Efficient numerical diagonalization of hermitian $3 \times 3$ matrices

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A very common problem in science is the numerical diagonalization of symmetric or hermitian $3 \times 3$ matrices. Since standard “black box” packages may be too inefficient if the number of matrices is large, we study several alternatives. We consider optimized implementations of the Jacobi, QL, and Cuppen algorithms and compare them with an analytical method relying on Cardano’s formula for the eigenvalues and on vector cross products for the eigenvectors. Jacobi is the most accurate, but also the slowest method, while QL and Cuppen are good general purpose algorithms. The analytical algorithm outperforms the others by more than a factor of 2, but becomes inaccurate or may even fail completely if the matrix entries differ greatly in magnitude. This can mostly be circumvented by using a hybrid method, which falls back to QL if conditions are such that the analytical calculation might become too inaccurate. For all algorithms, we give an overview of the underlying mathematical ideas, and present detailed benchmark results. C and Fortran implementations of our code are available for download from http://www.mpi-hd.mpg.de/~globes/3x3/.

1. INTRODUCTION

In many scientific problems, the numerical diagonalization of a large number of symmetric or hermitian $3 \times 3$ matrices plays a central role. For a matrix $A$, this means calculating a set of eigenvalues $\lambda_i$ and eigenvectors $v_i$, satisfying

$$Av_i = \lambda_i v_i. \quad (1)$$

An example from classical mechanics or molecular science is the determination of the principal axes of a solid object [1]. The author’s interest in the problem arises from the numerical computation of neutrino oscillation probabilities in matter [2–4], which requires the diagonalization of the Hamiltonian operator

$$H = U \begin{pmatrix} 0 & \Delta m^2_{21} & \Delta m^2_{31} \\ \Delta m^2_{21} & 0 & 0 \\ \Delta m^2_{31} & 0 & 0 \end{pmatrix} U^\dagger + \begin{pmatrix} V \\ 0 \\ 0 \end{pmatrix}. \quad (2)$$

Here, $U$ is the leptonic mixing matrix, $\Delta m^2_{21}$ and $\Delta m^2_{31}$ are the differences of the squared neutrino masses, and $V$ is the MSW (Mikheyev-Smirnov-Wolfenstein) Potential describing coherent forward scattering in matter. If certain non-standard physics contributions are considered, the MSW matrix can also contain more than one non-zero entry [5].

There exist many publicly available software packages for the calculation of matrix eigensystems, e.g. LAPACK [6], the GNU Scientific Library [7], or the Numerical Recipes algorithms [8]. These packages exhibit excellent accuracy, but being designed mainly for very large matrices, they may produce a lot of computational overhead in the simple $3 \times 3$ case. This overhead comes partly from the algorithms themselves, and partly from the implementational details.

In this letter, we will study the performance of several algorithms which were optimized specifically for $3 \times 3$ matrices. We will discuss the well-known Jacobi, QL and Cuppen algorithms, and compare their speed and accuracy to that of a direct analytical calculation using Cardano’s formula for the eigenvalues, and vector cross products for the eigenvectors. The application of Cardano’s formula to the $3 \times 3$ eigenproblem has been suggested previously in [9], and formulas for the eigenvectors based on the computation of the Euler angles have been presented in [10].

The outline of the paper is as follows: In Secs. 2 and 3, we will describe the mathematical background of the considered algorithms as well as the most important implementational issues, and discuss their numerical properties. In Sec. 4, we will briefly mention some other algorithms capable of solving the $3 \times 3$ eigenproblem, and give reasons why we do not consider them to be the optimal choice for such small matrices. Our purely theoretical discussion will be complemented in Sec. 5 by the presentation of detailed benchmark results. Finally, we will draw our conclusions in Sec. 6. The appendix contains two alternative derivations of Cardano’s formulas, and the documentation of our C and Fortran code, which is available for download from http://www.mpi-hd.mpg.de/~globes/3x3/.

2. ITERATIVE ALGORITHMS

2.1. The Jacobi method

One of the oldest methods for the diagonalization of an arbitrary symmetric or hermitian $n \times n$ matrix $A$ is the Jacobi algorithm. Discussions of this algorithm can be found in [8, 11–14]. Its basic idea is to iteratively zero the off-diagonal elements of $A$ by unitary transformations of

\[a_{i,j} = 0 \quad \text{for } i \neq j.\]
the form

\[
P_{pq} = \begin{pmatrix}
1 & & & \\
& c & \cdots & se^{i\alpha} \\
& \vdots & 1 & \vdots \\
-\bar{s}e^{-i\alpha} & \cdots & c & 1
\end{pmatrix}
\]  \quad (3)

The matrices \(P_{pq}\) differ from the unit matrix only in the \((pp), (pq), (qp),\) and \((qq)\) elements; \(c\) and \(s\) are required to satisfy \(s^2 + c^2 = 1\), and can thus be expressed in the form

\[
c = \cos \phi,
\]

\[
s = \sin \phi
\]

for some real angle \(\phi\). The complex phase \(\alpha\) is absent if \(A\) has only real entries. \(\phi\) and \(\alpha\) are chosen in such a way that the similarity transformation

\[
A \rightarrow P^\dagger_{pq} A P_{pq}
\]

eliminates the \((pq)\) element (and thus also the \((qp)\) element) of \(A\). Of course it will in general become nonzero again in the next iteration, where \(p\) or \(q\) is different, but one can show that the iteration (5) converges to a diagonal matrix, with the eigenvalues of \(A\) along the diagonal, if \(p\) and \(q\) cycle through the rows or columns of \(A\) [14].

The normalized eigenvectors are given by the columns of the matrix

\[
Q = P_{p_1 q_1} P_{p_2 q_2} P_{p_3 q_3} \cdots
\]

\quad (6)

2.2. The QR and QL algorithms

The QR and QL algorithms are among the most widely used methods in large scale linear algebra because they are very efficient and accurate although their implementation is a bit more involved than that of the Jacobi method [8, 12, 15]. They are only competitive if applied to real symmetric tridiagonal matrices of the form

\[
T = \begin{pmatrix}
0 & \times & \times & \\
\times & 0 & \cdots & \times \\
\times & \cdots & \ddots & \times \\
\times & \times & \cdots & 0
\end{pmatrix}
\]

\quad (7)

Therefore, as a preliminary step, \(A\) has to be brought to this form.

2.2.1. Reduction of \(A\) to tridiagonal form

There are two main ways to accomplish the tridiagonalization: The Givens method, which consists of successively applying plane rotations of the form of Eq. (3) (in contrast to the Jacobi reduction to diagonal form, the Givens reduction to tridiagonal form is non-iterative), and the Householder method, which we will discuss here. A Householder transformation is defined by the unitary transformation matrix

\[
P = I - \omega uu^\dagger
\]

\quad (8)

with

\[
u = x \mp |x| e_i
\]

and

\[
\omega = \frac{1}{|u|^2} \left( 1 + \frac{u^\dagger x}{u^\dagger u} \right).
\]

\quad (9)

Here, \(x\) is arbitrary for the moment, and \(e_i\) denotes the \(i\)-th unit vector. From a purely mathematical point of view, the choice of sign in Eq. (9) is arbitrary, but in the actual implementation we choose it to be equal to the sign of the real part of \(x_i\) to avoid cancellation errors. \(P\) has the property that \(Px \sim e_i\) because

\[
(I - \omega uu^\dagger)x = x - \frac{1 + \frac{u^\dagger x}{u^\dagger u}}{|x|^2 + |x|(x_i + x_i^*)} u u^\dagger x 
\]

\[
= x - \frac{(u^\dagger x + x^\dagger u)(x \mp |x|e_i)}{2|x|^2 + |x|(x_i + x_i^*)} 
\]

\[
= x - \frac{(|x|^2 + |x| x_i + |x|^2 \mp |x| x_i^*)(x \mp |x|e_i)}{2|x|^2 + |x|(x_i + x_i^*)} 
\]

\[
= \pm |x| e_i.
\]

\quad (10)

This means, that if we choose \(x\) to contain the lower \(n - 1\) elements of the first column of \(A\) and set \(x_1 = 0\), \(e_1 = e_2\), then

\[
P_1 A P_1^\dagger = \begin{pmatrix}
\times & \times & \cdots & \times \\
\times & 0 & \cdots & \times \\
\times & \cdots & \ddots & \times \\
\times & \times & \cdots & 0
\end{pmatrix}
\]

\quad (11)

Note that the first row and the first column of this matrix are real even if \(A\) is not. In the next step, \(x\) contains the lower \(n - 2\) elements of the second column of \(P_1 A P_1^\dagger\), \(x_1 = x_2 = 0\), and \(e_1 = e_3\), so that the second row (and column) is brought to the desired form, while the first remains unchanged. This is repeated \(n - 1\) times, until \(A\) is fully tridiagonal and real.

For the actual implementation of the Householder method, we do not calculate the matrix product \(PAP^\dagger\) directly, but instead evaluate

\[
p = \omega^* A u,
\]

\quad (12)

\[
K = \frac{\omega}{2} u^\dagger p,
\]

\quad (13)

\[
q = p - K u.
\]

\quad (14)
With these definitions, we have the final expression
\[ PA^i P = P(A - pu^i) \]
\[ = A - pu^i - up^i + 2Kuu^i \]
\[ = A - qu^i - uq^i. \] \hspace{1cm} (16)

Note that in the last step we have made use of the fact that \( K \) is real, as can be seen from Eqs. (14) and (13), and from the hermiticity of \( A \).

2.2.2. The QL algorithm for real tridiagonal matrices

The QL algorithm is based on the fact that any real matrix can be decomposed into an orthogonal matrix \( Q \) and a lower triangular matrix \( L \) according to
\[ A = QL. \] \hspace{1cm} (17)

Equivalently, one could also start from a decomposition of the form \( A = QR \), with \( R \) being upper triangular, to obtain the QR algorithm, which has similar properties. For tridiagonal \( A \), the QL decomposition is most efficiently calculated by a sequence of plane rotations of the form of Eq. (3). The iteration prescription is
\[ A \rightarrow Q^T A Q. \] \hspace{1cm} (18)

but to accelerate convergence it is advantageous to use the method of shifting, which means decomposing \( A - kI \) instead of \( A \). In each step, \( k \) is chosen in such a way that the convergence to zero of the uppermost non-zero off-diagonal element of \( A \) is maximized (see [15] for a discussion of the shifting strategy and for corresponding convergence theorems). Since in practice, the subtraction of \( k \) from the diagonal elements of \( A \) can introduce large numerical errors, the most widely used form of the QL algorithm is one with implicit shifting, where not all of these differences need to be evaluated explicitly, although the method is mathematically equivalent to the ordinary QL algorithm with shifting.

2.3. Efficiency and accuracy of the Jacobi and QL algorithms

As we have mentioned before, one of the main benefits of the QL algorithm is its efficiency: For matrices of large dimension \( n \), it requires \( \approx 30n^2 \) floating point operations (combined multiply/add) if only the eigenvalues are to be computed, or \( \approx 6n^3 \) operations if also the complex eigenvectors are desired [8]. Additionally, the preceding complex Householder transformation requires \( 8n^2/3 \) resp. \( 16n^2/3 \) operations. In contrast, the complex Jacobi algorithm takes about \( 3n^2 \) to \( 5n^2 \) complex Jacobi rotations, each of which involves \( 12n \) operations for the eigenvalues, or \( 24n \) operations for the complete eigensystem. Therefore, the total workload is \( \approx 35n^3 - 60n^3 \) resp. \( 70n^3 - 120n^3 \) operations.

For the small matrices considered here, these estimates are not reliable. In particular, the QL method suffers from the fact that the first few eigenvalues require more iterations than the later ones, since for these the corresponding off-diagonal elements have already been brought close to zero in the preceding steps. Furthermore, the operations taking place before and after the innermost loops will play a role for small matrices. Since these are more complicated for QL than for Jacobi, they will give an additional penalty to QL. For these reasons we expect the performance bonus of QL over Jacobi to be smaller for \( 3 \times 3 \) matrices than for larger problems.

The numerical properties of both iterative methods are independent of the matrix size and have been studied in great detail by others, so we will only give a brief overview here. For real symmetric positive definite matrices, Demmel and Veselić have shown that the Jacobi method is more accurate than the QL algorithm [16, 17]. In particular, if the eigenvalues are distributed over many orders of magnitude, QL may become inaccurate for the small eigenvalues. In the example given in [17], the extremely fast convergence of this algorithm is also its main weakness: In the attempt to bring the lowest diagonal element close to the smallest eigenvalue of the matrix, a difference of two almost equal numbers has to be taken.

If the requirement of positive definiteness is omitted, one can also find matrices for which QL is more accurate than Jacobi [18].

3. NON-ITERATIVE ALGORITHMS

3.1. Direct analytical calculation of the eigenvalues

For \( 3 \times 3 \) matrices, the fastest way to calculate the eigenvalues is by directly solving the characteristic equation
\[ P(\lambda) = |A - \lambda I| = 0 \] \hspace{1cm} (19)

If we write
\[ A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{pmatrix}, \] \hspace{1cm} (20)

Eq. (19) takes the form
\[ P(\lambda) = \lambda^3 + c_2\lambda^2 + c_1\lambda + c_0 = 0 \] \hspace{1cm} (21)

with the coefficients
\[ c_2 = -a_{11} - a_{22} - a_{33}, \] \hspace{1cm} (22)
\[ c_1 = a_{11}a_{22} + a_{11}a_{33} + a_{22}a_{33} - |a_{12}|^2 - |a_{13}|^2 - |a_{23}|^2, \] \hspace{1cm} (23)
\[ c_0 = a_{11}|a_{23}|^2 + a_{22}|a_{13}|^2 + a_{33}|a_{12}|^2 - a_{11}a_{22}a_{33} - 2\text{Re}(a_{13}a_{12}a_{23}). \] \hspace{1cm} (24)
To solve Eq. (21), we follow the method proposed by del Ferro, Tartaglia, and Cardano in the 16th century [19]. In Appendix A we will discuss two alternative approaches and show that they lead to the same algorithm as Cardano's method if numerical considerations are taken into account.

Cardano's method requires first transforming Eq. (21) to the form
\[ x^3 - 3x = t, \]  
by defining
\[ p = c_2^2 - 3c_1, \]  
\[ q = -\frac{27}{4}c_0 - c_2^3 + \frac{9}{2}c_2c_1, \]  
\[ t = 2p^{-3/2}q, \]  
\[ x = \frac{t}{\sqrt{p}}(\lambda + \frac{1}{3}c_2). \]

It is easy to check that a solution to Eq. (25) is then given by
\[ x = \frac{1}{u} + u, \]  
with
\[ u = \sqrt{\frac{t}{2} \pm \sqrt{\frac{t^2}{4} - 1}}. \]

There is a sixfold ambiguity in \( u \) (two choices for the sign of the square root and three solutions for the complex cube root), but it reduces to the expected threefold ambiguity in \( x \).

To achieve optimal performance, we would like to avoid complex arithmetic as far as possible. Therefore, we will now show that \( \sqrt{p} \) and, thus \( t \), are always real. We know from linear algebra that the characteristic polynomial \( P(\lambda) \) of the hermitian matrix \( A \) must have three real roots, which is only possible if the stationary points of \( P(\lambda) \), \( \lambda_{1/2} = -\frac{1}{2}c_2 \pm \frac{1}{2}\sqrt{c_2^2 - 3c_1} = -\frac{1}{2}c_2 \pm \frac{1}{2}\sqrt{p} \) are real. Since \( c_2 \) is real, this implies that also \( \sqrt{p} \) must be real.

Furthermore, from the same argument, we have the requirement that \( P(\lambda_1) \geq 0 \geq P(\lambda_2) \), which in turn implies that \( -2 \leq t \leq 2 \). Therefore, \( \sqrt{t^2/4 - 1} \) is always purely imaginary, and from this it is easy to see that \( |u| = 1 \). Therefore we can write \( u = e^{i\phi} \), with
\[ \phi = \frac{1}{3} \arctan \frac{\sqrt{t^2/4 - 1}}{t/2} = \frac{1}{3} \arctan \frac{\sqrt{p^3 - q^2}}{q} \]
\[ = \frac{1}{3} \arctan \frac{27q(c_0 - (p - c_1)) + c_0(q^2 - 4pc_0)}{q}. \]  
(32)

The last step is necessary to improve the numerical accuracy, which would suffer dramatically if we computed the difference \( p^3 - q^2 \) directly.

When evaluating Eq. (32), care must be taken to correctly resolve the ambiguity in the arctan by taking into account the sign of \( q \): For \( q > 0 \), the solution must lie in the first quadrant, for \( q < 0 \) it must be located in the second. In contrast to this, solutions differing by multiples of \( 2\pi \) are equivalent, so \( x \) can take three different values,
\[ x_1 = 2\cos \phi, \]
\[ x_2 = 2\cos \left( \phi + \frac{2\pi}{3} \right) = -\cos \phi - \sqrt{3}\sin \phi, \]
\[ x_3 = 2\cos \left( \phi - \frac{2\pi}{3} \right) = -\cos \phi + \sqrt{3}\sin \phi. \]

These correspond to the three eigenvalues of \( A \):
\[ \lambda_i = \frac{\sqrt{3}}{3}x_i - \frac{1}{3}c_2. \]

Similar formulas have been derived previously in [9].

The most expensive steps of Cardano’s algorithm are the evaluations of the trigonometric functions. Nevertheless, the method is extremely fast, and will therefore be the best choice for many practical problems. However, from Eq. (34) we can see that it becomes unstable for matrices with largely different eigenvalues: In general, \( c_2 \) is of the order of the largest eigenvalue \( \lambda_{\text{max}} \). Therefore, in order to obtain the smaller eigenvalues, considerable cancellation between \( \frac{\sqrt{3}}{3}x_i \) and \( \frac{1}{3}c_2 \) must occur, which can yield large errors and is very susceptible to tiny relative errors in the calculation of \( c_2 \).

In general, the roots of Eq. (21) can be very sensitive to small errors in the coefficients which might arise due to cancellations in Eqs. (22) – (24).

If \( \varepsilon \) is the machine precision, we can estimate the absolute accuracy of the eigenvalues to be of \( O(\varepsilon \lambda_{\text{max}}) \), which may imply a significant loss of relative accuracy for the small eigenvalues.

Consider for example the matrix
\[ \begin{pmatrix} 10^{40} & 10^{19} & 10^{20} \\ 10^{19} & 10^9 & 10^9 \\ 10^{19} & 10^9 & 1 \end{pmatrix}. \]
(35)
which has the (approximate) eigenvalues \( 10^{40}, 10^{20}, \) and \( 1 \). However, Cardano’s method yields \( 10^{40}, 5 \cdot 10^{19}, \) and \(-5 \cdot 10^{19} \). Note that for the matrix (35), also the QL algorithm has problems and delivers one negative eigenvalue. Only Jacobi converges to a reasonable relative accuracy. See [16] for a discussion of this.

### 3.2. Direct analytical calculation of the eigenvectors

Once the eigenvalues \( \lambda_i \) of \( A \) have been computed, the eigenvectors \( \mathbf{v}_i \) can be calculated very efficiently by using vector cross products, which are a unique tool in three-dimensional space.

The \( \mathbf{v}_i \) satisfy by definition
\[ (A - \lambda_i I) \cdot \mathbf{v}_i = 0. \]  
(36)
taking the hermitian conjugate of this equation and multiplying it with an arbitrary vector \( x \in \mathbb{C}^3 \), we obtain
\[
\mathbf{v}_i^\dagger \cdot (\mathbf{A} - \lambda_i \mathbf{I}) \cdot \mathbf{x} = 0.
\]
In particular, if \( x \) is the \( j \)-th unit vector \( \mathbf{e}_j \), this becomes
\[
\mathbf{v}_i^\dagger \cdot (\mathbf{A}_j - \lambda_i \mathbf{e}_j) = 0 \quad \forall \ j,
\]
where \( \mathbf{A}_j \) denotes the \( j \)-th column of \( \mathbf{A} \). Consequently, as long as \( \mathbf{A}_1 \mathbf{A}_2 - \lambda_i \mathbf{e}_1 \mathbf{e}_2 \) are linearly independent, we have
\[
\mathbf{v}_i = [(\mathbf{A}_1 - \lambda_i \mathbf{e}_1) \times (\mathbf{A}_2 - \lambda_i \mathbf{e}_2)]^*.
\]
In the special case that \( \mathbf{A}_1 - \lambda_i \mathbf{e}_1 = \mu(\mathbf{A}_2 - \lambda_i \mathbf{e}_2) \), \( \mathbf{v}_i \) is immediately given by
\[
\mathbf{v}_i = \frac{1}{\sqrt{1 + |\mu|^2}} \begin{pmatrix} 1 \\ -\mu \\ 0 \end{pmatrix}.
\]

When implementing the above procedure, care must be taken if there is a degenerate eigenvalue because in this case, the algorithm will only find one of the two corresponding eigenvectors. Therefore, if we detect a degenerate eigenvalue, say \( \lambda_1 = \lambda_2 \), we calculate the second eigenvector as the cross product of \( \mathbf{v}_1 \) with one of the columns of \( \mathbf{A} - \lambda_1 \mathbf{I} \). In principle, this alternative formula would also work for non-degenerate eigenvalues, but we try to avoid it as far as possible because it abets the propagation of errors. On the other hand, we have to keep in mind that the test for degeneracy may fail if the eigenvalues have been calculated too inaccurately. If this happens, the algorithm will deliver wrong results.

The calculation of the third eigenvalue can be greatly accelerated by using the formula \( \mathbf{v}_3^\dagger = \mathbf{v}_1 \times \mathbf{v}_2 \). Of course, this is again vulnerable to error propagation, but it turns out that this is usually tolerable.

For many practical purposes that require only moderate accuracy, the vector product algorithm is the method of choice because it is considerably faster than all other approaches. However, the limitations to its accuracy need to be kept in mind. First, the eigenvectors suffer from errors in the eigenvalues. Under certain circumstances, these errors can even be greatly enhanced by the algorithm. For example, the matrix
\[
\begin{pmatrix}
10^{20} & 10^9 & 10^9 \\
10^9 & 10^{20} & 10^9 \\
10^9 & 10^9 & 1
\end{pmatrix}
\]
has the approximate eigenvalues \((1 + 10^{-11}) \cdot 10^{20}, (1 - 10^{-11}) \cdot 10^{20}, \) and 0.98. The corresponding eigenvectors are approximately
\[
\mathbf{v}_1 = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{pmatrix}, \quad \mathbf{v}_3 = \begin{pmatrix} 10^{-11} \\ 10^{-11} \\ 1 \end{pmatrix}.
\]

If we erroneously start the vector product algorithm with the approximate eigenvalues \( 10^{20}, 10^{20}, \) and 0.98, the error that is introduced when subtracting \( \lambda_1 \) from the diagonal elements is of order \( O(10^9) \) and thus comparable to the off-diagonal elements. Consequently, the calculated eigenvectors
\[
\mathbf{v}_1 = \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ -1/\sqrt{3} \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 2/\sqrt{6} \\ -1/\sqrt{6} \\ 1/\sqrt{6} \end{pmatrix}, \quad \mathbf{v}_3 = \begin{pmatrix} 0 \\ 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}
\]
are completely wrong.

Another flaw of the vector product algorithm is the fact that the subtractions \( (\mathbf{A}_j - \lambda_i \mathbf{e}_j) \) and the subtractions in the evaluation of the cross products are very prone to cancellation errors.

### 3.3. A hybrid algorithm

To circumvent the cases where the cross product method fails or becomes too inaccurate, we have devised a hybrid algorithm, which uses the analytical calculations from Secs. 3.1 and 3.2 as the default branch, but falls back to QL if this procedure is estimated to be too error-prone. The condition for the fallback is
\[
||\mathbf{v}_i||^2 \leq 2^8 \epsilon \Lambda^2
\]
Here, \( \mathbf{v}_i \) is the analytically calculated and yet unnormalized eigenvector from Eq. (39), \( \epsilon \) is the machine precision, \( \Lambda = \max(\lambda_3^2, \lambda_{\text{max}}) \) is an estimate for the largest number appearing in the problem, and \( 2^8 \) is introduced as a safety factor.

Since in typical problems only a small fraction of matrices will fulfill condition (44), the hybrid approach can be expected to retain the efficiency of the analytical algorithm. In reality, it is even slightly faster because fewer conditional branches are used.

### 3.4. Cuppen’s Divide and Conquer algorithm

In recent years, the “Divide and Conquer” paradigm for symmetric eigenproblems has received considerable attention. The idea was originally invented by Cuppen [20], and current implementations are faster than the QL method for large matrices [6]. One can estimate, that for \( 3 \times 3 \) matrices, a divide and conquer strategy might also be beneficial, because it means splitting the problem into a trivial \( 1 \times 1 \) and an analytically accessible \( 2 \times 2 \) problem.

However, let us first discuss Cuppen’s algorithm in its general form for \( n \times n \) matrices. As a preliminary step, the matrix has to be reduced to symmetric tridiagonal form, as discussed in Sec. 2.2.1. The resulting matrix \( \mathbf{T} \) is then split up in the form
\[
\mathbf{T} = \begin{pmatrix} \mathbf{T}_1 & 0 \\ 0 & \mathbf{T}_2 \end{pmatrix} + \mathbf{H},
\]
where \( \mathbf{T}_1 \) and \( \mathbf{T}_2 \) are again tridiagonal, and \( \mathbf{H} \) is a very simple rank 1 matrix, e.g.

\[
\mathbf{H} = \begin{pmatrix}
0 & \beta & 0 \\
\beta & \beta & \beta \\
0 & \beta & 0
\end{pmatrix}.
\]

(46)

Then, the smaller matrices \( \mathbf{T}_1 \) and \( \mathbf{T}_2 \) are brought to the diagonal form \( \mathbf{T}_i = \mathbf{Q}_i \mathbf{D}_i \mathbf{Q}_i^T \), so that \( \mathbf{T} \) becomes

\[
\mathbf{T} = \begin{pmatrix}
\mathbf{Q}_1 \mathbf{D}_1 \mathbf{Q}_1^T & 0 \\
0 & \mathbf{Q}_2 \mathbf{D}_2 \mathbf{Q}_2^T
\end{pmatrix} + \mathbf{H}
\]

\[
= \begin{pmatrix}
\mathbf{Q}_1 & 0 \\
0 & \mathbf{Q}_2
\end{pmatrix} \begin{pmatrix}
\mathbf{D}_1 & 0 \\
0 & \mathbf{D}_2
\end{pmatrix} + \mathbf{H}' \begin{pmatrix}
\mathbf{Q}_1^T & 0 \\
0 & \mathbf{Q}_2^T
\end{pmatrix}.
\]

(47)

Here, \( \mathbf{H}' = \mathbf{z} \mathbf{z}^T \) is another rank 1 matrix with a generating vector \( \mathbf{z} \) consisting of the last row of \( \mathbf{Q}_1 \) and the first row of \( \mathbf{Q}_2 \), both multiplied with \( \beta \). The remaining problem is to find an eigenvalue \( \lambda \) and an eigenvector \( \mathbf{v} \), satisfying

\[
\begin{pmatrix}
\mathbf{D}_1 & 0 \\
0 & \mathbf{D}_2
\end{pmatrix} \mathbf{v} + \mathbf{z} \mathbf{z}^T - \lambda \mathbf{I} = 0.
\]

(48)

By multiplying this equation from the left with \( \mathbf{z}^T \cdot \text{diag}((\mathbf{D}_1 - \lambda \mathbf{I})^{-1}, (\mathbf{D}_2 - \lambda \mathbf{I})^{-1}) \) and dividing off the scalar \( \mathbf{z}^T \mathbf{v} \), we obtain the characteristic equation in the form

\[
1 + \sum_i \frac{z_i^2}{d_i - \lambda} = 0,
\]

(49)

where the \( d_i \) are the diagonal entries of \( \mathbf{D}_1 \) and \( \mathbf{D}_2 \).

There are several obvious strategies for solving this equation in the \( 3 \times 3 \) case: First, by multiplying out the denominators we obtain a third degree polynomial which can be solved exactly as discussed in Sec. 3.1. This is very fast, but we have seen that it can be numerically unstable. Second, one could apply the classical Newton-Raphson iteration, which is fast and accurate in the vicinity of the root, but may fail altogether if a bad starting value is chosen. Finally, the fact that the roots of Eq. (49) are known to be separated by the singularities \( d_1, d_2 \) and \( d_3 \) suggests the usage of a bisection method to obtain the eigenvalues very accurately, but with slow convergence.

To get the optimum results, we apply Cardano’s analytical method to get estimates for the roots, and refine them with a hybrid Newton-Raphson/Bisection method based on [8]. This method usually takes Newton-Raphson steps, but if the convergence gets too slow or if Newton-Raphson runs out of the bracketing interval, it falls back to bisection.

The elements \( \tilde{v}_{ij} \) of the eigenvectors \( \tilde{\mathbf{v}}_i \) of \( \text{diag}(\mathbf{D}_1, \mathbf{D}_2) + \mathbf{H}' \) are then obtained by the simple formula

\[
\tilde{v}_{ij} = \frac{z_j}{d_j - \lambda_i}
\]

(50)

and just need to be transformed back to the original basis by undoing the transformations \( \mathbf{Q}_1, \mathbf{Q}_2 \), and the tridiagonalization.

If implemented carefully, Cuppen’s method can reach an accuracy comparable to that of the QL method. A major issue is the calculation of the differences \( d_i - \lambda_j \) in the evaluation of the characteristic equation, Eq. (49), and in the calculation of the eigenvectors, Eq. (50). To keep the errors as small as possible when solving for the eigenvalue \( \lambda_j \), we subtract our initial estimate for \( \lambda_j \) from all \( d_i \) before starting the iteration. This ensures that the thus transformed eigenvalue is very close to zero and therefore small compared to the \( d_i \).

As we have mentioned before, the Divide and Conquer algorithm is faster than the QL method for large matrices. It also required \( O(n^3) \) operations, but since the expensive steps — the reduction to tridiagonal form and the back-transformation of the eigenvectors — are both outside the iterative loops, the coefficient of \( n^3 \) is significantly smaller. For the small matrices that we are considering, however, the most expensive part is solving the characteristic equation. Furthermore, many conditional branches are required to implement necessary case differentiations, to avoid divisions by zero, and to handle special cases like multiple eigenvalues. Therefore, we expect the algorithm to be about as fast as the QL method.

It is of course possible to reduce the calculational effort at the expense of reducing the accuracy and stability of the algorithm, but it will always be slower than Cardano’s method combined with the vector product algorithm.

4. OTHER ALGORITHMS

Apart from the Jacobi, QL, Cuppen, and vector product algorithms there are several other methods for finding the eigensystems of symmetric matrices. We will briefly outline some of them here, and give reasons why they are inappropriate for \( 3 \times 3 \) problems.

4.1. Iterative root finding methods

In order to avoid the instabilities of Cardano’s method which were discussed in Sec. 3.1, one can use an iterative root finding method to solve the characteristic equation. Root bracketing algorithms like classical bisection or the Dekker-Brent method start with an interval which is known to contain the root. This interval is then iteratively narrowed until the root is known with the desired accuracy. Their speed of convergence is fair, but they are usually superseded by the Newton-Raphson method which follows the gradient of the function until it finds the root. However, the Newton-Raphson algorithm is not guaranteed to converge in all cases.

Although these problems can partly be circumvented by using a hybrid method like the one discussed in
Sec. 3.4, iterative root finders are still unable to find multiple roots, and these special cases would have to be treated separately. Furthermore, the accuracy is limited by the accuracy with which the characteristic polynomial can be evaluated. As we have already mentioned in Sec. 3.1, this can be spoiled by cancellations in the calculation of the coefficients $c_0$, $c_1$, and $c_2$.

4.2. Inverse iteration

Inverse iteration is a powerful tool for finding eigenvectors and improving the accuracy of eigenvalues. The method starts with some approximation $\tilde{\lambda}_i$ for the desired eigenvalue $\lambda_i$, and a random vector $b$. One then solves the linear equation

$$ (A - \tilde{\lambda}_i I) \cdot \tilde{v}_i = b $$

(51)

to find and approximation $\tilde{v}_i$ for the eigenvector $v_i$. An improved estimate for $\lambda_i$ is calculated by using the formula

$$ (A - \tilde{\lambda}_i I) \cdot \tilde{v}_i \approx (\lambda_i - \tilde{\lambda}_i) \cdot \tilde{v}_i. $$

(52)

We estimate that inverse iteration is impractical for small matrices because there are many special cases that need to be detected and handled separately. This would slow the computation down significantly.

4.3. Vectorization

In a situation where a large number $N$ of small matrices needs to be diagonalized, and all these matrices are available at the same time, it may be advantageous to vectorize the algorithm, i.e., to make the loop from 1 to $N$ the innermost loop. This makes consecutive operations independent of each other (because they affect different matrices), and allows them to be pipelined and executed very efficiently.

A detailed discussion of this approach is beyond the scope of the present work, but our estimate is that, as long as only the eigenvalues are to be computed, a vectorization of Cardano’s method would be most beneficial, because this method requires only few performance-limiting conditional branches, so that the number of processor pipeline stalls is reduced to a minimum. However, the accuracy limitations discussed above would still apply in the vectorized version.

If we want to calculate the full eigensystem, a vectorized vector product method can only give a limited performance bonus because in the calculation of the vector products, many special cases can arise which need to be detected and treated separately. This renders efficient vectorization impossible. The same is true for Cuppen’s Divide and Conquer algorithm. On the other hand, the iterative methods are problematic if the required number of iterations is not approximately the same for all matrices. Then, only the first few iterations can be vectorized efficiently. Afterwards, matrices for which the algorithm has not converged yet need to be treated separately.

5. BENCHMARK RESULTS

In this section we report on the computational performance and on the numerical accuracy of the above algorithms. For the iterative methods we use implementations which are similar to those discussed in [8]. Additionally, we study the LAPACK implementation of the QL/QR algorithm [6] and the QL routine from the GNU Scientific Library [7]. For the analytical methods we use our own implementations. Some ideas in our Cuppen routine are based on ideas realized in LAPACK.

Note that we do not show results for the LAPACK implementation of a Divide and Conquer algorithm (routine ZHEEVR) because this algorithm falls back to QL for small matrices ($n < 25$) and would therefore not yield anything new. We also neglect the new LAPACK routine ZHEEVR because for the $3 \times 3$ problems considered here it is significantly slower than the other algorithms.

We have implemented our code in C and Fortran, but here we will only discuss results for the Fortran version. We have checked that the C code yields a similar numerical accuracy, but is about 10% slower. This performance deficit can be ascribed to the fact that C code is harder to optimize for the compiler.

Our code has been compiled with the GNU compiler, using the standard optimization flag `-O3`. We did not use any further compiler optimizations although we are aware of the fact that it is possible to increase the execution speed by about 10% if options like `-ffast-math` are used to allow optimizations that violate the IEEE 754 standard for floating point arithmetic.

Our numerical tests were conducted in double precision arithmetic (64 bit, 15 – 16 decimal digits) on an AMD Opteron 250 (64-bit, 2.4 GHz) system running Linux. To maximize the LAPACK performance on this system, we used the highly optimized AMD Core Math Library for the corresponding tests. Note that on some platforms, in particular on Intel and AMD desktop processors, you may obtain a higher numerical accuracy than is reported here because these processors internally use 80 bit wide floating point registers.

To measure the accuracy of the calculated eigensystems we use three different benchmarks:

- The relative difference of the eigenvalue $\tilde{\lambda}$ and the corresponding result of the LAPACK QL routine

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1 We thank Charles van Loan for drawing our attention to this possibility.
ZHEEV, $\tilde{\lambda}^{\text{LAPACK}}$.

\[
\Delta_1 \equiv \frac{|\tilde{\lambda} - \tilde{\lambda}^{\text{LAPACK}}|}{\tilde{\lambda}^{\text{LAPACK}}}. \tag{53}
\]

We use the LAPACK QL implementation as a reference because it is very well tested and stable.

- The relative difference of the eigenvector $\tilde{v}$ and the corresponding LAPACK result, $v^{\text{LAPACK}}$:

\[
\Delta_2 \equiv \frac{||\tilde{v} - \tilde{v}^{\text{LAPACK}}||_2}{||\tilde{v}^{\text{LAPACK}}||_2}, \tag{54}
\]

where $|| \cdot ||_2$ denotes the Euclidean norm. This definition of $\Delta_2$ is of course not meaningful for matrices with degenerate eigenvalues because for these, different algorithms might find different bases for the multidimensional eigenspace. Even for non-degenerate eigenvalues, $\Delta_2$ is only meaningful if the same phase convention is chosen for $\tilde{v}$ and $v^{\text{LAPACK}}$. Therefore, when computing $\Delta_2$, we reject matrices with degenerate eigenvalues, and for all others we re-phase the eigenvectors in such a way that the component which has the largest modulus in $\tilde{v}^{\text{LAPACK}}$ is real.

- The deviation of the eigenvalue/eigenvector pair $(\tilde{\lambda}, \tilde{v})$ from its defining property $A v = \lambda v$:

\[
\Delta_3 \equiv \frac{||A \tilde{v} - \tilde{\lambda} \tilde{v}||_2}{||\tilde{\lambda} \tilde{v}||}. \tag{55}
\]

Note that for the algorithms considered here, $||\tilde{v}||_2 = 1$, so the definitions of $\Delta_2$ and $\Delta_3$ can be slightly simplified.

We have first verified the correctness of the algorithms by diagonalizing $10^7$ random hermitian resp. symmetric matrices with integer entries from the interval $[-10, 10]$ and (automatedly) checking that $\Delta_1$, $\Delta_2$ and $\Delta_3$ were as small as expected. We have repeated this test with logarithmically distributed integer entries from the interval $[0, 10^{10}]$. Such matrices tend to have largely different eigenvalues and are therefore a special challenge to the algorithms.

For the results that we are going to present here, we have used similar tests, but we have allowed the matrix entries to be real, which corresponds more closely to what is found in actual scientific problems. Furthermore, for the logarithmically distributed case we have changed the interval to $[10^{-5}, 10^5]$.

### 5.1. Performance

The results of our timing tests are summarized in Table I. The most important observation from this table is the fact that the standard libraries are slower by a substantial factor than the specialized algorithms. This is due to the fact that in both LAPACK and the GSL, only the innermost loops, which determine the performance for large scale problems, are optimized. Outside these loops, the libraries spend a lot of time evaluating their parameters and preparing data structures. LAPACK QL additionally takes some time to decide at runtime whether a QR or QL algorithm is more favorable.

On the other hand, our implementations of the iterative algorithms have a very simple parameter set, they do not require any internal reorganization of data structures, avoid function calls as far as possible, and contain some optimizations specific to the $3 \times 3$ case. On the downside, they do not perform any pre-treatment of the matrix such as rescaling it to avoid overflows and underflows. We believe that for pathological matrices, LAPACK may be more accurate than our QL method.

It is interesting to observe that the iterative algorithms are slightly faster for matrices with logarithmically distributed entries. The reason is that for many of these matrices, the off-diagonal entries are already small initially.
so fewer iterations are required for the diagonalization. This is one of the reasons why QL is always faster than Cuppen in the logarithmically distributed scenario, but may be slower in the linear case. Another reason for this is the fact that logarithmically distributed matrices are more likely to create situations in which the hybrid root finder, which is used to solve Eq. (49), converges very slowly. This happens for example if the analytically calculated starting values have large errors.

However, even in favorable situations, neither QL nor Cuppen can compete with the analytical methods. These do not require any pre-treatment of the matrix (like the transformation to tridiagonal form in the case of QL and Cuppen), and though their implementation may look a bit lengthy due to the many special cases that can arise, the number of floating point operations that are finally executed for each matrix is very small.

If we compare the performance for real symmetric vs. complex hermitian matrices, we find that purely real problems can be solved much more efficiently. This is especially true for the Jacobi algorithm since real Jacobi transformations are much cheaper than complex ones. For QL and Cuppen, the performance bonus is less dramatic because large parts of these algorithms always operate on purely real data structures. The Cardano and vector product algorithms contain complex arithmetic, but their speed is also limited by the evaluation of trigonometric functions (Cardano) and by several conditional branches (vector product), therefore they too do not benefit as much as the Jacobi method.

### 5.2. Numerical accuracy

The excellent performance of the analytical and hybrid algorithms is relativized by the results of our accuracy tests, which are shown in Table II. While for linearly distributed matrix entries, all algorithms get close to the machine precision of about $2 \cdot 10^{-16}$, the Cardano and vector product methods become unstable for the logarithmically distributed case. In particular, the large average values of $\Delta_3 > O(10^{-3})$ show that the calculated eigenvalues and eigenvectors often fail to fulfill their defining property $A\mathbf{v} = \lambda \mathbf{v}$. This problem is mitigated by the hybrid technique, but even this approach is still far less accurate than the Jacobi, QL, and Cuppen algorithms. For these, $\Delta_3$ is still of order $10^{-3}$ (QL & Cuppen) resp. $10^{-10}$ (Jacobi). The fact that Jacobi is more accurate than QL and Cuppen confirms our expectations from Sec. 2.3.

Note that the values of $\Delta_1$ and $\Delta_2$ for the LAPACK QL algorithm are zero in the case of complex matrices and extremely small for real matrices. The reason is that LAPACK QL is the reference algorithm used in the definition of these quantities. In the case of real matrices, $\Delta_1$ and $\Delta_2$ reveal the tiny differences between the LAPACK ZHEEV and DSYEV routines.

It is interesting to observe that in the logarithmically distributed scenario, $\Delta_1$ and $\Delta_2$ are systematically larger for real than for complex matrices. This does not have a deeper reason but is simply due to the fact that in the real case, there are fewer random degrees of freedom, so there is a higher chance for ill-conditioned matrices to occur. The effect is not visible in $\Delta_3$ because there it is compensated by the fact that this quantity receives large contributions mainly when in the evaluation of $A\mathbf{v}$, in Eq. (55), a multiplication of a large matrix entry with a small and thus relatively inaccurate vector component occurs. It follows from combinatorics that this is more likely to happen if $A$ and $\mathbf{v}$ are complex.

### 6. Conclusions

In this article, we have studied the numerical three-dimensional eigenproblem for symmetric and hermitian matrices. We have discussed the Jacobi, QL, and Cuppen algorithms as well as an analytical method using Cardano’s formula and vector cross products. Our benchmarks reveal that standard packages are very slow for small matrices. Optimized versions of the standard algorithms are a lot faster while retaining similar numerical properties, but even their speed is not competitive with that of the analytical methods. We have, however, seen that the latter have limited numerical accuracy in extreme situations. Moreover, they were not designed to avoid overflow and underflow conditions. To partly circumvent these problems, we have devised a hybrid algorithm, which employs analytical calculations as the standard branch, but falls back to QL if it estimates the problem to be ill-conditioned.

Depending on what kind of problem is to be solved, we give the following recommendations:

- **The hybrid algorithm** is recommended for problems where computational speed is more important than accuracy, and the matrices are not too ill-conditioned in the sense that their eigenvalues do not differ by more than a few orders of magnitude. For example, in the initial example of the neutrino oscillation Hamiltonian, where the physical uncertainties in the parameters are much larger than the numerical errors, the hybrid algorithm turns out to be the optimal choice [4].

- **The QL algorithm** is a good general purpose “black box” method since it is reasonably fast and — except in some very special situations like the example given in Eq. (35) — also very accurate. If speed is not an issue, one can use standard implementations of QL like the LAPACK function ZHEEV. For better performance we recommend simpler implementations like our function ZHEEVRQ3 or the function tqli from Ref. [8], on which our routine is based.

- **Cuppen’s Divide and Conquer method** can
### Linearly distributed real matrix entries

| Algorithm    | $\Delta_1$ | $\Delta_2$ | $\Delta_3$ |
|--------------|-------------|-------------|-------------|
|              | Avg. | Max. | Avg. | Max. | Avg. | Max. |
| Jacobi       | 1.34 × 10^{-15} | 3.52 × 10^{-9} | 4.01 × 10^{-16} | 1.32 × 10^{-12} | 2.01 × 10^{-15} | 1.02 × 10^{-8} |
| QL           | 1.89 × 10^{-15} | 5.59 × 10^{-9} | 4.09 × 10^{-16} | 2.05 × 10^{-12} | 3.58 × 10^{-15} | 1.24 × 10^{-8} |
| Cuppen       | 1.95 × 10^{-15} | 9.53 × 10^{-9} | 6.83 × 10^{-16} | 1.80 × 10^{-12} | 4.21 × 10^{-15} | 1.45 × 10^{-8} |
| GSL          | 1.29 × 10^{-15} | 3.18 × 10^{-9} | 3.56 × 10^{-16} | 2.18 × 10^{-12} | 2.40 × 10^{-15} | 5.02 × 10^{-9} |
| LAPACK QL    | 5.80 × 10^{-17} | 3.61 × 10^{-11} | 3.17 × 10^{-17} | 6.10 × 10^{-13} | 2.69 × 10^{-15} | 8.28 × 10^{-9} |
| Analytical   | 1.87 × 10^{-15} | 9.53 × 10^{-9} | 6.19 × 10^{-15} | 1.80 × 10^{-8} | 1.36 × 10^{-14} | 4.32 × 10^{-8} |
| Hybrid       | 1.87 × 10^{-15} | 9.53 × 10^{-9} | 4.91 × 10^{-15} | 6.49 × 10^{-9} | 1.16 × 10^{-14} | 2.91 × 10^{-8} |

### Linearly distributed complex matrix entries

| Algorithm    | $\Delta_1$ | $\Delta_2$ | $\Delta_3$ |
|--------------|-------------|-------------|-------------|
|              | Avg. | Max. | Avg. | Max. | Avg. | Max. |
| Jacobi       | 1.96 × 10^{-15} | 7.66 × 10^{-9} | 4.64 × 10^{-16} | 1.13 × 10^{-14} | 1.42 × 10^{-14} | 3.44 × 10^{-7} |
| QL           | 2.08 × 10^{-14} | 5.46 × 10^{-7} | 4.83 × 10^{-16} | 8.16 × 10^{-14} | 4.27 × 10^{-14} | 1.14 × 10^{-6} |
| Cuppen       | 4.37 × 10^{-15} | 6.54 × 10^{-8} | 6.60 × 10^{-16} | 2.03 × 10^{-13} | 3.95 × 10^{-14} | 1.03 × 10^{-6} |
| GSL          | 8.01 × 10^{-15} | 1.88 × 10^{-7} | 4.56 × 10^{-16} | 8.36 × 10^{-14} | 2.14 × 10^{-14} | 5.26 × 10^{-7} |
| LAPACK QL    | 0.0 | 0.0 | 0.0 | 0.0 | 2.41 × 10^{-14} | 6.03 × 10^{-7} |
| Analytical   | 4.19 × 10^{-15} | 6.54 × 10^{-8} | 5.66 × 10^{-16} | 3.17 × 10^{-11} | 3.05 × 10^{-14} | 7.95 × 10^{-7} |
| Hybrid       | 4.19 × 10^{-15} | 6.54 × 10^{-8} | 5.56 × 10^{-16} | 3.17 × 10^{-11} | 3.03 × 10^{-14} | 7.95 × 10^{-7} |

### Logarithmically distributed real matrix entries

| Algorithm    | $\Delta_1$ | $\Delta_2$ | $\Delta_3$ |
|--------------|-------------|-------------|-------------|
|              | Avg. | Max. | Avg. | Max. | Avg. | Max. |
| Jacobi       | 2.96 × 10^{-10} | 1.94 × 10^{-4} | 3.05 × 10^{-12} | 3.91 × 10^{-7} | 8.16 × 10^{-11} | 1.10 × 10^{-4} |
| QL           | 4.88 × 10^{-10} | 4.29 × 10^{-4} | 2.59 × 10^{-12} | 7.14 × 10^{-7} | 1.03 × 10^{-9} | 1.18 × 10^{-3} |
| Cuppen       | 4.28 × 10^{-10} | 4.29 × 10^{-4} | 3.58 × 10^{-12} | 6.55 × 10^{-7} | 8.90 × 10^{-10} | 1.12 × 10^{-3} |
| GSL          | 1.86 × 10^{-10} | 1.62 × 10^{-4} | 2.78 × 10^{-12} | 4.01 × 10^{-7} | 9.87 × 10^{-10} | 2.04 × 10^{-3} |
| LAPACK QL    | 8.36 × 10^{-12} | 1.14 × 10^{-5} | 1.28 × 10^{-13} | 1.81 × 10^{-7} | 1.11 × 10^{-9} | 1.18 × 10^{-3} |
| Analytical   | 1.87 × 10^{-9} | 7.20 × 10^{-3} | 1.80 × 10^{-7} | 1.36 × 10^{-10} | 3.47 × 10^{-1} | 1.07 × 10^{-6} |
| Hybrid       | 1.40 × 10^{-9} | 1.16 × 10^{-3} | 3.84 × 10^{-11} | 2.03 × 10^{-4} | 2.19 × 10^{-4} | 4.75 × 10^{-11} |

### Logarithmically distributed complex matrix entries

| Algorithm    | $\Delta_1$ | $\Delta_2$ | $\Delta_3$ |
|--------------|-------------|-------------|-------------|
|              | Avg. | Max. | Avg. | Max. | Avg. | Max. |
| Jacobi       | 1.55 × 10^{-10} | 1.64 × 10^{-4} | 2.23 × 10^{-13} | 7.43 × 10^{-8} | 1.19 × 10^{-10} | 8.24 × 10^{-5} |
| QL           | 2.25 × 10^{-10} | 6.84 × 10^{-4} | 1.96 × 10^{-13} | 1.17 × 10^{-7} | 7.85 × 10^{-10} | 5.93 × 10^{-4} |
| Cuppen       | 2.03 × 10^{-10} | 6.02 × 10^{-4} | 2.71 × 10^{-13} | 1.30 × 10^{-7} | 7.59 × 10^{-10} | 5.86 × 10^{-4} |
| GSL          | 1.06 × 10^{-10} | 8.69 × 10^{-5} | 2.17 × 10^{-13} | 1.30 × 10^{-7} | 1.38 × 10^{-9} | 1.15 × 10^{-3} |
| LAPACK QL    | 0.0 | 0.0 | 0.0 | 0.0 | 1.27 × 10^{-9} | 1.24 × 10^{-3} |
| Analytical   | 1.16 × 10^{-9} | 7.10 × 10^{-4} | 6.10 × 10^{-9} | 8.29 × 10^{-2} | 2.88 × 10^{-3} | 2.84 × 10^{-3} |
| Hybrid       | 1.11 × 10^{-9} | 6.84 × 10^{-4} | 8.55 × 10^{-12} | 3.55 × 10^{-5} | 1.15 × 10^{-4} | 8.81 × 10^{-11} |

Table II: Numerical accuracy of different algorithms for calculating the eigenvalues and eigenvectors of symmetric or hermitian 3 × 3 matrices. This table refers to the Fortran implementation, but we have checked that the values obtained with the C code are similar.
achieve an accuracy similar to that of the QL algorithm and may be slightly faster for complex problems if the input matrix is not already close to diagonal. The choice between Cuppen and QL will therefore depend on the details of the problem that is to be solved.

- If the highest possible accuracy is desired, **Jacobi’s method** is the algorithm of choice. It is extremely accurate even for very pathological matrices, but it is significantly slower than the other algorithms, especially for complex problems.

- The **purely analytical method** is not recommended for practical applications because it is superseded by the hybrid algorithm. It is, however, of academic interest since it reveals both the strengths and the limitations of analytical eigensystem calculations.

Let us remark that in scenarios where the diagonalization of a hermitian $3 \times 3$ matrix is only part of a larger problem, it may be advantageous to choose a slower but more accurate algorithm because this may improve the convergence of the surrounding algorithm, thus speeding up the overall process. The final choice of diagonalization algorithm will always depend strongly on the details of the problem which is to be solved.

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**Appendix A: ALTERNATIVE DERIVATIONS OF CARDANO’S METHOD**

In this appendix, we will discuss two alternative solution strategies for the third degree polynomial equations (21), and show that in the end, numerical considerations lead again to Eq. (33).

1. **A trigonometric approach**

   If we substitute $x = 2 \cos \frac{\theta}{3}$ on the left hand side of Eq. (25) and use trigonometric transformations to obtain
   \[ 2 \cos \frac{\theta}{3} = t, \]  
   (A1)
   we can show that the solutions to Eq. (25) can be written as
   \[ x = 2 \cos \frac{\theta}{3} = 2 \cos \left( \frac{1}{3} \arccos \frac{t}{2} \right). \]  
   (A2)

   Our previous result $-2 \leq t \leq 2$ (see Sec. 3.1) ensures that this is well-defined. If we replace the arccos by a numerically more stable arctan, we immediately recover Eq. (33).

2. **Lagrange resolvents**

   The second alternative to Cardano’s derivation that we are going to consider employs the concept of Lagrange resolvents. We start from the observation that the coefficients of Eq. (21) can be expressed in terms of the roots $\lambda_1$, $\lambda_2$, and $\lambda_3$ of $P(\lambda)$, because we can write
   \[ P(\lambda) = \prod_{i=1,2,3} (\lambda - \lambda_i). \]
   In particular, $c_0$, $c_1$, and $c_2$ are the so-called **elementary symmetric polynomials** in $\lambda_1$, $\lambda_2$, and $\lambda_3$:
   \[ -c_2 = \sum_{i<j} \lambda_i \lambda_j, \]
   \[ c_1 = \sum \lambda_i \lambda_j, \]
   \[ -c_0 = \prod \lambda_i. \]  
   (A3)

   Next, we consider the **Lagrange resolvents** of Eq. (21), which are defined by
   \[ r_1 = \lambda_1 + \lambda_2 + \lambda_3, \]
   \[ r_2 = \lambda_1 + e^{\frac{2 \pi i}{3}} \lambda_2 + e^{-\frac{2 \pi i}{3}} \lambda_3, \]
   \[ r_3 = \lambda_1 + e^{-\frac{2 \pi i}{3}} \lambda_2 + e^{\frac{2 \pi i}{3}} \lambda_3. \]  
   (A4)

   We observe, that $r_3^2$ is invariant under permutation of the $\lambda_i$, and so, by the fundamental theorem of symmetric functions [21], can be expressed in terms of $c_0$, $c_1$, and $c_2$. Indeed, with the definitions from Eq. (29), we obtain
   \[ r_1^3 = -c_2^3, \]
   \[ r_2^3 = q + \sqrt{q^2 - p^3}, \]
   \[ r_3^3 = q - \sqrt{q^2 - p^3}. \]  
   (A5)

   We can then recover $\lambda_1$, $\lambda_2$, and $\lambda_3$ according to
   \[ \lambda_1 = \frac{1}{3} (r_1 + r_2 + r_3), \]
   \[ \lambda_2 = \frac{1}{3} (r_1 + e^{\frac{2 \pi i}{3}} r_2 + e^{-\frac{2 \pi i}{3}} r_3), \]
   \[ \lambda_3 = \frac{1}{3} (r_1 + e^{-\frac{2 \pi i}{3}} r_2 + e^{\frac{2 \pi i}{3}} r_3). \]  
   (A6)

   For a practical implementation of these formulas, one would like to avoid complex arithmetic. This is possible because we have seen before that $\sqrt{q^2 - p^3}$ is always purely imaginary. This observation allows us to write
   \[ r_2 = \sqrt{p} e^{i \phi}, \]
   \[ r_3 = \sqrt{p} e^{-i \phi}, \]  
   (A7)
   with $\phi = \frac{1}{3} \arctan \sqrt{p^3 - q^2} / q$ as before, and thus
   \[ \lambda_1 = \frac{1}{3} (-c_2 + 2 \rho \cos \phi), \]
   \[ \lambda_2 = \frac{1}{3} (-c_2 - \rho \cos \phi - \sqrt{3} \rho \sin \phi), \]
   \[ \lambda_3 = \frac{1}{3} (-c_2 - \rho \cos \phi + \sqrt{3} \rho \sin \phi). \]  
   (A8)
These expressions are equivalent to Eq. (33) after substituting back Eqs. (29), so the practical implementation of the Lagrange method is again identical to the previous algorithms.

Appendix B: DOCUMENTATION OF THE C AND FORTRAN CODE

Along with the publication of this article, we provide C and Fortran implementations of the algorithms discussed here for download. They are intended to be used for further numerical experiments or for the solution of actual scientific problems.

Our C code follows the C99 standard which provides the complex data type `double complex`. In gcc, this requires the usage of the compiler option `-std=c99`. The Fortran code is essentially Fortran 77, except for the fact that not all variable and function names obey the 6-character limitation.

Both versions of the code contain detailed comments, describing the structure of the routines, the purpose of the different functions, and their arguments. The C version also contains detailed information about local variables, which was omitted in the Fortran version to keep the code compact.

Our nomenclature conventions for functions and subroutines may seem a bit cryptical because we tried to keep as close as possible to the LAPACK conventions: The first letter indicates the data type ("D" for double or "Z" for complex), the second and third letters indicate the matrix type ("SY" for symmetric and "HE" for hermitian), while the remaining characters specify the purpose of the function: "EV" means eigenvalues and/or eigenvectors, "F" stands for Jacobi, "Q" for QL, "D" for Divide & Conquer (Cuppen), "V" for vector product, and "C" for Cardano. We also add the suffix "3" to indicate that our routines are designed for 3 × 3 matrices.

In the following we will describe the interface of the different functions, and their arguments. The C version also contains detailed information about local variables, which was omitted in the Fortran version to keep the code compact.

Our nomenclature conventions for functions and subroutines may seem a bit cryptical because we tried to keep as close as possible to the LAPACK conventions: The first letter indicates the data type ("D" for double or "Z" for complex), the second and third letters indicate the matrix type ("SY" for symmetric and "HE" for hermitian), while the remaining characters specify the purpose of the function: "EV" means eigenvalues and/or eigenvectors, "F" stands for Jacobi, "Q" for QL, "D" for Divide & Conquer (Cuppen), "V" for vector product, and "C" for Cardano. We also add the suffix "3" to indicate that our routines are designed for 3 × 3 matrices.

In the following we will describe the interface of the individual routines. We will discuss only those functions which are relevant to the complex case, because their real counterparts are similar, with the data types `COMPLEX*16` resp. `double complex` being replaced by `DOUBLE PRECISION` resp. `double`.

Furthermore, we will only discuss the Fortran code here because the corresponding C functions have identical names and arguments. For example the Fortran subroutine

```fortran
SUBROUTINE ZHEEV3(A, Q, W)
  COMPLEX*16 A(3, 3)
  COMPLEX*16 Q(3, 3)
  DOUBLE PRECISION W(3)
END
```

This routine calculates the eigenvalues and stores them in `W`, and in the columns of `Q`.

The function accesses only the diagonal and upper triangular parts of `A`. The access is read-only.

```fortran
SUBROUTINE ZHEEVQ3(A, Q, W)
  COMPLEX*16 A(3, 3)
  COMPLEX*16 Q(3, 3)
  DOUBLE PRECISION W(3)
END
```

This is our implementation of the QL algorithm from Sec. 2.2. It finds the eigenvalues and normalized eigenvectors of a hermitian 3 × 3 matrix `A` and stores them in `W`, while the eigenvectors are returned in the columns of `Q`.

The upper triangular part of `A` is destroyed during the calculation, the diagonal elements are read but not destroyed, and the lower triangular elements are not referenced at all.

```fortran
SUBROUTINE ZHEEVD3(A, Q, W)
  COMPLEX*16 A(3, 3)
  COMPLEX*16 Q(3, 3)
  DOUBLE PRECISION W(3)
END
```

This is Cuppen's Divide and Conquer algorithm, optimized for 3-dimensional problems (see Sec. 3.4). The function assumes `A` to be a hermitian 3 × 3 matrix, and calculates its eigenvalues `W`, as well as its normalized eigenvectors. The latter are returned in the columns of `Q`.

The function accesses only the diagonal and upper triangular parts of `A`. The access is read-only.

```fortran
SUBROUTINE ZHEEVC3(A, W)
  COMPLEX*16 A(3, 3)
  DOUBLE PRECISION W(3)
END
```

This routine calculates the eigenvalues `W`, of a hermitian 3 × 3 matrix `A` using Cardano’s analytical algorithm (see Sec. 3.1). Only the diagonal and upper triangular parts of `A` are accessed, and the access is read-only.

```fortran
SUBROUTINE ZHEEVC3(A, W)
  COMPLEX*16 A(3, 3)
  DOUBLE PRECISION W(3)
END
```

This function first calls `ZHEEVC3` to find the eigenvalues of the hermitian 3 × 3 matrix `A`, and then uses vector cross products to analytically calculate the normalized eigenvectors (see Sec. 3.2). The eigenvalues are stored in `W`, the normalized eigenvectors in the columns of `Q`.

```fortran
SUBROUTINE ZHEEVJ3(A, Q, W)
  COMPLEX*16 A(3, 3)
  COMPLEX*16 Q(3, 3)
  DOUBLE PRECISION W(3)
END
```

1. Main driver function
Only the diagonal and upper triangular parts of $A$ need to contain meaningful values, but all of $A$ may be used as temporary storage and might hence be destroyed.

**SUBROUTINE ZHEEVH3(A, Q, W)**

COMPLEX*16 A(3, 3)
COMPLEX*16 Q(3, 3)
DOUBLE PRECISION W(3)

This is the hybrid algorithm from Sec. 3.3. Its default behavior is identical to that of ZHEEV3, but under certain circumstances, it falls back to calling ZHEEVQ3. As for the other routines, $A$ has to be a hermitian $3 \times 3$ matrix, and the eigenvalues and eigenvectors are stored in $W$ resp. in the columns of $Q$.

Only the diagonal and upper triangular parts of $A$ need to contain meaningful values, and access to $A$ is read-only.

### 2. Helper functions

**SUBROUTINE DSYEV2(A, B, C, RT1, RT2, CS, SN)**

DOUBLE PRECISION A, B, C
DOUBLE PRECISION RT1, RT2, CS, SN

This subroutine calculates the eigenvalues and eigenvectors of a real symmetric $2 \times 2$ matrix

\[
\begin{pmatrix}
A & B \\
B & C
\end{pmatrix}
\]

The result satisfies

\[
\begin{pmatrix}
RT1 & 0 \\
0 & RT2
\end{pmatrix} = 
\begin{pmatrix}
CS & SN \\
-SN & CS
\end{pmatrix}
\begin{pmatrix}
A & B \\
B & C
\end{pmatrix}
\begin{pmatrix}
CS & -SN \\
SN & CS
\end{pmatrix}
\]

(B2)

and $RT1 \geq RT2$. Note that this convention is different from the convention used in the corresponding LAPACK function DLAEV2, where $|RT1| \geq |RT2|$. We use a different convention here because it helps to avoid several conditional branches in ZHEEVD3 and DSYEVD3.

**SUBROUTINE ZHETRD3(A, Q, D, E)**

COMPLEX*16 A(3, 3)
COMPLEX*16 Q(3, 3)
DOUBLE PRECISION D(3)
DOUBLE PRECISION E(2)

This routine reduces a hermitian matrix $A$ to real tridiagonal form by applying a Householder transformation $Q$ according to Sec. 2.2:

\[
A = Q \cdot \begin{pmatrix}
D_1 & E_1 \\
E_1 & D_2 \\
& E_2 \\
& & D_3
\end{pmatrix} \cdot Q^T.
\]

(B3)

The function accesses only the diagonal and upper triangular parts of $A$. The access is read-only.

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