Likewise

\[ D^2 \log(B) = \sum_{k=2}^{\infty} D^2 \log^{(k)}(B) \]  \hspace{1cm} (54)

where

\[ D^2 \log^{(2)}(B) = \frac{1}{2} D^2 B^2 \]  \hspace{1cm} (55)

\[ D^2 \log^{(k+1)}(B) = -\frac{k}{k+1} \{D^2 \log^{(k)}(B)(A - I) + 2\text{sym}[D \log^{(k)}(B)\partial B]\}, \quad k = 2, \ldots \]  \hspace{1cm} (56)

In components

\[ D^2 \log^{(2)}(B)_{ijklmn} = \frac{1}{2} (\delta_{ik} \delta_{lm} \delta_{jn} + \delta_{in} \delta_{jm} \delta_{jl}) \]  \hspace{1cm} (57)

\[ D^2 \log^{(k+1)}(B)_{ijklmn} = -\frac{k}{k+1} [D^2 \log^{(k)}(B)_{ipklmn}(A_{pj} - \delta_{pj}) \]

\[ + D \log^{(k)}(B)_{mkl} \delta_{jn} + D \log^{(k)}(B)_{kmn} \delta_{jl}], \quad k = 2, \ldots \]  \hspace{1cm} (58)

The above recursive formulae are in a form which lends itself to a convenient numerical implementation. In practice, the recursive evaluation terminates when the norm of the next term is less than a prespecified tolerance, or when convergence fails to be attained within a fixed maximum number of iterations.

3. COMPARISON BETWEEN TAYLOR AND SPECTRAL REPRESENTATIONS

In the foregoing, we have described two different representations of the exponential and logarithmic mappings and their first and second derivatives. The Taylor expansion of the
Figure 1. Execution times for the Taylor-expansion and spectral representations of the exponential mapping as a function of matrix size.

Figure 2. Execution times for the Taylor-expansion and spectral representations of the logarithmic mapping as a function of the distance to the identity matrix.

The rate of convergence of the Taylor expansion of the exponential (resp. logarithm) is dictated by the magnitude of the maximum eigenvalue of $A$ (resp. $B - I$). Consequently, we choose the abscissae of Figures 1 and 2 to correspond to $|A|$ and $|B|$, respectively.
The execution times are computed in C language as follows:

```c
int time_0 = clock();

for (repetitions=0; repetitions < number_of_repetitions; repetitions++)
{
    compute exponential/logarithmic mapping
    including 1st and 2nd derivatives
}

int time_1 = clock();

printf("Execution time= %f ", (double) (time_1 -
      time_0)/CLOCKS_PER_SECOND);
```

The calculations were carried out on a PC computer with a Pentium II processor (400 MHz) and 128 Mb of memory. The variable number_of_repetitions was set to 1000. All eigenvalue calculations were carried out using the `rg` subroutine from the fortran library EISPACK (http://www.netlib.org/eispack). This subroutine computes the eigenvalues and eigenvectors of a general matrix using Jacobi rotations.

It is evident from these data that the cross-over from a Taylor expansion to a spectral representation should be effected when the magnitude of the maximum eigenvalue of $A$ or $B - I$ is of the order of $0.15-0.20$. A practical cross-over criterion which avoids the computation of eigenvalues may be based simply on the Euclidean norms $\|A\| = \sqrt{\text{tr}A^TA}$ and $\|B - I\| = \sqrt{\text{tr}((B - I)^T(B - I))}$.

### 4. SUMMARY AND CONCLUSIONS

We have analysed two methods for the evaluations of the exponential and logarithmic mappings based on the Taylor expansion and the spectral function theorem. Based on the results of selected numerical tests, we have provided guidelines for switching between those representations on the basis of the size of the argument. In addition, we have presented a representation of the first and second linearizations of the exponential and logarithmic mappings based on the well-known exponential formula for the solutions of systems of linear ordinary differential equations. This representation does not require the use of perturbation formulae for eigenvalues and eigenvectors. Our approach leads to workable and straightforward expressions for the first and second linearizations of the exponential and logarithmic mappings regardless of degeneracies in the spectral decomposition of the argument.

Our numerical tests suggest switching from the Taylor expansion to the spectral representation roughly when the Euclidean norms $\|A\|$ or $\|B - I\|$ become of the order of $0.15-0.20$. The implications of this empirical criterion as regards applications to constitutive updates are noteworthy. Thus, in explicit-dynamics calculations, which are characterized by small incremental deformations, the Taylor-expansion representation may be expected to be always advantageous. Contrarywise, the spectral representation may be expected to become cost-effective in
implicit calculations involving large incremental deformations, e.g., in the vicinity of stress-risers such as crack tips. In this regime, the Taylor expansion may become unacceptably slow, or simply fail to converge. It is clear, therefore, that a general and efficient implementation of the exponential and logarithmic mappings requires the use of both expansions and spectral representations.

REFERENCES