

Accurate complex Jacobi rotations^{*}

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Abstract

This note shows how to compute, to high relative accuracy under mild assumptions, complex Jacobi rotations for diagonalization of Hermitian matrices of order two, using the correctly rounded functions `cr_hypot` and `cr_rsqrtd`, proposed for standardization in the C programming language as recommended by the IEEE-754 floating-point standard. The rounding to nearest (ties to even) and the non-stop arithmetic are assumed. The numerical examples compare the observed with theoretical bounds on the relative errors in the rotations' elements, and show that the maximal observed departure of the rotations' determinants from unity is smaller than that of the transformations computed by LAPACK.

Keywords: Jacobi rotation, Hermitian eigenproblem of order two, rounding error analysis
2020 MSC: 65F15, 65-04, 65G50

1. Introduction

Given A , a Hermitian matrix of order two, a complex Jacobi rotation is a unitary matrix U such that $\det U = 1$ and $AU = U\Lambda$, i.e., $U^*AU = \Lambda$. Here, Λ is a real diagonal matrix of the eigenvalues of A , and U is a matrix of the associated eigenvectors. Let the representation of A , U , and Λ be fixed, with $\varphi \in [-\pi/4, \pi/4]$ and $\alpha \in (-\pi, \pi]$, as

$$A = \begin{bmatrix} a_{11} & \overline{a_{21}} \\ a_{21} & a_{22} \end{bmatrix}, \quad U = \begin{bmatrix} \cos \varphi & -e^{-i\alpha} \sin \varphi \\ e^{i\alpha} \sin \varphi & \cos \varphi \end{bmatrix}, \quad \Lambda = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}. \quad (1)$$

It is shown here how to compute \tilde{U} , a floating-point approximation of U , from the rounded, floating-point value of A , $\text{fl}(A)$. Empirically, such \tilde{U} is closer, in the worst case, to a unitary matrix than the worst-case transformation from the `xLAEV2` LAPACK [1] routine, as long as $\text{fl}(A)$ can be exactly scaled to A' , which has no non-zero subnormal values.

Applications of the eigendecomposition (EVD) of a Hermitian matrix of order two are numerous (see [13] for a more exhaustive list), the most prominent being the Jacobi method for the EVD of general Hermitian matrices [9], and the implicit (i.e., one-sided) Jacobi (also known as Hestenes) method for the singular value decomposition (SVD) of $m \times n$, $m \geq n$ matrices, which is implemented in LAPACK following [5, 6, 7] as `xGESVJ` and `xGEJSV` routines.

This work simplifies, and improves accuracy of, the complex Jacobi rotations' floating-point computation from [13], by relying on *correctly rounded* functions `cr_hypot`(x, y) = $\text{fl}(\sqrt{x^2 + y^2})$ and `cr_rsqrtd`(x) = $\text{fl}(1/\sqrt{x})$, expected to be standardized as optional in C [11, §7.33.8]. These functions have been provided¹ by the CORE-MATH project [14] for the default rounding to nearest-even, in single (binary32) and double (binary64) precision. The latter function has also been considered in [4], and one approach towards the former has been described in [3]. It is therefore assumed here that the non-stop floating-point arithmetic [10] is used, with gradual underflow and rounding to nearest-even.

Usage of `hypot` for improving accuracy of real Jacobi rotations has been considered in [2], in a different way and without the assumption on correct rounding. As shown in [13], `cr_rsqrtd` can be safely avoided when it is unavailable.

The special case of symmetric matrices and real Jacobi rotations is not detailed for brevity, but the corresponding theoretical and numerical results as well as the implementations can be derived from the presented ones, and are included in the supplement. Performance of the code is not considered due to novelty of the correctly rounded routines.

^{*}The supplementary material is available in `AccJac` and `libpvn` repositories from <https://github.com/venovako> or by request.

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¹The source code and other resources are freely available at <https://core-math.gitlabpages.inria.fr> at the time of writing.

2. Floating-point computation of complex Jacobi rotations

Listing 1 presents ZJAEV2², the proposed algorithm for the Hermitian EVD in the form of (1), as a simplification of [13, Listing 1]. In single precision, CJAEV2 can be obtained straightforwardly. The derivation of the algorithm can be found in [13], including the scaling of $\text{fl}(A)$ by a suitable power of two to avoid overflow of the scaled eigenvalues.

Two accuracy-improving (but possibly performance-degrading) modifications of [13] are proposed. With ν being the largest finite floating-point value, and using the C language functions as defined in [11], [13, Eq. (2.6)] has become

$$\tan(2\tilde{\varphi}) = \text{copysign}(\text{fmin}(\text{fmax}(\text{fl}((2|\tilde{a}'_{21}|)/|\tilde{a}|), 0), \nu), \tilde{a}), \quad \tilde{a} = \text{fl}(a'_{11} - a'_{22}), \quad A' = \text{fl}(2^\zeta \text{fl}(A)), \quad (2)$$

with all roundings explicitly stated, and $|\tilde{a}'_{21}| = \text{cr_hypot}(\Re a'_{21}, \Im a'_{21})$. Also, [13, Eq. (2.5)] has been simplified as³

$$\tan \tilde{\varphi} = \text{fl}(\tan(2\tilde{\varphi}) / \text{fl}(1 + \text{cr_hypot}(\tan(2\tilde{\varphi}), 1))), \quad \sec^2 \tilde{\varphi} = \text{fma}(\tan \tilde{\varphi}, \tan \tilde{\varphi}, 1), \quad \cos \tilde{\varphi} = \text{cr_rsqrt}(\sec^2 \tilde{\varphi}), \quad (3)$$

where $\text{fma}(x, y, z) = \text{fl}(x \cdot y + z)$. The symbols having a tilde indicate the computed approximations of the exact values; e.g., $\tan \tilde{\varphi}$ approximates $\tan \varphi$. The elements of $\text{fl}(A)$ are considered exact for the purposes of this paper, i.e., $A = \text{fl}(A)$. For all but extremely badly scaled matrices A no element underflows when scaled as in (2), so A' is exact in such cases.

Listing 1: ZJAEV2: the EVD of a double precision Hermitian matrix of order two in pseudo-C when rounding to nearest

```

1 // input: fl(A) as a11, a22, ℜa21, ℑa21; output: cos ϕ̃, cos α̃ sin ϕ̃, sin α̃ sin ϕ̃; λ̃1, λ̃2, ζ' or λ̃1, λ̃2
2 int ζ11, ζ22, ζ21ℜ, ζ21ℑ, ζ, ζ', η' = DBL_MAX_EXP - 3; double μ̃ = DBL_TRUE_MIN, ν = DBL_MAX;
3 // determine ζ assuming all inputs are finite; avoid taking the exponent of 0
4 frexp(fmax(fabs(a11), μ̃), &ζ11); frexp(fmax(fabs(a22), μ̃), &ζ22);
5 frexp(fmax(fabs(ℜa21), μ̃), &ζ21ℜ); frexp(fmax(fabs(ℑa21), μ̃), &ζ21ℑ);
6 ζ = η' - max{ζ11, ζ22, ζ21ℜ, ζ21ℑ}; ζ' = -ζ; // max{...} has to be expanded using the >= operator
7 // scale the input matrix A by 2ζ as A' = 2ζA; the results might be inexact only due to underflow
8 a'11 = scalbn(a11, ζ); a'22 = scalbn(a22, ζ); ℜa'21 = scalbn(ℜa21, ζ); ℑa'21 = scalbn(ℑa21, ζ);
9 // find the polar form of a'21 = 2ζa21 as |ā'21|eiα̃ = |ā'21|(|cos α̃ + i · sin α̃|); |ℜā'21| = |ℑā'21| = μ̃ is dangerous
10 |ℜā'21| = fabs(ℜa'21); |ℑā'21| = fabs(ℑa'21); |ā'21| = cr_hypot(|ℜā'21|, |ℑā'21|);
11 cos α̃ = copysign(fmin(|ℜā'21| / |ā'21|, 1.0), ℜā'21); sin α̃ = ℑa'21 / fmax(|ā'21|, μ̃); // underflows possible
12 // compute the complex Jacobi rotation
13 ò = |ā'21| * 2.0; ā = a'11 - a'22; |ā| = fabs(a); // underflow of ā possible
14 tan(2ϕ̃) = copysign(fmin(fmax(ò / |ā|, 0.0), ν), ā); // filter out possible non-finite partial results
15 tan ϕ̃ = tan(2ϕ̃) / (1.0 + cr_hypot(tan(2ϕ̃), 1.0)); // rounding to nearest: denominator cannot overflow
16 sec2 ϕ̃ = fma(tan ϕ̃, tan ϕ̃, 1.0); cos ϕ̃ = cr_rsqrt(sec2 ϕ̃); sin ϕ̃ = tan ϕ̃ * cos ϕ̃;
17 cos α̃ sin ϕ̃ = cos α̃ * sin ϕ̃; sin α̃ sin ϕ̃ = sin α̃ * sin ϕ̃; // tan ϕ̃, sin ϕ̃, ℜ(eiα̃ sin ϕ̃), ℑ(eiα̃ sin ϕ̃) can underflow
18 // compute the eigenvalues scaled by 2ζ (always finite)
19 λ̃1' = fma(tan ϕ̃, fma(a'22, tan ϕ̃, ò), a'11) / sec2 ϕ̃; λ̃2' = fma(tan ϕ̃, fma(a'11, tan ϕ̃, -ò), a'22) / sec2 ϕ̃;
20 λ̃1 = scalbn(λ̃1', ζ'); λ̃2 = scalbn(λ̃2', ζ'); // optionally backscale (over/under-flows possible)

```

ZJAEV2, unlike ZLAEV2, does not attempt to sort the computed eigenvalues decreasingly, leaving it to users instead.

3. Rounding error analysis

Theorem 1 shows that the elements of \tilde{U} computed by xJAEV2 have high relative accuracy, with the error bounds tighter than in [13, Proposition 2.4], if no computed inexact value underflows. Exact subnormals and zeros are allowed.

²See https://github.com/venovako/libpvn/blob/master/src/pvn_ev2.c, along with `pvn.h` and `pvn_crm.h` in the same subdirectory, and <https://github.com/venovako/AccJac/blob/master/src/zjaev2.f90>, for the mostly LAPACK-compatible implementation.

³If Λ is not needed, $\sec \tilde{\varphi} = \text{cr_hypot}(\tan \tilde{\varphi}, 1)$, $\cos \tilde{\varphi} = 1 / \sec \tilde{\varphi}$, and $\sin \tilde{\varphi} = \tan \tilde{\varphi} / \sec \tilde{\varphi}$ could be used instead for possibly better accuracy.

Theorem 1. *In at least single precision arithmetic with rounding to nearest, and barring any inexact underflow, the elements of \tilde{U} computed by xJAEV2 have the relative error bounds as specified, with ε being the machine precision:*

$$\cos \tilde{\varphi} = \delta_c \cos \varphi, \quad 1 - 6.00000017 \varepsilon < \delta_c < 1 + 6.00000000 \varepsilon, \quad (4)$$

$$\cos \tilde{\alpha} \sin \tilde{\varphi} = \delta_{21}^{\Re} \cos \alpha \sin \varphi, \quad \sin \tilde{\alpha} \sin \tilde{\varphi} = \delta_{21}^{\Im} \sin \alpha \sin \varphi, \quad 1 - 19.00000000 \varepsilon < \delta_{21}^{\Re}, \delta_{21}^{\Im} < 1 + 19.00000950 \varepsilon.$$

PROOF. Since `cr_hypot` is correctly rounded, $|\tilde{a}'_{21}| = |a'_{21}|(1 + \epsilon_1)$, $|\epsilon_1| \leq \varepsilon$, and $|\tilde{a}'_{21}| = 0$ if and only if $a'_{21} = 0$. With ϵ_2 and ϵ_3 , $\max\{|\epsilon_2|, |\epsilon_3|\} \leq \varepsilon$, from line 11 of Listing 1, when $|\tilde{a}'_{21}| > 0$, the relative errors δ_α^{\Re} and δ_α^{\Im} in $\cos \tilde{\alpha}$ and $\sin \tilde{\alpha}$ are

$$\cos \tilde{\alpha} = \frac{\Re a'_{21}}{|a'_{21}|(1 + \epsilon_1)}(1 + \epsilon_2) = \cos \alpha \frac{1 + \epsilon_2}{1 + \epsilon_1} = \delta_\alpha^{\Re} \cos \alpha, \quad \sin \tilde{\alpha} = \frac{\Im a'_{21}}{|a'_{21}|(1 + \epsilon_1)}(1 + \epsilon_3) = \sin \alpha \frac{1 + \epsilon_3}{1 + \epsilon_1} = \delta_\alpha^{\Im} \sin \alpha.$$

The minimal value of $(1 + \epsilon_i)/(1 + \epsilon_1)$, $i \in \{2, 3\}$, is $\delta_\alpha^- = (1 - \varepsilon)/(1 + \varepsilon)$, and the maximal value is $\delta_\alpha^+ = (1 + \varepsilon)/(1 - \varepsilon)$. When \tilde{a}'_{21} is real or imaginary (let $\beta = 1$ then, and otherwise $\beta = 2$), $\cos \tilde{\alpha}$ and $\sin \tilde{\alpha}$ are exact, so $\delta_\alpha^- = \delta_\alpha^+ = 1$. The scaling in lines 4–8 of Listing 1 prevents $|\tilde{a}'_{21}|$, as well as \tilde{o} , from overflowing (see [13, Proposition 2.4 and Corollary 2.5]).

Multiplication by a power of two is exact if the result is normal, so $\tilde{o} = o(1 + \epsilon_1)^{\beta-1}$ in line 13 of Listing 1. It is assumed that \tilde{a} is exact (i.e., $\tilde{a} = a$) or has not underflowed, so $|\tilde{a}| = |a|(1 + \epsilon_4)$, $|\epsilon_4| \leq \varepsilon$. With $|\epsilon_5| \leq \varepsilon$ it holds

$$\text{fl}\left(\frac{\tilde{o}}{|\tilde{a}|}\right) = \frac{o(1 + \epsilon_1)^{\beta-1}}{|a|(1 + \epsilon_4)}(1 + \epsilon_5) = \delta_2 \frac{o}{|a|}, \quad \delta_2 = \frac{(1 + \epsilon_1)^{\beta-1}(1 + \epsilon_5)}{1 + \epsilon_4}, \quad \frac{(1 - \varepsilon)^\beta}{1 + \varepsilon} = \delta_2^- \leq \delta_2 \leq \frac{(1 + \varepsilon)^\beta}{1 - \varepsilon} = \delta_2^+. \quad (5)$$

If $\tilde{o} = 0$, then $\tan(2\tilde{\varphi}) = \pm 0$, so it is exact. Else, if $\tilde{a} = \pm 0$, then $\tan \tilde{\varphi} = \pm 1$ is exact, regardless of the error in $\tan(2\tilde{\varphi})$. Else, if \tilde{a} causes overflow of the result of the division in line 14 of Listing 1, $\tan(2\tilde{\varphi}) = \pm \nu$ instead of $\pm \infty$. Its relative error is then not easily bounded, but is irrelevant, since $\tan \varphi$ is a monotonically non-decreasing function of $\tan(2\varphi)$, as well as $\tan \tilde{\varphi}$ with respect to $\tan(2\tilde{\varphi})$, due to monotonicity of all floating-point operations involved in computing it (addition, division, and hypotenuse, with the associated roundings) as in (3). The relative error in $\tan \tilde{\varphi}$ largest by magnitude, i.e., $\tan \tilde{\varphi} = \pm 1$, computed when $|\tan(2\varphi)| \leq \nu$ for which $|\tan(2\tilde{\varphi})| = \nu$, can only decrease for $\tan(2\varphi)$ larger in magnitude, since $\tan(2\varphi) \rightarrow \pm \infty$ implies $\tan \varphi \rightarrow \pm 1$. Moreover, $\tan(2\tilde{\varphi})$ is not an output value of xJAEV2.

The equation $\tan^2(2\tilde{\varphi}) + 1 = (\tan^2(2\varphi) + 1)(1 + \epsilon_6)$ has to be solved for ϵ_6 , to relate the exact with the computed hypotenuse in line 15 of Listing 1. By substituting $\delta_2 \tan(2\varphi)$ for $\tan(2\tilde{\varphi})$, what can be done when $|\tan(2\varphi)| \leq \nu$, and rearranging the terms, while noting that $0 < \delta_2^- < 1$, $\delta_2^+ > 1$, and $0 \leq x/(x+1) < 1$ for all $x \geq 0$, it follows that

$$\epsilon_6 = \frac{\tan^2(2\varphi)}{\tan^2(2\varphi) + 1}(\delta_2^- - 1), \quad (\delta_2^-)^2 - 1 < \epsilon_6 < (\delta_2^+)^2 - 1, \quad \delta_2^- < \sqrt{1 + \epsilon_6} < \delta_2^+. \quad (6)$$

Let $z = \sqrt{\tan^2(2\varphi) + 1}$. Then, $\sqrt{\tan^2(2\tilde{\varphi}) + 1} = z\sqrt{1 + \epsilon_6}$, so $\tilde{z} = \text{cr_hypot}(\tan(2\tilde{\varphi}), 1) = z\sqrt{1 + \epsilon_6}(1 + \epsilon_7) = z \cdot y$, where $|\epsilon_7| \leq \varepsilon$. Now, $1 + \tilde{z} = (1 + z)(1 + \epsilon_8)$ has to be solved for ϵ_8 , to relate the exact and the computed denominator in line 15 of Listing 1. Similarly as above, since $z \geq 0$ and, due to (6), $\delta_2^-(1 - \varepsilon) = y^- < y < y^+ = \delta_2^+(1 + \varepsilon)$, it follows

$$\epsilon_8 = \frac{z}{z+1}(y-1), \quad y^- - 1 < \epsilon_8 < y^+ - 1, \quad y^- < 1 + \epsilon_8 < y^+. \quad (7)$$

Therefore, $\text{fl}(1 + \tilde{z}) = (1 + z)(1 + \epsilon_8)(1 + \epsilon_9)$, where $|\epsilon_9| \leq \varepsilon$. Let $x = \tan(2\varphi)$ and $\tilde{x} = \tan(2\tilde{\varphi})$. Then, with $|\epsilon_{10}| \leq \varepsilon$,

$$\tan \tilde{\varphi} = \text{fl}\left(\frac{\tilde{x}}{\text{fl}(1 + \tilde{z})}\right) = \frac{x}{1 + z} \frac{\delta_2(1 + \epsilon_{10})}{(1 + \epsilon_8)(1 + \epsilon_9)} = \delta_t \tan \varphi, \quad \delta_t = \frac{\delta_2}{1 + \epsilon_8} \frac{1 + \epsilon_{10}}{1 + \epsilon_9}. \quad (8)$$

It is easy to minimize the second factor of δ_t in (8) to $(1 - \varepsilon)/(1 + \varepsilon)$, and to maximize it to $(1 + \varepsilon)/(1 - \varepsilon)$, irrespectively of the first factor. Using (7), $1 + \epsilon_8$ is minimized to $\delta_2^-(1 - \varepsilon)$ and maximized to $\delta_2^+(1 + \varepsilon)$. Therefore, from (5) follows

$$\delta_t^- = \frac{\delta_2^-}{\delta_2^+(1 + \varepsilon)} \frac{1 - \varepsilon}{1 + \varepsilon} = \frac{(1 - \varepsilon)^{\beta+2}}{(1 + \varepsilon)^{\beta+3}}, \quad \delta_t^+ = \frac{\delta_2^+}{\delta_2^-(1 - \varepsilon)} \frac{1 + \varepsilon}{1 - \varepsilon} = \frac{(1 + \varepsilon)^{\beta+2}}{(1 - \varepsilon)^{\beta+3}}, \quad \delta_t^- < \delta_t < \delta_t^+. \quad (9)$$

Similarly as in (6), the equation $\delta_t^2 \tan^2 \varphi + 1 = (\tan^2 \varphi + 1)(1 + \epsilon_{11})$ has to be solved for ϵ_{11} , what, due to (9), leads to

$$\epsilon_{11} = \frac{\tan^2 \varphi}{\tan^2 \varphi + 1}(\delta_t^2 - 1), \quad 0 \leq \frac{\tan^2 \varphi}{\tan^2 \varphi + 1} \leq \frac{1}{2}, \quad \frac{1}{\sqrt{2}} \sqrt{(\delta_t^-)^2 + 1} = \delta_r^- < \sqrt{1 + \epsilon_{11}} < \delta_r^+ = \frac{1}{\sqrt{2}} \sqrt{(\delta_t^+)^2 + 1}. \quad (10)$$

Then, from line 16 of Listing 1, $\sec^2 \tilde{\varphi} = (\delta_r^2 \tan^2 \varphi + 1)(1 + \epsilon_{12}) = \delta_q^2 \sec^2 \varphi$, where $|\epsilon_{12}| \leq \epsilon$ and $\delta_q^2 = (1 + \epsilon_{11})(1 + \epsilon_{12})$, while, from (10), $\delta_r^- \sqrt{1 - \epsilon} = \delta_q^- < \delta_q < \delta_q^+ = \delta_r^+ \sqrt{1 + \epsilon}$. With $|\epsilon_{13}| \leq \epsilon$, the relative error in $\cos \tilde{\varphi}$ can be bounded as

$$\cos \tilde{\varphi} = \frac{1 + \epsilon_{13}}{\sqrt{\sec^2 \tilde{\varphi}}} = \frac{1 + \epsilon_{13}}{\delta_q} \cos \varphi = \delta_c \cos \varphi, \quad \frac{1 - \epsilon}{\delta_q^+} = \delta_c^- < \delta_c < \delta_c^+ = \frac{1 + \epsilon}{\delta_q^-}. \quad (11)$$

Now, $\sin \tilde{\varphi} = \delta_s \sin \varphi$, where $\delta_s = \delta_r \delta_c (1 + \epsilon_{14})$, $|\epsilon_{14}| \leq \epsilon$, and $\delta_r^- \delta_c^- (1 - \epsilon) = \delta_s^- < \delta_s < \delta_s^+ = \delta_r^+ \delta_c^+ (1 + \epsilon)$. It holds

$$\cos \tilde{\alpha} \sin \tilde{\varphi} = \delta_{21}^{\mathfrak{R}} \cos \alpha \sin \varphi, \quad \delta_{21}^{\mathfrak{R}} = \delta_\alpha^{\mathfrak{R}} \delta_s (1 + \epsilon_{15})^{\beta-1}, \quad \sin \tilde{\alpha} \sin \tilde{\varphi} = \delta_{21}^{\mathfrak{I}} \sin \alpha \sin \varphi, \quad \delta_{21}^{\mathfrak{I}} = \delta_\alpha^{\mathfrak{I}} \delta_s (1 + \epsilon_{16})^{\beta-1}, \quad (12)$$

$$\max\{|\epsilon_{15}|, |\epsilon_{16}|\} \leq \epsilon, \quad \delta_\alpha^- \delta_s^- (1 - \epsilon)^{\beta-1} = \delta_{21}^- < \delta_{21}^{\mathfrak{R}}, \delta_{21}^{\mathfrak{I}} < \delta_{21}^+ = \delta_\alpha^+ \delta_s^+ (1 + \epsilon)^{\beta-1}.$$

Given p , the number of non-implied bits of the significand of a floating-point value ($p = 23, 52, 112$ for the binary32, binary64, and binary128 types, respectively), and thus $\epsilon = 2^{-p-1}$, the bounds δ_c^- and δ_c^+ from (11), and δ_{21}^- and δ_{21}^+ from (12) were evaluated symbolically by the Wolfram Language script⁴ from the supplement. The expressions $1 - \delta_c^-$, $\delta_c^+ - 1$, $1 - \delta_{21}^-$, and $\delta_{21}^+ - 1$ were then divided by ϵ , approximated to $n = 100$ digits, and rounded away from zero to $d = 8$ decimal places, to calculate by how many ϵ each bound differs from unity. This was repeated for all three aforementioned datatypes, although only for the first two the required correctly rounded functions exist at present, and could have been similarly done for another (e.g., half) precision. Among the three bounds of the same (e.g., δ_c^-) kind, the one with the largest respective multiple of ϵ became the overall worst-case bound of its kind (the lower bound for δ_c in this case). The worst-case bounds were finally collected in (4), what concludes the proof for the standard datatypes. \square

Even tighter error bounds hold when a'_{21} is real or imaginary, as indicated in the proof of Theorem 1 (take $\beta = 1$), and can as well hold for one or more datatypes in the general ($\beta = 2$) case, as shown in (13) for double precision ($p = 52$),

$$\delta_c^- \gtrsim 1 - 6.00000001\epsilon, \quad \delta_c^+ \lesssim 1 + 6.00000000\epsilon, \quad \delta_{21}^- \gtrsim 1 - 19.00000000\epsilon, \quad \delta_{21}^+ \lesssim 1 + 19.00000001\epsilon. \quad (13)$$

4. Numerical testing

Let, for an exact quantity $x \neq 0$, the relative error in an approximation \tilde{x} in the terms of the machine precision ϵ be

$$\rho(\tilde{x}) = (\tilde{x} - x)/(x \cdot \epsilon).$$

If $x = 0$, then $\rho(\tilde{x}) = 0$ if $\tilde{x} = 0$ and $\pm\infty$ otherwise. For a computed Jacobi rotation \tilde{U} , take as a measure of its non-unitarity the difference of its determinant from unity, in the terms of ϵ to keep the measure's values comparable across the spectrum of floating-point datatypes. Since $\tilde{u}_{11} = \tilde{u}_{22} = \cos \tilde{\varphi}$ and $\tilde{u}_{21} = -\tilde{u}_{12} = \cos \tilde{\alpha} \sin \tilde{\varphi} + i \cdot \sin \tilde{\alpha} \sin \tilde{\varphi}$, define

$$\Delta(\tilde{U}) = \rho(\det \tilde{U}) = (\det \tilde{U} - 1)/\epsilon = (\cos^2 \tilde{\varphi} + (\cos \tilde{\alpha} \sin \tilde{\varphi})^2 + (\sin \tilde{\alpha} \sin \tilde{\varphi})^2 - 1)/\epsilon.$$

Each of 33 test runs generated random Hermitian matrices A_k , $1 \leq k \leq 2^{30}$, and computed $\tilde{U}_{k;Z}^{[X]}$, Δ_X^- , Δ_X^+ , $\rho_J^-(\cos \tilde{\varphi})$, $\rho_J^+(\cos \tilde{\varphi})$, $\rho_J^-(\mathfrak{R}\tilde{u}_{21})$, $\rho_J^+(\mathfrak{R}\tilde{u}_{21})$, $\rho_J^-(\mathfrak{I}\tilde{u}_{21})$, and $\rho_J^+(\mathfrak{I}\tilde{u}_{21})$, where $X = J$ stands for ZJAEV2 and $X = L$ for ZLAEV2, and the superscripts $-$ and $+$ denote the minimal and the maximal relative error in a particular quantity in the run; i.e.,

$$\Delta_X^- = \min_k \Delta(\tilde{U}_{k;Z}^{[X]}), \quad \Delta_X^+ = \max_k \Delta(\tilde{U}_{k;Z}^{[X]}), \quad \rho_J^-(\tilde{x}) = \min_k \rho(\tilde{x}_k), \quad \rho_J^+(\tilde{x}) = \max_k \rho(\tilde{x}_k), \quad \tilde{x} \in \{\cos \tilde{\varphi}, \mathfrak{R}\tilde{u}_{21}, \mathfrak{I}\tilde{u}_{21}\}. \quad (14)$$

The error values were obtained in quadruple precision (the MPFR library [8] could have been used for higher precision). For ρ_J^\pm from (14), $\tilde{U}_{k;Q}^{[J]}$ was computed by QJAEV2, using the `_float128` C datatype and the corresponding functions from the GCC's `libquadmath`⁵ library (substituting `hypotq` for `cr_hypot` and `1/sqrtq` for `cr_rsqrtd`, and calculating $\sin \tilde{\varphi} \operatorname{atan} \tilde{\varphi} / \sqrt{\sec^2 \tilde{\varphi}}$), and was taken to be the exact U_k from (1), while the inexact was $\tilde{U}_{k;Z}^{[J]}$.

⁴<https://github.com/venovako/AccJac/blob/master/etc/thm1.wls>, with the command-line arguments p, n, β , and d

⁵Some of its functions might not be correctly rounded, as noted in [12] for `sqrtq`, but this was not checked with the present implementation.

The testing was performed on an Intel Xeon Phi 7210 machine, with the GNU C (gcc) and Fortran (gfortran) compilers, version 13.2.1, on a 64-bit Linux. Random numbers were harvested from /dev/random and discarded if not within $[\mu, v/4]$ by magnitude, with μ being the smallest positive normal value. Each Hermitian matrix was defined by four such random numbers, two for the offdiagonal element and two for the diagonal. The reference LAPACK⁶ routines were compiled from the modernized but semantically faithful sources, because it is not easy to determine exactly how the optimized routines in vendors' libraries compute nor whether or when their behavior will change.

Figure 1 shows the values of $\Delta_{\tilde{X}}^-$ and $\Delta_{\tilde{X}}^+$, between which all $\Delta(\tilde{U}_{k;2}^{[X]})$ in a particular run lie. It can be concluded that in the worst case ZJAEV2 outputs a transformation that is almost twice “closer” to a unitary matrix than the worst-case one from ZLAEV2 as long as the elements of A' are normal (otherwise, see the comments on accuracy in [13, Sect. 5.2]).

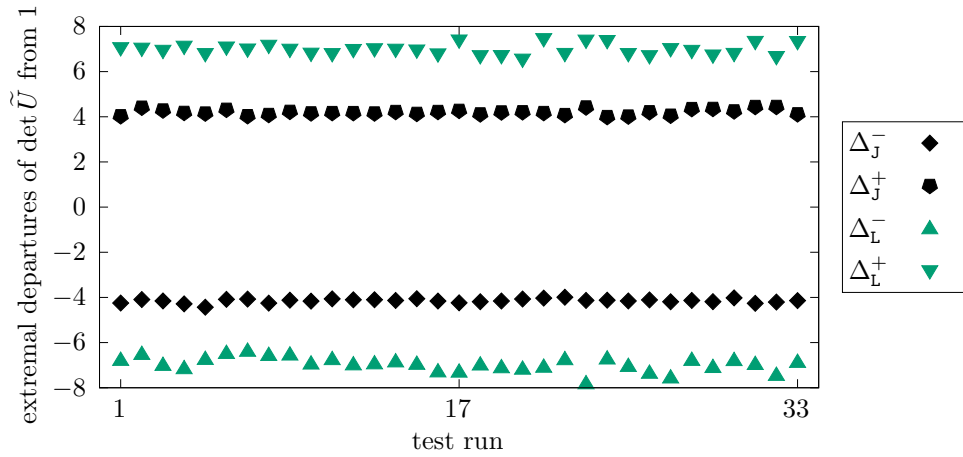


Figure 1: Extremal departures of $\det \tilde{U}$ from unity in multiples of ε , for ZJAEV2 and ZLAEV2.

Figure 2 depicts the observed relative errors in the elements of \tilde{U} computed by ZJAEV2, which fall well within the ranges from (4). This shows that the bounds from Theorem 1 can probably be tightened, what is left for future work.

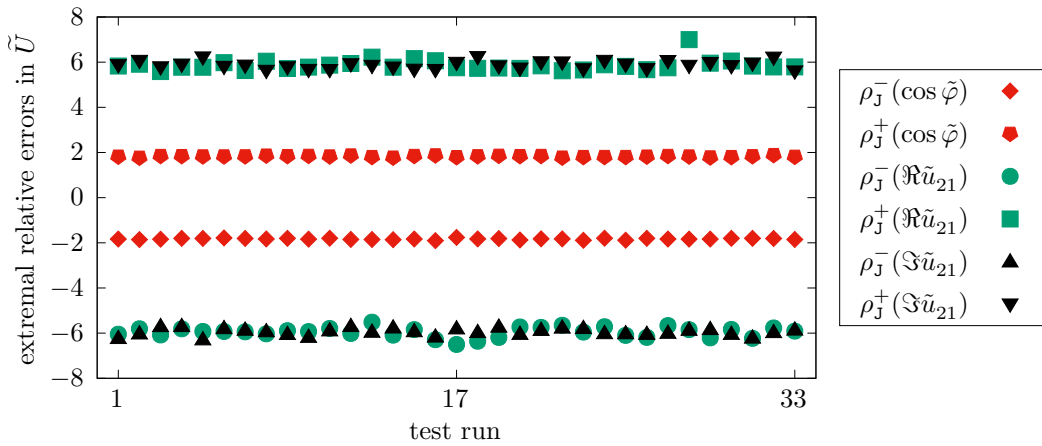


Figure 2: Observed extremal relative errors, in multiples of ε , in the elements of \tilde{U} computed by ZJAEV2.

As a practical application of the proposed algorithm, a Jacobi eigensolver for Hermitian matrices [9] of any order n has been implemented, that annihilates a pair of pivot elements of the largest magnitude in each sequential step by

⁶See <https://github.com/Reference-LAPACK> and <https://github.com/venovako/AccJac/blob/master/src/zlaev2.f90>.

pre-multiplying the pivot rows of the iteration matrix by \widetilde{U}^* and post-multiplying the pivot columns of the iteration matrix and of the eigenvector matrix \mathbf{U} by \widetilde{U} , where \widetilde{U} is computed either by ZJAEV2 or by ZLAEV2. The former variant is called ZJAEVD and the latter ZLAEVD. Figure 3 shows that the final \mathbf{U} is closer to a unitary matrix with ZJAEV2 than with ZLAEV2, for the given Hermitian matrices with eigenvalues i , $1 \leq i \leq n$, where $n = 4j$, $1 \leq j \leq 32$.

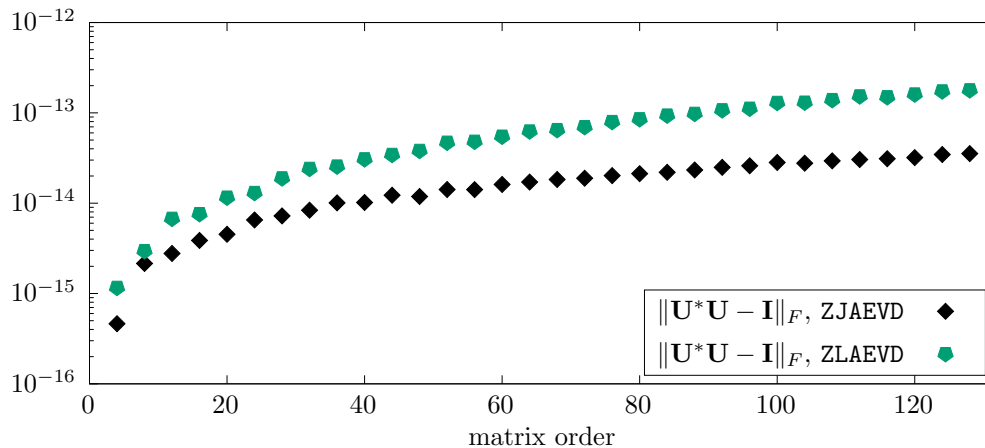


Figure 3: Departures from unitarity of the accumulated eigenvector matrices \mathbf{U} of order n from ZJAEVD and ZLAEVD.

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