SYMBOLIC SPECTRAL DECOMPOSITION OF 3X3 MATRICES

ABSTRACT

Spectral decomposition of matrices is a recurring and important task in applied mathematics, physics and engineering. Many application problems require the consideration of matrices of size three with spectral decomposition over the real numbers. If the functional dependence of the spectral decomposition on the matrix elements has to be preserved, then closed-form solution approaches must be considered. Existing closed-form expressions are based on the use of principal matrix invariants which suffer from a number of deficiencies when evaluated in the framework of finite precision arithmetic. This paper introduces an alternative form for the computation of the involved matrix invariants (in particular the discriminant) in terms of sum-of-products expressions as function of the matrix elements. We prove and demonstrate by numerical examples that this alternative approach leads to increased floating point accuracy, especially in all important limit cases (e.g. eigenvalue multiplicity). It is believed that the combination of symbolic algorithms with the accuracy improvements presented in this paper can serve as a powerful building block for many engineering tasks.

Keywords spectral decomposition over real numbers · symbolic computation · differentiation through eigenvalues

1 Introduction

Spectral decomposition of real-valued matrices (eigendecomposition) is a task of utmost importance for mathematicians, physicists and engineers. Specifically, the decomposition of $3 \times 3$ matrices plays a central role in three dimensional space as it is characteristic to many real-world application contexts. This special spectral decomposition problem was studied for centuries, especially due to its close relation to the roots of the cubic equation. Closed-form solutions found increasingly more use with the advent of computers and powerful symbolic systems as Mathematica [18] or SymPy [10]. The symbolic approach represents an efficient tool for computation of eigenvalues and eigenvectors while preserving their functional dependence on the matrix elements. It has the potential to be exploited together with automatic differentiation (AD) in problems where derivatives of spectral decomposition are required (e.g. non-linear problems in principal space, sensitivity analysis).

Unfortunately, when results of such eigendecomposition are implemented and evaluated in computer software with finite precision arithmetic, not all closed-form approaches are equivalent\(^1\). Very few existing papers address accuracy and sensitivity of this decomposition in the context of a symbolic algorithm, see e.g. [8,4]. Papers that study finite precision accuracy of closed-form roots to the cubic equation are more common, but less so in the context of eigenvalues and eigenvectors, [7]. Heuristic approaches were developed by the engineering community in order to overcome rounding issues, but none effectively improves the accuracy of results, see [15,11,6].

\(^1\)It might sound confusing to talk about a symbolic algorithm having finite precision issues. What is meant here is that when a symbolic expression gets evaluated for finite precision inputs the result will contain rounding error. It is implicitly assumed that the symbolic engine which evaluates expressions does not perform any aggressive simplifications or optimisations on the expression tree.
While well-established iterative methods can provide eigenvalues and eigenvectors up to very high precision, their inherent nature (presence of loops, non-predetermined number of required iterations, stopping criteria and conditionals) renders them not suitable for use within symbolic algorithms. Common implementations of iterative schemes can be found in LAPACK [1]. Numerical Recipes in C [14] or GNU Scientific Library [2].

The aim of this paper is to study rounding errors in closed-form solution to the spectral decomposition. Alternative – but mathematically equivalent – expressions are sought such that rounding effects are diminished. An ideal set of symbolic expressions must not require the evaluation of loops or taking advantage of any finite precision specific tricks, such that the resulting mathematical expression is robust and ready for direct use within a symbolic framework.

## 2 Spectral decomposition

For a diagonalisable matrix $A \in \mathbb{R}^{n \times n}$ the multiplicative spectral decomposition over the real numbers

$$A = U \Lambda V$$

is given in terms of the real-valued matrices $U = [u_1, \ldots, u_n]$ and $V = [v_1^\top, \ldots, v_n^\top]^\top$ (which, respectively, contain the right eigenvectors $u_k$ column-wise and the left eigenvectors $v_k$ row-wise) and the diagonal matrix $\Lambda$, holding the $n$ real-valued eigenvalues $\lambda_k$. The (scaled) eigenvectors in $U$ and $V$ fulfil the requirement $UV = I$. The equivalent additive real-valued spectral decomposition

$$A = \sum_{k=1}^{n} \lambda_k E_k$$

can be written in terms of the product of the eigenvalue $\lambda_k$ and its associated eigenprojector $E_k = u_k \otimes v_k$. Independent of eigenvalue multiplicities, $n$ distinct eigenprojectors could always be found such that they have then the following properties

$$\sum_{k=1}^{n} E_k = I, \quad E_i E_j = \delta_{ij} E_j, \quad \text{tr}\{E_k\} = 1, \quad \det\{E_k\} = 0. \quad (3)$$

### 2.1 Eigenvalues and discriminant

The formulation of the eigenvalue problems

$$AE_k = \lambda_k E_k$$

$$A^\top E_k^\top = \lambda_k E_k^\top$$

(or, alternatively, $AU = UA$ and $VA = \Lambda V$) leads to the characteristic polynomial

$$P_A(\lambda) = \det(\lambda I - A) = \det(\lambda I - A^\top) = \prod_{k=1}^{n}(\lambda - \lambda_k) \quad (5)$$

of matrix $A$. The discriminant of the characteristic polynomial $P_A$ is defined as the product of the squared distances of the roots

$$\Delta := \prod_{i<j}^{n}(\lambda_i - \lambda_j)^2 \quad (6)$$

and is zero in the case of repeated eigenvalues. The discriminant associated with matrix $A$ is a function of the matrix elements and it has been shown by Parlett [13] that the discriminant can be expressed as the determinant of a symmetric matrix

$$\Delta = \det\{B\} = \det\{XY\} \quad (7)$$

with elements $B_{ij} = \text{tr}\{A^{i+j-2}\} = A^{i-1} : (A^{j-1})^\top = \text{vec}^\top\{A^{i-1}\} \text{ vec}\{(A^{j-1})^\top\}$ for $1 \leq i, j \leq n$ and a factorisation into the $n \times n^2$ matrix $X$ and the $n^2 \times n$ matrix $Y$, which are – similar to the Vandermonde matrix – constructed from powers of $A$ as follows (the vec operator represents column-stacking)

$$X = \begin{bmatrix} \text{vec}^\top\{A^{0}\} \\ \vdots \\ \text{vec}^\top\{A^{n-1}\} \end{bmatrix}, \quad Y = \begin{bmatrix} \text{vec}\{(A^{0})^\top\} & \ldots & \text{vec}\{(A^{n-1})^\top\} \end{bmatrix}. \quad (8)$$
Using the Cauchy-Binet formula for the determinant of a matrix product, the discriminant is identified as a sum-of-products
\[ \Delta = \sum_{m} \det(x_m) \det(y_m) = x^\top y \] (9)
where the determinants of the \( \binom{n}{2} \) minors, \( \det(x_m) \) and \( \det(y_m) \), are collected in the vectors \( x \) and \( y \), respectively. The expansion (9) has \( \binom{n}{2} - \binom{n-1}{2} \) nonzero terms of which several may occur repeatedly. Thus, a condensed form of the sum-of-products discriminant representation can be established
\[ \Delta = \bar{x}^\top D \bar{y} \] (10)
in which \( \bar{x} \) and \( \bar{y} \) contain only unique factors and the diagonal matrix \( D \) holds the respective product multiplier.

2.1.1 Sub-discriminants

The expression for the discriminant based on the determinant of matrix \( B \) suggests a generalisation into certain invariants (in this paper called sub-discriminants). The matrix \( B = X Y \) is factored into two rectangular matrices which represent column and row-stacked powers \( A^0, A^1, \ldots, A^{n-1} \). The sub-discriminant \( \Delta_{kl} \) corresponding to multi-indices \( k = (k_0, k_1, \ldots, k_r) \) and \( l = (l_0, l_1, \ldots, l_s) \) is defined based on subsets \( k \) and \( l \) of powers, i.e.
\[ \Delta_{kl} := \det(B_{kl}) = \det(X_k Y_l) \] (11)
where
\[ X_k = \begin{bmatrix} \text{vec}^\top \{ A^{k_0} \} \\ \vdots \\ \text{vec}^\top \{ A^{k_r} \} \end{bmatrix}, \quad Y_l = \begin{bmatrix} \text{vec} \{ (A^{l_0})^\top \} & \ldots & \text{vec} \{ (A^{l_s})^\top \} \end{bmatrix}. \] (12)
It is important to note, that all sub-discriminants \( \Delta_{kl} \) are proper invariants of matrix \( A \) (they are invariant under similarity transformations). Moreover, each component of the matrix \( B_{kl} \) is an invariant, since \( (B_{kl})_{ij} = \text{tr} \{ A^{i+j-2} \} \) for all \( i \in k \) and all \( j \in l \).

Following its definition simple identities are identified,
\[ \Delta_{(0)(1)} = \Delta_{(1)(0)} = \text{tr} \{ \lambda \}, \] (13)
\[ \Delta_{(0,1,\ldots,n-1)(0,1,\ldots,n-1)} = \Delta. \] (14)

2.2 Eigenprojectors

The \( n \) eigenvalues – as roots \( \lambda_k \) of the characteristic polynomial – are nonlinear functions of the \( n^2 \) elements of \( A \). A relation for the eigenprojector \( E_k \) is obtained by forming the inner product of the total differential of (16) with \( E_k \) and by using equation (15a) together with identities (13) as follows
\[ 0 = E_k : d \left[ (\lambda_k I - A^\top) E_k \right] \] (15a)
\[ = E_k : \left[ (d\lambda_k I - dA^\top) E_k + (\lambda_k I - A^\top) dE_k^\top \right] \] (15b)
\[ = (d\lambda_k I - dA) E_k : E_k + (\lambda_k I - A) E_k : dE_k^\top \] (15c)
\[ = d\lambda_k \text{tr} \{ E_k E_k \} - \text{tr} \{ dA E_k E_k \} + 0 : dE_k^\top \] (15d)
\[ = d\lambda_k - E_k^\top : dA \] (15e)
\[ = \left( \frac{\partial \lambda_k}{\partial A} - E_k^\top \right) : dA \] (15f)
from which, for arbitrary \( dA \), one extracts an expression for the eigenprojector
\[ E_k^\top = \frac{\partial \lambda_k}{\partial A} \] (16)
in terms of differentiation through the eigenvalue. If \( \lambda_k = \lambda_k(A) \) is available as differentiable symbolic expression (as it is the object of this paper), then Equation (16) presents advantages over the direct computation of the Frobenius covariants as Lagrange interpolants
\[ E_k = \prod_{i=1,i\neq k}^{n} \frac{A - \lambda_i I}{\lambda_k - \lambda_i} \] (17)
obtained as a consequence of Equations (2) and (3) for strictly distinct eigenvalues \(\lambda_k\). Alternatively, the eigenprojectors can be computed from
\[
E_k = U \text{ diag } \{e_k\} V
\]
where \(e_k\) is a canonical unit vector (having 1 in the \(k\)-th component and 0 elsewhere) and the \(\text{diag}\) operator mapping vectors into diagonal matrices. In this case matrices \(U\) and \(V\) must be otherwise known, so this approach is useful only for testing purposes.

3 Spectral decomposition of 3 \times 3 matrices

In the following we consider the case of a 3 \times 3 matrix \(A\) with real-valued elements \(A_{ij}\) and 1 \(\leq i, j \leq 3\) under the (above stated) assumption that \(A\) is diagonalisable over the real numbers.

3.1 Eigenvalues

The characteristic polynomial of a 3 \times 3 matrix \(A\)
\[
P_A(\lambda) = \lambda^3 - I_1(A)\lambda^2 + I_2(A)\lambda - I_3(A) = (\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3)
\]
can be expressed in terms of the principal invariants of \(A\)
\[
I_1(A) = \text{tr}\{A\}, \quad I_2(A) = \frac{1}{2} (\{\text{tr}\{A\}\}^2 - \text{tr}\{A^2\}), \quad I_3(A) = \text{det}\{A\}
\]
or in terms of its three roots \(\lambda_1, \lambda_2\) and \(\lambda_3\).

3.1.1 Roots of the characteristic polynomial

In order to facilitate the identification of the roots \(\lambda_k\) of the cubic equation \(P_A(\lambda) = 0\) the substitution
\[
\lambda = \mu + r \cos \varphi
\]
is introduced, with \(\mu, r, \varphi \in \mathbb{R}\) to be determined. This leads, in a first step, to
\[
P_A(\mu, r, \varphi) = (r^3) \cos^3 \varphi + r^2 (3\mu - I_1) \cos^2 \varphi + r (3\mu^2 - 2I_1\mu + I_2) \cos \varphi + (\mu^3 - I_1\mu^2 + I_2\mu - I_3)
\]
and is transformed to
\[
P_A(\mu, r, \varphi) = \frac{r^3}{4} \cos 3\varphi + r^2 (3\mu - I_1) \cos^2 \varphi + \frac{r}{4} (12\mu^2 - 8I_1\mu + 4I_2 + 3r^2) \cos \varphi + (\mu^3 - I_1\mu^2 + I_2\mu - I_3)
\]
using the triple-angle trigonometric identity \(4 \cos^3 \varphi = \cos 3\varphi - 3 \cos \varphi\). In the above expression for \(P_A\) the factors to \(\cos^2 \varphi\) and \(\cos \varphi\) become zero for suitable choices of \(\mu\) and \(r\). The non-trivial solution of the associated system of equations
\[
\begin{align*}
r^2 (3\mu - I_1) &= 0 \\
\frac{r}{4} (12\mu^2 - 8I_1\mu + 4I_2 + 3r^2) &= 0
\end{align*}
\]
is given by
\[
\mu = \frac{1}{3} I_1, \quad r = \pm \frac{2}{3} \sqrt{I_1^2 - 3I_2}
\]
and allows to eliminate \(\mu\) and \(r\) in \(P_A(\mu, r, \varphi)\). This provides
\[
P_A(\varphi) = \pm \frac{2}{27} (I_1^3 - 3I_2)^{\frac{3}{2}} \cos 3\varphi + \left(-\frac{2}{27} I_1^3 + \frac{1}{3} I_1 I_2 - I_3\right)
\]
and with
\[
0 = \pm 2 (I_1^3 - 3I_2)^{\frac{3}{2}} \cos 3\varphi + (-2I_1^3 + 9I_1 I_2 - 27I_3)
\]
the relation to determine the cosine of the triple angle
\[
\cos 3\varphi = \pm \frac{1}{2} \left(2I_1^3 - 9I_1 I_2 + 27I_3\right) (I_1^2 - 3I_2)^{-\frac{3}{2}}
\]
with \(-1 \leq \cos 3\varphi \leq +1\).

The three eigenvalues of matrix \(A\)
\[
\lambda_k = \frac{1}{3} \left[I_1 + 2\sqrt{I_1^2 - 3I_2 \cos \left(\varphi + \frac{2\pi k}{3}\right)}\right], \quad k = 1, 2, 3
\]
are then highly nonlinear functions of the principal matrix invariants.
3.1.2 Discriminant and sub-discriminants

The discriminant of the (cubic) polynomial can be expressed in terms of its coefficients (referred to as “naive” expression in this paper)

\[
\Delta = 18I_1I_2I_3 + I_1^2I_2 - 4I_1^3I_3 - 4I_2^3 - 27I_3^2 \quad (27a)
\]

\[
= \frac{1}{27} \left[ 4(I_1^2 - 3I_2)^3 - (2I_1^3 - 9I_1I_2 + 27I_3)^2 \right] = \frac{1}{27} (4\Delta_p^3 - \Delta_q^2) \quad (27b)
\]

where invariants \( \Delta_p \) and \( \Delta_q \) are defined as

\[
\Delta_p := I_1^2 - 3I_2, \quad (28a)
\]

\[
\Delta_q := 2I_1^3 - 9I_1I_2 + 27I_3. \quad (28b)
\]

Alternatively, for \( n = 3 \) the condensed sum-of-products representation of the discriminant, see Equation (10), is given by 14 products with

\[
\bar{x} = \begin{bmatrix}
A_{12}A_{21}A_{31} - A_{11}A_{22}A_{32} \\
A_{22}A_{31} - A_{12}A_{31}A_{22} + A_{12}A_{31}A_{32} - A_{21}A_{31}A_{21} \\
A_{11}A_{12}A_{32} - A_{12}A_{32} + A_{12}A_{32} + A_{31}A_{32} + A_{11}A_{32}A_{32} - A_{11}A_{32}A_{32} \\
A_{11}A_{13}A_{32} - A_{13}A_{32} + A_{13}A_{32} + A_{21}A_{32}A_{32} - A_{21}A_{32}A_{32} \\
A_{12}A_{13}A_{22} - A_{12}A_{22} + A_{12}A_{22} + A_{12}A_{22} + A_{12}A_{22}A_{22} - A_{12}A_{22}A_{22} \\
A_{11}A_{12}A_{22} - A_{12}A_{22} + A_{12}A_{22} + A_{12}A_{22} + A_{12}A_{22}A_{22} - A_{12}A_{22}A_{22} \\
A_{11}A_{13}A_{22} - A_{13}A_{22} + A_{13}A_{22} + A_{13}A_{22} + A_{13}A_{22}A_{22} - A_{13}A_{22}A_{22} \\
A_{12}A_{13}A_{22} - A_{12}A_{22} + A_{12}A_{22} + A_{12}A_{22} + A_{12}A_{22}A_{22} - A_{12}A_{22}A_{22} \\
A_{11}A_{13}A_{32} - A_{13}A_{32} + A_{13}A_{32} + A_{13}A_{32} + A_{13}A_{32}A_{32} - A_{13}A_{32}A_{32} \\
A_{12}A_{13}A_{32} - A_{13}A_{32} + A_{13}A_{32} + A_{13}A_{32} + A_{13}A_{32}A_{32} - A_{13}A_{32}A_{32} \\
A_{11}A_{12}A_{33} - A_{12}A_{33} + A_{12}A_{33} + A_{12}A_{33} + A_{12}A_{33}A_{33} - A_{12}A_{33}A_{33} \\
A_{12}A_{13}A_{33} - A_{13}A_{33} + A_{13}A_{33} + A_{13}A_{33} + A_{13}A_{33}A_{33} - A_{13}A_{33}A_{33} \\
\end{bmatrix}, \quad (29a)
\]

\[
\bar{y} = \begin{bmatrix}
A_{13}A_{21}A_{31} - A_{12}A_{21}A_{31} \\
A_{22}A_{32} - A_{12}A_{22}A_{31} + A_{21}A_{31}A_{31} - A_{21}A_{31}A_{31} \\
A_{11}A_{12}A_{32} - A_{12}A_{32} + A_{12}A_{32} + A_{21}A_{32}A_{32} - A_{21}A_{32}A_{32} \\
A_{11}A_{13}A_{32} - A_{13}A_{32} + A_{13}A_{32} + A_{21}A_{32}A_{32} - A_{21}A_{32}A_{32} \\
A_{12}A_{13}A_{22} - A_{13}A_{22} + A_{13}A_{22} + A_{13}A_{22} + A_{13}A_{22}A_{22} - A_{13}A_{22}A_{22} \\
A_{11}A_{12}A_{22} - A_{12}A_{22} + A_{12}A_{22} + A_{12}A_{22} + A_{12}A_{22}A_{22} - A_{12}A_{22}A_{22} \\
A_{11}A_{13}A_{22} - A_{13}A_{22} + A_{13}A_{22} + A_{13}A_{22} + A_{13}A_{22}A_{22} - A_{13}A_{22}A_{22} \\
A_{12}A_{13}A_{22} - A_{13}A_{22} + A_{13}A_{22} + A_{13}A_{22} + A_{13}A_{22}A_{22} - A_{13}A_{22}A_{22} \\
A_{11}A_{13}A_{32} - A_{13}A_{32} + A_{13}A_{32} + A_{13}A_{32} + A_{13}A_{32}A_{32} - A_{13}A_{32}A_{32} \\
A_{12}A_{13}A_{32} - A_{13}A_{32} + A_{13}A_{32} + A_{13}A_{32} + A_{13}A_{32}A_{32} - A_{13}A_{32}A_{32} \\
\end{bmatrix}, \quad (29b)
\]

\[
D = \text{diag}\{9, 6, 6, 6, 8, 8, 8, 2, 2, 2, 2, 2, 1\}. \quad (29c)
\]

It should be noted that symmetric matrices allow for further reduction of the number of products and presentation of the discriminant as a sum-of-squares, as demonstrated by Kummer [9] (7 squares) and Watson [17] (5 squares).

With the notion of sub-discriminants it can be shown that

\[
\Delta_{(0,1)(0,1)} = 2\Delta_p = 2(I_1^2 - 3I_2). \quad (30)
\]

It follows from

\[
\det\{B_{(0,1)(0,1)}\} = \det\{\begin{bmatrix} 3 & \text{tr}\{A\} \\ \text{tr}\{A\} & \text{tr}\{A^2\} \end{bmatrix}\} = 3 \text{tr}\{A^2\} - \text{tr}\{A\}^2 = 2\Delta_p. \quad (31)
\]
With similar factorisation into sum-of-products an alternative expression for the $\Delta_p$ invariant reads

$$\Delta_p = \frac{1}{2} \bar{x}_p^T D_p \bar{y}_p,$$

(32a)

$$\bar{x}_p = \begin{bmatrix} A_{10} \\ A_{20} \\ A_{21} \\ -A_{00} + A_{11} \\ -A_{00} + A_{22} \\ -A_{11} + A_{22} \end{bmatrix}, \quad \bar{y}_p = \begin{bmatrix} A_{01} \\ A_{02} \\ A_{12} \\ -A_{00} + A_{11} \\ -A_{00} + A_{22} \\ -A_{11} + A_{22} \end{bmatrix},$$

(32b)

$$D_p = \text{diag}\{\{6, 6, 6, 1, 1, 1\}\}.$$  

(32c)

A similar expression cannot be identified for $\Delta_q$, however, this invariant can partially be expressed on the basis of sum-of-products as follows

$$\Delta_q = 3\Delta_{(0,1)(0,2)} - 4 \text{tr}\{A\} \Delta_p.$$  

(33)

### 4 Finite precision and rounding errors

The above formulas for the computation of eigenvalues and eigenprojectors are not all equivalent when finite precision floating point arithmetic is involved. This is, of course, the case when these expressions are implemented in a computer program. The discrepancies will be explained and addressed below.

Machine epsilon, $\varepsilon$, is here defined as the difference between 1 and the next larger floating point number. Let $b$ be the radix (base) and $p$ a precision of a floating point number representation, then $\varepsilon = b^{-(p-1)}$. For example, the standard double precision floating point representation used in this paper has $\varepsilon = 2.22 \times 10^{-16}$. Only the magnitude of the rounding error is considered in this paper, so there is no distinction made between units in the last place and relative error in terms of machine epsilon.

#### 4.1 Rounding errors in principal invariants

An inherent property of the analytical approach to spectral decomposition follows as a consequence of its use of matrix invariants $I_1$, $I_2$ and $I_3$. As noted in [7], this approach is not suitable when the distances between eigenvalues are large. As a simple example, consider a matrix with $\lambda_1 = 1$, $\lambda_2 = 2$ and $\lambda_3 = 10^{17}$. Any computation which then makes use of matrix trace $I_1 = \lambda_1 + \lambda_2 + \lambda_3$ will suffer from rounding error (in standard double precision), to the effect that the presence of the two small eigenvalues is not measurable in the matrix trace.

Due to non-associativity of the floating point arithmetic the case with eigenvalues $\lambda_1 = -10^{17}$, $\lambda_2 = 1$ and $\lambda_3 = 10^{17}$ would also introduce large relative error into the computation of the trace $I_1 = \text{fl}(\lambda_1 + \lambda_2 + \lambda_3)$. Here, $\text{fl}(x)$ denotes floating point representation of number $x$. Such issues could be solved using techniques as the Kahan summation algorithm (or the improved Kahan-Babuška algorithm [12]). Unfortunately, tricks based on benign cancellation are not applicable when developing a symbolic algorithm, since the actual execution order of floating point operations is not strictly preserved.

In [7] the alternative use of iterative methods is recommended (Jacobi/QR and QL). These methods, however, are not relevant in the context of symbolic computation.

#### 4.2 Catastrophic cancellation in the discriminant

Catastrophic cancellation is a numerical phenomenon where the subtraction of the good approximation to two close numbers results in a bad approximation in the result. The formula for discriminant based on principal invariants (Equation (27a) and (27b)) suffers from this effect.

Let $A \in \mathbb{R}^{3\times3}$ be a diagonalisable traceless matrix with real eigenvalues $\lambda_1 = 1 + \delta, \lambda_2 = 1$ and $\lambda_3 = -2 - \delta$. The parameter $\delta$ is a distance between two largest eigenvalues and for $\delta \rightarrow 0$ there is $\Delta \rightarrow 0$. For this matrix

$$I_1 = 0, \quad I_2 = -3 - 3\delta - \delta^2, \quad I_3 = -2 - 3\delta - \delta^2.$$  

If $\delta^2$ is smaller than machine epsilon, then the computation and storage of $I_2$ and $I_3$ introduces a rounding error, such that

$$\text{fl}(I_2) = -3 - 3\delta, \quad \text{fl}(I_3) = -2 - 3\delta.$$
The discriminant computed using formula based on principal invariants (27a) then leads to
\[
\text{fl}(\Delta) = \text{fl}(-4 \text{fl}(I_2)^3) - \text{fl}(27 \text{fl}(I_3)^2)
\]
\[
= \text{fl}(108 + 324\delta + 324\delta^2 + 108\delta^3) - \text{fl}(108 + 324\delta + 243\delta^2)
\]
\[
= 0.
\]
This situation occurs for standard double precision when \( \delta < 10^{-8} \). In other words, the discriminant computed from the naive expression (27a) becomes insignificant when the distance between two eigenvalues is smaller than half precision. The loss of precision could be avoided if a different expression for the discriminant is used, which motivates the following discussion.

Fortunately, the sum-of-products expression for the discriminant (Equation (10)) does not suffer from catastrophic cancellation when the discriminant goes to zero. This observation is the foundation for computation of eigenvalues (and determination of eigenvalues multiplicity) with improved accuracy and is proved in the following.

For the special case of symmetric matrix, sum-of-products reduces to sum-of-squares, i.e. the vectors \( \bar{x} \) and \( \bar{y} \) are equal. Assuming that the distance between the two closest eigenvalues is some \( \delta << 1 \), the discriminant is proportional to \( \delta^2 \) (since the discriminant is the square of eigenvalue distances) and every (positive) summand in the scalar product \( \bar{x}^\top D \bar{x} \) is thus either zero or a small number proportional to \( \delta^2 \). Every non-zero element in the vector \( \bar{x} \) is therefore proportional to \( \delta \) and could be computed up to machine precision. Finally, the sum-of-squares of small numbers of the same magnitude does not introduce a significant rounding error.

In the general non-symmetric case, it must be shown that each non-zero element in \( \bar{x} \) and \( \bar{y} \) approaches zero dominated by terms linear in \( \delta \). First, the limit case for \( \delta = 0 \) (i.e. \( \Delta = 0 \)) is proven. Equivalently, it is required that
\[
\Delta = 0 \implies \det\{X_m\} = \det\{Y_m\} = 0, \quad \forall m, \tag{34}
\]
where \( m \) runs through all \( n \times n \) square sub-matrices of \( X \) and \( Y \). This is a stronger statement than \( \Delta = 0 \implies \det(XY) = 0 \) which follows easily from Equation (7).

It could be shown, that for a diagonalisable matrix \( A \in \mathbb{R}^{n \times n} \), which has zero discriminant, the following matrices
\[
I, A, A^2, \ldots, A^{n-1}
\]
are linearly dependent\(^2\). In other words, there exist coefficients \( \{c_i\} \in \mathbb{R}^n \) such that
\[
c_0 I + c_1 A + \ldots + c_{n-1} A^{n-1} = 0. \tag{36}
\]
Alternatively, (36) could be written using the vec operator as
\[
c_0 \text{vec}^\top I + c_1 \text{vec}^\top A + \ldots + c_{n-1} \text{vec}^\top A^{n-1} = 0. \tag{37}
\]
This equation states that the rows in matrix \( X \) are linearly dependent, thus the rows in all sub-matrices \( X_m \) are linearly dependent too. Hence, \( \det\{X_m\} = 0 \) for each \( m \). The same observation applies to the transpose of (36) and columns of \( Y_m \), so that equally, \( \det\{Y_m\} = 0 \). Moreover, since the discriminant is a continuous function of distances between eigenvalues – follows from its definition (6) –, if \( \delta \to 0 \) then each \( \det\{X_m\} \to 0 \) and \( \det\{Y_m\} \to 0 \). Finally, since discriminant is proportional to \( \delta^2 \), each non-zero element in \( \bar{x} \) and \( \bar{y} \) is proportional to \( \delta \).

Note: Catastrophic cancellation occurs also in (26) for \( \varphi \to 0, I_1 > 0 \) or \( \varphi \to \pi, I_1 < 0 \). If the distance between eigenvalues \( \delta \) becomes large, Equation (26) results in the subtraction of two large numbers in order to produce the small eigenvalue \( \lambda_2 = 1 \) (for the example introduced at the beginning of this subsection).

4.3 Catastrophic cancellation in the \( \Delta_p \) invariant

The invariant \( \Delta_p \) plays a foremost role in the computation of eigenvalues. For \( A \in \mathbb{R}^{3 \times 3} \) being a diagonalisable matrix with eigenvalues \( \lambda_1 = 1, \lambda_2 = 1 \) and \( \lambda_3 = 1 + \delta \) one obtains \( \Delta_p = \delta^2 \). For this matrix
\[
I_1 = 3 - \delta, \quad I_2 = 3 - 2\delta.
\]
Similarly to arguments for cancellation in the discriminant, when \( I_1^2 \) is computed and stored for \( \delta^2 \) smaller than machine epsilon, one observes that
\[
\text{fl}(I_1^2) = \text{fl}(9 - 6\delta + \delta^2) = 9 - 6\delta, \quad \text{fl}(\Delta_p) = \text{fl}(9 - 6\delta - 3\text{fl}(3 - 2\delta)) = 0.
\]
\(^2\)Matrix \( A \) is a root of its minimal polynomial, which is of order \( k \leq n \). For a diagonalisable matrix every eigenvalue has its algebraic multiplicity equal to geometric multiplicity. Therefore, a zero discriminant implies that the degree of minimal polynomial is strictly smaller than the matrix size \( n \).
Thankfully, the sum-of-products expression for $\Delta_p$, see Equation (32), does not suffer from catastrophic cancellation by similar arguments as used in the proof for the discriminant. It could be shown that for $\Delta_p$ proportional to $\delta^2$ every non-zero term in vectors $\bar{x}_p$ and $\bar{y}_p$ is proportional to $\delta$. It is a consequence of the linear dependence of matrices $I$ and $A$, which follows from that fact that degree of minimal polynomial $k = 1$ in the case of $3 \times 3$ matrix with $\Delta_p = 0$.

### 4.4 Rounding error in the triple angle

The evaluation of the triple angle $\varphi$ in Equation (25) suffers from dangerous rounding errors in the vicinity of $\Delta = 0$. In order to demonstrate these effects, let again consider a traceless matrix with eigenvalues $\lambda_1 = 1 + \delta, \lambda_2 = 1$ and $\lambda_3 = -2 - \delta$. Direct inversion of (25) gives

$$\varphi = \frac{1}{3} \arccos \left( \frac{1}{2} \Delta_q \Delta_p^{-3/2} \right)$$

and series expansion of the inverse cosine argument around the critical point $\Delta = 0$ (i.e. $\delta = 0$) for the chosen example matrix leads to

$$\frac{1}{2} \Delta_q \Delta_p^{-3/2} = -1 + \frac{3\delta^2}{8} + \mathcal{O}(\delta^3).$$

Similar to the discussion above, when the argument is evaluated and stored in floating point representation rounding error becomes significant if the eigenvalue distance is smaller than square root of machine epsilon. This effect could be avoided in two ways.

The first approach is based on the generalised (Puiseux) series approximation to the inverse cosine

$$\arccos(1 - x) = \sqrt{2x} + \frac{x^{3/2}}{6\sqrt{2}} + \frac{3x^{5/2}}{80\sqrt{2}} + \frac{x^{7/2}}{448\sqrt{2}} + \mathcal{O}(x^{9/2})$$

around point $x = 0^+$. The presence of the square root in the expansion suggests a possible series approximation of the angle which would contain linear terms in the eigenvalue distance $\delta$ (or equivalently, terms proportional to $\sqrt{\Delta}$). Indeed, the expansion of the angle $\varphi$ around $\Delta = 0$ reads

$$\varphi = \frac{1}{3} \arccos \left( \frac{\Delta_q}{\sqrt{\Delta_q^2 + 27\Delta}} \right) = \frac{1}{3} \left[ \arccos(\text{sign}(\Delta_q)) + \frac{3\sqrt{3}\sqrt{\Delta}}{\Delta_q} - \frac{27\sqrt{3}(\sqrt{\Delta})^3}{5\Delta_q^5} + \mathcal{O}(\Delta^3) \right].$$

In the alternative second approach, a trigonometric identity for $\arccos$ is used to transform its argument, such that the evaluation of problematic arguments (like $-1 + \delta^2$ in the above example) is avoided. If the argument is transformed to the vicinity of zero, then the evaluation does not suffer from finite-precision round-off. Applying the Pythagorean theorem to the right-angled triangle with unit hypotenuse leads to

$$\tan(\arccos x) = \frac{\sqrt{1 - x^2}}{x}. \quad (41)$$

The inverse tangent could be applied to this identity. However, $\arccos$ maps to $[0, \pi]$, so for $x < 0$ the standard arctan must be shifted by $\pi$. Hence,

$$\arccos x = \arctan \left( \frac{\sqrt{1 - x^2}}{x} \right) - \frac{\text{sign}(x) - 1}{2\pi} \quad (42)$$

With $x = \Delta_q/\sqrt{\Delta_q^2 + 27\Delta}$ the angle $\varphi$ is equivalently expressed as

$$\varphi = \frac{1}{3} \left[ \arctan \left( \frac{3\sqrt{3}\sqrt{\Delta}}{\Delta_q} \right) - \frac{\text{sign}(\Delta_q) - 1}{2\pi} \right]. \quad (43)$$

The use of the $\arctan$ identity was already noted in [16] for better accuracy, but without thorough explanation. In addition, the sum-of-products expression for the discriminant must be employed along the $\arctan$ identity in order to obtain a consistently increased accuracy in the eigenvalues.
Table 1: Summary of rounding errors in invariants

| invariant | expression | critical case          | eigenvalues                  | absolute error |
|-----------|------------|------------------------|------------------------------|----------------|
| $I_1$     | (20)       | large eigenvalue distances | $\lambda_1 = 1, \lambda_2 = 1, \lambda_3 = 10^{17}$ | 1              |
| $\Delta$  | "naive", (27a) | $\Delta \rightarrow 0$ | $\lambda_1 = -1, \lambda_2 = 1, \lambda_3 = 1 + \varepsilon$ | $\varepsilon^2$ |
|           | sum-of-products, (29) |                     |                              |                |
| $\Delta_p$| "naive", (28a) | $\Delta_p \rightarrow 0$ | $\lambda_1 = 1, \lambda_2 = 1, \lambda_3 = 1 + \varepsilon$ | $\varepsilon^2$ |
|           | sum-of-products, (32) |                 |                              |                |
| $\Delta_q$| "naive", (28b) | $\Delta_q \rightarrow 0$ | $\lambda_1 = 0, \lambda_2 = 1, \lambda_3 = 2$ | $\varepsilon$  |

Table 2: Critical cases studied in the numerical benchmarks.

| $\Delta \rightarrow 0$ | $\Delta_p \rightarrow 0$ | $\Delta_q \rightarrow 0$ |
|-------------------------|--------------------------|--------------------------|
| $\Lambda$ diag\{(−1, 1, 1 + \delta)\} | diag\{(1, 1, 1 + \delta)\} | diag\{(0, 1, 2 + \delta)\} |

4.5 Summary of the rounding errors

The improved expression for eigenvalues is given in terms of three invariants $I_1$, $\Delta_p$ and $\Delta_q$:

$$\lambda_k = \frac{1}{3} \left[ I_1 + 2 \sqrt{\Delta_p} \cos \left( \varphi + \frac{2\pi}{3} k \right) \right], \quad k = 1, 2, 3,$$

where Equation (43) is used to compute $\varphi$ based on $\Delta$ and $\Delta_q$. With the use of the sum-of-products expression rounding errors are significantly reduced, see Table 1.

Remark: The authors are not aware of an alternative expression for the invariant $\Delta_q$ which would exhibit an error smaller than machine precision in the critical case. One could show that $\Delta_q = 3\Delta_{(0,1)(0,2)} - 4 \text{tr} \{A\} \Delta_p$, but this formula shows cancellation and larger error too. An expression based on the sum of small products would be required. There are approaches derived from Kahan’s algorithm for the determinant of $2 \times 2$ matrices [5]. Unfortunately, these techniques benefit from benign cancellation and fused multiply-add instructions, and are thus not suitable in the symbolic scope of this work.

Remark: Errors in Table 1 are included for eigenvalues of order 1. A simple scaling argument could be used for rough estimates of the error for a matrix with elements of different order. The discriminant $\Delta$ is a sixth order polynomial in the matrix elements, thus its error in Table 1 could be scaled with $|\text{max}(A_{ij})|^6$. Similarly, the $\Delta_p$ invariant as a second order polynomial scales with $|\text{max}(A_{ij})|^2$ and $\Delta_q$ with $|\text{max}(A_{ij})|^3$.

5 Numerical benchmarks

In order to test the improved accuracy of eigenvalues (and invariants) computation a non-symmetric diagonalisable matrix $B = U\Lambda U^{-1} \in \mathbb{R}^{3 \times 3}$ is considered.

There are three critical cases where invariants $\Delta$, $\Delta_p$ or $\Delta_q$ vanish. In the following benchmarks a distance parameter $\delta$ is used to approach these limit states. It can be modelled on the basis of the diagonal matrix $\Lambda$, see Table 2.

The similarity transformation matrix $U$ does not change the value of eigenvalues (or invariants) in infinite precision. However, it effectively propagates the distance parameter $\delta$ into the elements of the final matrix $A$ as well as into the principal invariants. For this reason two different non-singular transformation matrices are tested, see Table 3.

5.1 Invariants

Absolute errors in the computation of matrix invariants $\Delta_q$, $\Delta_p$ and $\Delta$ are shown in Figure 1. Plots are produced for the transformation matrix Case I and various critical cases. Invariants computed using the sum-of-products formulas (29), (32) and (33) are included on the left while naive expressions (27a), (28a) and (28b) are used for the results plotted on the right.
With formulas (44) the absolute eigenvalues errors for the transformation matrix Case I are computed, see Figure 2.

The eigenprojectors can be computed as eigenvalues derivatives, see (16). The observed absolute error of this approach

\[
\bar{y} = \mathbf{U}(\gamma) \mathbf{A}(\delta) \mathbf{U}(\gamma)^{-1}
\]

The first critical case \( \Delta \rightarrow 0 \) (Figure 1a and Figure 1b) shows decreased error for the discriminant (blue points) for distances \( \delta < 1 \). The naive expressions exhibit large rounding error and there is no measurable dependence for smaller \( \delta \) distances. Note, that the absolute error should be decreasing, since the actual value of the discriminant \( \Delta \) goes to zero. The sum-of-products expressions, however, consistently remain sensitive to distances \( \delta \) as small as machine precision.

For the scenario of triple eigenvalues, as represented by the case \( \Delta_p \rightarrow 0 \), and shown in Figure 1c and Figure 1d, the important difference is in the sensitivity of \( \Delta_p \) (green squares) with respect to the distance \( \delta \). Again, the sum-of-products approach shows improved accuracy where the absolute error in \( \Delta_p \) decreases for smaller \( \delta \).

There is no significant difference between approaches for the last critical case \( \Delta_q \rightarrow 0 \) (see Figure 1e and Figure 1f) since the (almost) sum-of-products expression for the \( \Delta_q \) invariant is expected to suffer from subtractive cancellation between the terms \( 3\Delta_{(0,1)(0,2)} \) and \( 4 \text{tr} \{ \mathbf{A} \} \Delta_p \).

5.2 Eigenvalues

With formulas (44) the absolute eigenvalues errors for the transformation matrix Case I are computed, see Figure 2.

The error in each case is a direct consequence of the error shown for matrix invariants \( \Delta, \Delta_p, \Delta_q \) and \( I_1 \). In general, accuracy is improved for sum-of-products expressions (left column).

For the critical case \( \Delta_p \rightarrow 0 \) (Figure 2c and Figure 2d) there is an increase in the error around \( \delta \approx 10^{-6} \). The reason for this error is contained in formula for the arctan argument in (43), namely \( \frac{3\sqrt{\Delta_p}}{\Delta_q} \). The discriminant \( \Delta \) should be equal to zero (in infinite precision arithmetic, two smallest eigenvalues are equal), but rounding causes the discriminant to be nonzero (see e.g. Figure 1c). The floating point value of the discriminant is dominated by rounding error, so it has no significance (the relative error is infinitely large). As \( \Delta_q \) becomes sufficiently small it amplifies insignificant values in the discriminant and increases the error of the fraction.

Remark: Absolute errors in Figure 1 and Figure 2 were computed for the transformation matrix \( \mathbf{U} \), Case I, see Table 3. Case II contains the parameter \( \gamma > 0 \) which controls the conditioning number \( \kappa(\mathbf{U}) \) of the transformation matrix (the smaller \( \gamma \), the larger the conditioning number). For the critical case \( \Delta \rightarrow 0 \) the test matrix \( \mathbf{B} \) is expressed as a function of the distance \( \delta \) and the parameter \( \gamma \),

\[
\mathbf{B} = \mathbf{U}(\gamma) \mathbf{A}(\delta) \mathbf{U}(\gamma)^{-1} = \begin{bmatrix}
-\frac{\delta+\gamma-2}{\gamma} & -\frac{\delta+2}{\gamma} & \frac{\delta+2}{\gamma} \\
-\frac{\delta+2}{\gamma} & -\frac{\delta+\gamma+2}{\gamma} & -\frac{\delta+2}{\gamma} \\
\frac{\gamma-(\delta+1)(\gamma+2)-2}{\gamma} & -\delta - \frac{2\delta}{\gamma} - 4 & \frac{(\delta+1)(\gamma+2)+2}{\gamma}
\end{bmatrix}.
\]

The important observation is that for \( \gamma \rightarrow 0 \) every component in the matrix goes to \( \pm \infty \) with increasing proportionality coefficients in \( \delta \). In formulas (29) the components of the vectors \( \bar{x} \) and \( \bar{y} \) could happen to be close to zero due to cancellation in products of matrix components. With a badly conditioned transformation matrix \( \mathbf{U} \) the error in the cancellation becomes larger. This scaling affects the naive formula for discriminant (27a) negatively too.

The effect of a badly conditioned matrix \( \mathbf{U} \) with \( \gamma = 10^{-3} \) is depicted in Figure 3. Both, sum-of-products and naive expressions, show decreased accuracy for all eigenvalues.

5.3 Eigenprojectors

The eigenprojectors can be computed as eigenvalues derivatives, see (16). The observed absolute error of this approach is outlined in Figure 4. This error shows different characteristics as the absolute error observed for invariants and eigenvalues. The computed eigenprojectors satisfy the "normalisation properties" according to (3), which makes their absolute error resemble more the relative error of eigenvalues.

| Case I | Case II |
|--------|---------|
| \( \mathbf{U} \) | \( \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ -1 & -1 & 1 \end{bmatrix} \) | \( \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 2 & 1 & 2+\gamma \end{bmatrix} \) |

Table 3: Similarity transformation matrices \( \mathbf{U} \) used in the numerical benchmarks.

The important observation is that for \( \gamma \rightarrow 0 \) every component in the matrix goes to \( \pm \infty \) with increasing proportionality coefficients in \( \delta \). In formulas (29) the components of the vectors \( \bar{x} \) and \( \bar{y} \) could happen to be close to zero due to cancellation in products of matrix components. With a badly conditioned transformation matrix \( \mathbf{U} \) the error in the cancellation becomes larger. This scaling affects the naive formula for discriminant (27a) negatively too.

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Symbolic spectral decomposition of 3x3 matrices

(a) Critical case $\Delta \to 0$, sum-of-products.

(b) Critical case $\Delta \to 0$, naive.

(c) Critical case $\Delta_p \to 0$, sum-of-products.

(d) Critical case $\Delta_p \to 0$, naive.

(e) Critical case $\Delta_q \to 0$, sum-of-products.

(f) Critical case $\Delta_q \to 0$, naive.

Figure 1: Absolute error in matrix invariants for transformation matrix Case I.
Symbolic spectral decomposition of 3x3 matrices

Figure 2: Absolute error in eigenvalues for transformation matrix Case I.
Symbolic spectral decomposition of 3x3 matrices

5.4 Matrix powers

A typical use case for symbolic spectral decomposition is the evaluation of matrix functions $f(A)$ according to Sylvester interpolating definition (see [3])

$$f(A) = \sum_{k=1}^{3} f(\lambda_k)E_k. \quad (46)$$

The upper bound for the error in this formula is then a consequence of errors in eigenvalues and eigenprojectors (due to trivial triangle inequality estimate). Benchmark results for the critical case $\Delta \to 0$ and a well conditioned transformation matrix (Case I) are included in Figure 5. In Figure 5a and Figure 5b, the main contribution to the error is due to eigenvalues errors, which is then scaled with a factor corresponding to the matrix power. There is a notable improvement in the accuracy for $A^2$ when the sum-of-products approach is used.
6 Conclusion

This paper studies the closed-form solution approach to spectral decomposition of real-valued matrices with real eigenvalues. Formulas based on trigonometric transformations are derived in the beginning. The notion of the matrix discriminant is then generalised based on the determinant of certain matrix powers. The special case of $3 \times 3$ matrices is studied for associated rounding errors in the symbolic computation of the spectral decomposition and several potential sources of catastrophic cancellation are identified. Discriminant and sub-discriminants are expressed on the basis of sum-of-products expressions. It is shown, that this mathematically equivalent procedure provides alternative expressions for particular matrix invariants (discriminant and invariant $\Delta_p$), which do not suffer catastrophic cancellation and consequently show much improved numerical floating point accuracy in all critical cases.

A set of numerical benchmarks is executed to test newly developed expressions. Absolute errors in matrix invariants $\Delta, \Delta_p$ and $\Delta_q$ show different characteristics and are in general superior to the naive expressions used in existing literature. With the employed techniques the error in computed eigenvalues can be decreased from half to full machine precision.

The overall improved algorithm is included in Appendix A and is believed to serve as basis for those who require near machine precision of eigenvalues and preserved symbolic, functional dependence of the eigendecomposition on the matrix elements.

An extension of the presented formalism to matrices having a spectral decomposition over the complex numbers or general complex-valued matrices is considered straightforward. While the advantages of the sum-of-products based (sub)-discriminant(s) persist, the main difference lies then in an appropriate choice for Equation (21) with trivial subsequent steps.
**A Improved algorithm for spectral decomposition**

Following algorithm is written in Python programming language and tested using **Python 3.9.7** and symbolic algebra package **SymPy 1.8**.

```python
import sympy as sy
import itertools

def subdiscriminant(A, subU, subV):
    U = sy.matrices.Matrix.vstack(*[A**p.vec().T for p in subU])
    V = sy.matrices.Matrix.hstack(*[A**p.T.vec() for p in subV])

    enums = list(itertools.combinations(range(U.cols), U.rows))
    u = [U[:, e].det() for e in enums]
    v = [V[e, :].det() for e in enums]
    return sum([uu * vv for uu, vv in zip(u, v)])

def eigenvalues(A):
    I1 = sy.Trace(A)
    dp = 1 / 2 * subdiscriminant(A, [0, 1], [0, 1])
    dq = 3 * subdiscriminant(A, [0, 1], [0, 2]) - 4 * I1 * dp
    disc = subdiscriminant(A, [0, 1, 2], [0, 1, 2])
    atan_arg = 3 * sy.sqrt(3) * sy.sqrt(disc) / dq
    phi = sy.atan(atan_arg) + (1 - sy.sign(dq)) * sy.pi / 2
    return [(I1 + 2 * sy.sqrt(dp) * sy.cos((phi + 2 * sy.pi * k) / 3)) / 3
            for k in [1, 2, 3]]

def eigenprojectors(A):
    eigenvals = eigenvalues(A)
    return [eigenval.diff(A).T for eigenval in eigenvals]
```

**References**

[1] E. Anderson, Z. Bai, C. Bischof, L. S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, et al. *LAPACK Users’ guide*. SIAM, 1999.

[2] M. Galassi, J. Davies, J. Theiler, B. Gough, G. Jungman, P. Alken, M. Booth, F. Rossi, and R. Ulerich. *GNU scientific library*. Network Theory Limited, 2002.

[3] N. J. Higham. *Functions of matrices: theory and computation*. SIAM, 2008.

[4] B. Hudobivnik and J. Korelc. Closed-form representation of matrix functions in the formulation of nonlinear material models. *Finite Elements in Analysis and Design*, 111:19–32, 2016.

[5] C.-P. Jeannerod, N. Louvet, and J.-M. Muller. Further analysis of kahan’s algorithm for the accurate computation of $2 \times 2$ determinants. *Mathematics of Computation*, 82:2245–2264, 2013.

[6] B. Jeremić and Z. Cheng. Significance of equal principal stretches in computational hyperelasticity. *Communications in numerical methods in engineering*, 21(9):477–486, 2005.

[7] J. Kopp. Efficient numerical diagonalization of hermitian $3 \times 3$ matrices. *International Journal of Modern Physics C*, 19(03):523–548, 2008.

[8] J. Korelc and S. Stupkiewicz. Closed-form matrix exponential and its application in finite-strain plasticity. *International Journal for Numerical Methods in Engineering*, 98(13):960–987, 2014.

[9] E. E. Kummer. Bemerkungen über die cubische Gleichung, durch welche die Haupt-Axen der Flächen zweiten Grades bestimmt werden. *Journal für die reine und angewandte Mathematik*, 26:268–272, 1843. doi:https://doi.org/10.1515/9783112367704-017

[10] A. Meurer, C. P. Smith, M. Paprocki, O. Čertík, S. B. Kirpichev, M. Rocklin, A. Kumar, S. Ivanov, J. K. Moore, S. Singh, T. Rathnayake, S. Vig, B. E. Granger, R. P. Muller, F. Bonazzi, H. Gupta, S. Vats, F. Johansson,
F. Pedregosa, M. J. Curry, A. R. Terrel, V. Roučka, A. Saboo, I. Fernando, S. Kulal, R. Cimrman, and A. Sco- 
patz. Sympy: symbolic computing in python. PeerJ Computer Science, 3:e103, Jan. 2017. ISSN 2376-5992. 
doi:10.7717/peerj-cs.103 URL https://doi.org/10.7717/peerj-cs.103

[11] C. Miehe. Computation of isotropic tensor functions. Communications in numerical methods in 
ingineering, 9 (11):889–896, 1993.

[12] A. Neumaier. Rundungsfehleranalyse einiger Verfahren zur Summation endlicher Summen. Univ., Inst. f. Prakt. 
Mathematik, 1973.

[13] B. N. Parlett. The (matrix) discriminant as a determinant. Linear Algebra and its Applications, 355:85–101, 2002. 
doi:https://doi.org/10.1016/S0024-3795(02)00335-X

[14] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. Numerical recipes in C, 1988.

[15] J. C. Simo and R. L. Taylor. Quasi-incompressible finite elasticity in principal stretches. continuum basis and 
numerical algorithms. Computer methods in applied mechanics and engineering, 85(3):273–310, 1991.

[16] O. K. Smith. Eigenvalues of a symmetric 3× 3 matrix. Communications of the ACM, 4(4):168, 1961.

[17] G. N. Watson. Some identities associated with a discriminant. Proceedings of the Edinburgh Mathematical 
Society, 10:101–107, 1956. doi:https://doi.org/10.1017/S0013091500021490

[18] S. Wolfram. Mathematica: a system for doing mathematics by computer. Addison Wesley Longman Publishing 
Co., Inc., 1991.