An Orthogonal and Symmetric High Relative Accuracy Algorithm for the Symmetric Eigenproblem

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Abstract (1)

- **INPUT:** Factors X and D of a decomposition $A = XDX^T$ of a symmetric matrix, where X is well-conditioned and D is diagonal, perhaps indefinite.
- We run the standard Jacobi algorithm to compute eigenvalues and eigenvectors but applying the rotations only on X.
- **BASIC STEP:** Compute a plane Jacobi rotation R such that $(R^T AR)_{ij} = 0$, for some $i \neq j$, then

$$XDX^T \longrightarrow (R^T X)D(R^T X)^T.$$

- From a decomposition of A we obtain a decomposition of $R^T AR$. The matrix A is never formed.

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- Algorithm stops when the off diagonal part of $A_f = X_f D X_f^T$ is small enough.
- **OUTPUT:**
  1. The eigenvalues of A are the computed diagonal entries of $X_f D X_f^T$.
  2. Eigenvectors are the columns of $R_1 R_2 \cdots R_f$
- Let ϵ be the unit roundoff. The **errors** in computed eigenvalues and eigenvectors are

$$\frac{|\hat{\lambda}_i - \lambda_i|}{|\lambda_i|} \leq O(\epsilon\kappa(X)) \quad \text{and} \quad \theta(v_i, \hat{v}_i) \leq \frac{O(\epsilon\kappa(X))}{\min_{j \neq i} \left| \frac{\lambda_i - \lambda_j}{\lambda_i} \right|} \quad \text{for all} \quad i,$$

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- This implicit Jacobi algorithm is mathematically equivalent to the standard one.

- This is the first algorithm that
  1. computes accurate eigenvalues an eigenvectors of symmetric (indefinite) matrices,
  2. respects and preserves the symmetry of the problem, and
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Outline

1. **Why is the Implicit Jacobi algorithm interesting?**
2. Why does Implicit Jacobi compute accurate eigenvalues and eigenvectors?
3. The rigorous roundoff error result
4. Numerical Experiments
5. Conclusions

Accurate eigencomputations for symmetric matrices

- In the last twenty years an intensive research effort has been made to compute eigenvalues and eigenvectors of $n \times n$ symmetric matrices **to high relative accuracy (hra)**.
- Given $A = A^T \in \mathbb{R}^{n \times n}$, we will say that an algorithm computes **all** its **eigenvalues and eigenvectors** to **hra** if the computed eigenvalues and eigenvectors satisfy

$$|\widehat{\lambda}_i - \lambda_i| = O(\epsilon)\,|\lambda_i| \quad \text{and} \quad \theta(v_i, \hat{v}_i) \leq \frac{O(\epsilon)}{\min\limits_{j \neq i} \left| \frac{\lambda_i - \lambda_j}{\lambda_i} \right|} \quad \text{for all} \quad i$$

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HRA is not obtained from standard algorithms

EXAMPLE: Symmetric INDEFINITE 100×100 Cauchy matrix A

$$a_{ij} = \frac{1}{x_i + x_j}, \quad \text{with} \quad \begin{cases} x_i = i - 0.5 \;\; for \;\; i = 1:99 \\ x_{100} = -99.5 \end{cases}$$

- $\kappa(A) = 3.5 \cdot 10^{147}$
- **Errors in accurate algorithm (Factorization + Imp. Jacobi)** compared to 200-decimal digits MATLAB's `eig` command

$$\max_i \frac{|\hat{\lambda}_i - \lambda_i|}{|\lambda_i|} = 1.2 \cdot 10^{-13} \quad \text{and} \quad \max_i \|\hat{v}_i - v_i\|_2 = 5.7 \cdot 10^{-14}.$$

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Key unifying idea: Rank Revealing Decompositions (RRD) (Demmel et al. 1999)

We restrict to symmetric RRDs of $A = A^T \in \mathbb{R}^{n \times n}$.

- Compute first an **accurate** RRD

$$A = XDX^T,$$

X is **well-conditioned** and D is **diagonal and nonsingular**.

Remark: **Accuracy** is only possible for special types of matrices through structured implementations of Gaussian elimination with complete pivoting (**GECP**), or variations of GECP.

- Compute eigenvalues and eigenvectors with **hra** from the **factors** X **and** D with a **Jacobi-type** method.

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A symmetric RRD determines accurately its eigenvalues and eigenvectors (I): multiplicative perturbations

Theorem

Let $A = A^T \in \mathbb{R}^{n \times n}$ *and* $A = XDX^T$ *be an RRD of* A*, where* $X \in \mathbb{R}^{n \times r}$*,* $n \geq r$*, and* $D = \mathrm{diag}(d_1, \ldots, d_r) \in \mathbb{R}^{r \times r}$*. Let* $\widehat{X}$ *and* $\widehat{D} = \mathrm{diag}(\widehat{d}_1, \ldots, \widehat{d}_r)$ *be perturbations of* X *and* D*, respectively, that satisfy*

$$\frac{\|\widehat{X} - X\|_2}{\|X\|_2} \leq \delta \quad \text{and} \quad \frac{|\widehat{d}_i - d_i|}{|d_i|} \leq \delta \quad \text{for } i = 1, \ldots, r,$$

where $\delta < 1$*. Then*

$$\widehat{X}\widehat{D}\widehat{X}^T = (I + F)A(I + F)^T,$$

with $\|F\|_2 \leq (2\delta + \delta^2)\kappa(X)$*.*

A symmetric RRD determines accurately its eigenvalues and eigenvectors (II): multiplicative perturbation theory

Theorem (Eisenstat, Ipsen (1995) and R. C. Li (2000))

Let $A = A^T \in \mathbb{R}^{n\times n}$ *and* $\widetilde{A} = (I+F)A(I+F)^T \in \mathbb{R}^{n\times n}$, *where* $\|F\|_2 < 1$. *Let* $\lambda_1 \geq \cdots \geq \lambda_n$ *and* $\widetilde{\lambda}_1 \geq \cdots \geq \widetilde{\lambda}_n$ *be, respectively, the eigenvalues of* A *and* $\widetilde{A}$. *Then*

- $$|\widetilde{\lambda}_i - \lambda_i| \leq (2\,\|F\|_2 + \|F\|_2^2)\; |\lambda_i|, \quad \text{for } i = 1, \ldots, n$$
- *For the corresponding eigenvectors,* v_i *and* $\widetilde{v}_i$,

$$\frac{1}{2}\sin\, 2\theta(v_i, \widetilde{v}_i) \leq \frac{2}{\displaystyle\min_{j\neq i}\left|\frac{\lambda_i - \lambda_j}{\lambda_i}\right|} \cdot \frac{1+\|F\|_2}{1-\|F\|_2}\,(2\,\|F\|_2 + \|F\|_2^2)$$

Accurate e-values and e-vectors from X and D (1): Positive definite case

Algorithm (Demmel, Veselić (1992))

Given RRD $A = XDX^T$ **positive definite**:

1. Compute SVD of
$$X\sqrt{D} = U\Sigma V^T$$
with **one-sided Jacobi on the left.**
2. The spectral decomposition is
$$A = X\sqrt{D}(X\sqrt{D})^T = U\Sigma^2 U^T.$$

Accurate e-values and e-vectors from X and D (2): General case

Two algorithms have been proposed for the **indefinite** case. They work well in practice, **they both have shortcomings**:

- **One-sided Hyperbolic Jacobi** (Slapničar, Veselić (1992,2003)).
  1. It uses hyperbolic transformations (symmetric matrices are diagonalizable by orthogonal similarity).
  2. The error bounds implied by the use of hyperbolic rotations are not rigorously bounded.
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Outline

Notation for Jacobi rotation ($c^2 + s^2 = 1$)

$$
R(i,j,c,s) \quad = \quad
\begin{array}{c}
\\ \\ i \\ \\ j \\ \\ \\
\end{array}
\begin{array}{c}
\begin{array}{ccccccc}
 & & i & & j & & \\
\end{array}
\\
\left[
\begin{array}{ccccccc}
1 & & & & & & \\
 & \ddots & & & & & \\
 & & c & & -s & & \\
 & & & \ddots & & & \\
 & & s & & c & & \\
 & & & & & \ddots & \\
 & & & & & & 1
\end{array}
\right]
\end{array}
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Implicit Jacobi for square factors

INPUT: $X \in \mathbb{R}^{n\times n}$ nonsingular and $D \in \mathbb{R}^{n\times n}$ diag. and nonsingular
OUTPUT: e-values, λ_i, and matrix of e-vectors, U, of $A = XDX^T$

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Jacobi rotations on X preserve accurate e-values and e-vectors

Lemma (Small multiplicative backward errors of Jacobi rotations)

Let R_i be **exact** *Jacobi rotations and $\widehat{R}_i$ their floating point approximations. Then*

1. $$\widehat{X}_N \equiv \mathtt{fl}(\widehat{R}_N^T \cdots \widehat{R}_1^T X) = (I+F) R_N^T \cdots R_1^T X,$$
   where $\|F\|_2 = O(N\,\epsilon\,\kappa(X))$, and
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Proof of Rounding Errors in Jacobi rotations

Proof.

Let $U^T = R_N^T \cdots R_1^T$.

- $\mathtt{fl}(\widehat{R}_N^T \cdots \widehat{R}_1^T X) = R_N^T \cdots R_1^T (X + E)$ with $\|E\|_2 = O(N\epsilon\|X\|_2)$.
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Errors on diagonal entries of almost diagonal RRDs (I)

Given $X \in \mathbb{R}^{n\times n}$ nonsingular and $D = \text{diag}(d_1, \ldots, d_n) \in \mathbb{R}^{n\times n}$ diagonal and nonsingular:

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Errors on diagonal entries of almost diagonal RRDs (II): EXAMPLE

INPUT: $\kappa(X) = 7.21$

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RUNNING IMPLICIT JACOBI UNTIL CONVERGENCE

$$X_f D X_f^T = \begin{bmatrix} 4.79 \cdot 10^{-48} & 5.35 \cdot 10^{-1} & 2.04 \cdot 10^{-47} \\ 3.8 \cdot 10^{-1} & 4.03 \cdot 10^{-2} & 1.64 \\ 2.42 & 1.65 & 5.67 \cdot 10^{-1} \end{bmatrix} \begin{bmatrix} 10^{50} & & \\ & 1 & \\ & & -10^{50} \end{bmatrix} X_f^T$$

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Errors on diagonal entries of almost diagonal RRDs (III): THE MAIN THEOREM

Theorem

Let $X, D \in \mathbb{R}^{n\times n}$ *be nonsingular and* $D = \mathrm{diag}(d_1, \ldots, d_n)$ *be diagonal. If the matrix* $A \equiv XDX^T$ *satisfies* $a_{ii} = \sum_{k=1}^{n} x_{ik}^2 d_k \neq 0$ *for all* i*, and*

$$\frac{|a_{ij}|}{\sqrt{|a_{ii}a_{jj}|}} \leq \delta, \quad \textit{for all } \; i \neq j, \quad \textit{where } \delta \leq \frac{1}{5n}, \textit{ then}$$

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Errors on diagonal entries of almost diagonal RRDs (IV): Corollary

Corollary

If $A = XDX^T$ *satisfies the stopping criterion then*

$$\left| \frac{\mathtt{fl}(a_{ii}) - a_{ii}}{a_{ii}} \right| \leq (n+1)\,\epsilon\,\kappa(X) + O(\kappa(X)\,\epsilon^2)$$

Key idea in the proof of THE MAIN THEOREM

Proof by contradiction

- $A = XDX^T$ is close to diagonal, then its diagonal entries are close to its eigenvalues.
- Assume

$$\frac{\sum_{k=1}^{n} x_{ik}^2 |d_k|}{|a_{ii}|} = \frac{\sum_{k=1}^{n} x_{ik}^2 |d_k|}{|\sum_{k=1}^{n} x_{ik}^2 d_k|} >> \kappa(X)$$

- Then there are perturbations $\widetilde{d}_k = d_k(1 + \delta_k)$, $|\delta_k| < \beta << 1$ such that $(X\widetilde{D}X^T)_{ii} = \sum_{k=1}^{n} x_{ik}^2 \widetilde{d}_k$, satisfy

$$\frac{|a_{ii} - (X\widetilde{D}X^T)_{ii}|}{|a_{ii}|} >> \beta\kappa(X).$$

- This is in contradiction with an RRD determining accurately its eigenvalues.

Key idea in the proof of THE MAIN THEOREM

Proof by contradiction

- $A = XDX^T$ is close to diagonal, then its diagonal entries are close to its eigenvalues.
- Assume

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Outline

Implicit Jacobi is multiplicative backward stable

Theorem

Let N *be the* **number of rotations** *applied by implicit Jacobi on* $A = XDX^T$ *until convergence, and* $\widehat{\Lambda}$ *and* $\widehat{U}$ *be the computed matrices of eigenvalues and eigenvectors. Then there exists an* **exact orthogonal** *matrix* $U \in \mathbb{R}^{n\times n}$ *such that*

$$U\widehat{\Lambda}U^T = (I+E)\, XDX^T\, (I+E)^T,$$

with

$$\|E\|_F = O(\epsilon\, N\, \kappa(X)) \quad \textit{and} \quad \|\widehat{U} - U\|_F = O(N\,\epsilon).$$

Corollary (Forward errors in e-values and e-vectors)

$$\frac{|\hat{\lambda}_i - \lambda_i|}{|\lambda_i|} \le O(\epsilon\, N\, \kappa(X)) \quad \text{and} \quad \theta(v_i, \hat{v}_i) \le \frac{O(\epsilon\, N\, \kappa(X))}{\min_{j\neq i} \left|\frac{\lambda_i - \lambda_j}{\lambda_i}\right|} \quad \textit{for all} \quad i,$$

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Technical comments

To establish the backward error result, we need to prove that

- The stopping criterion in finite arithmetic on $A = X_f D X_f^T$ gives *exact* information, i.e.,

$$\mathtt{fl}\left(\frac{|a_{ij}|}{\sqrt{|a_{ii}a_{jj}|}}\right) \leq \epsilon\,\kappa(X) \implies \frac{|a_{ij}|}{\sqrt{|a_{ii}a_{jj}|}} \leq n\,\epsilon\,\kappa(X) + O(\epsilon^2)$$

  for all $i \neq j$, which is the case if there is no cancellation in $fl(a_{ii})$.

- The stopping criterion introduces small multiplicative backward errors, i.e.,

$$\mathrm{diag}(\mathtt{fl}(a_{11}), \ldots, \mathtt{fl}(a_{nn})) = (I+F) X_f D X_f^T (I+F)^T,$$

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Outline

Numerical Experiments

- Thousands of numerical experiments confirm the high relative accuracy that we have rigorously proven.
- Traditional Jacobi is **slow**, then Implicit Jacobi is **slow**.
- **Speed is not our main issue**, but we have compared the number of sweeps performed by Implicit Jacobi with respect other high relative accuracy algorithms:
  1. One sided Hyperbolic Jacobi (Slapničar-Veselić): **not** rigorous bounds.
  2. SSVD-I (D-Molera-Moro): **not** rigorous bounds.
  3. SSVD-r (D-Molera-Moro): rigorous bounds.
- We have used `gallery('randsvd',...)` by N. Higham in MATLAB to generate random RRDs with X well-conditioned and D indefinite and **extremely** ill-conditioned.

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Number of sweeps: Increasing $\kappa(D)$ (I)

In all of these tests $\kappa(X) = 30$ and X, D are 100×100.

D has one entry with magnitude 1 and the rest $1/\kappa(D)$

$\kappa(D)$	Imp. Jac.	Hyp. Jac.	SSVD-l	SSVD-r
10^{10}	10	10.8	10	13
10^{30}	10	10.6	9.8	13.2
10^{50}	10.8	10.8	10	14
10^{70}	11	11	10.2	13.6
10^{90}	10.8	10.6	10	13.8
10^{110}	11	10.4	10	14.8

Number of sweeps: Increasing $\kappa(D)$ (II)

In all of these tests $\kappa(X) = 30$ and X, D are 100×100.

D has entries with magnitudes geometrically distributed

$\kappa(D)$	Imp. Jac.	Hyp. Jac.	SSVD-l	SSVD-r
10^{10}	16	9	6.2	27.2
10^{30}	24.8	9	4.8	39.6
10^{50}	32.4	9	4.4	47.2
10^{70}	35.8	9.4	4.4	52.6
10^{90}	40	9	4	57
10^{110}	43.2	9	3	59.6

$$|d_i| = \kappa(D)^{\frac{i-1}{n-1}}, \quad i = 1, \ldots, n$$

Numerical Experiments: Conclusions

- The comparison of the performance of the available high relative accuracy algorithms for symmetric indefinite RRDs depends heavily on the distribution of the eigenvalues
- The new Implicit Jacobi is the fastest algorithm with guaranteed errors bounds (the other one is SSVD-r).
- The new Implicit Jacobi may be considerably slower than Hyperbolic Jacobi and SSVD-l, both with errors not rigorously bounded.
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Conclusions

- The implicit Jacobi algorithm on symmetric rank revealing factorizations

$$A = XDX^T$$

is the first algorithm that:

1. computes the eigenvalues and eigenvectors of A to high relative accuracy,
2. preserves the symmetry, and
3. uses only orthogonal transformations.

- In addition, the error bounds are rigorously proven, and are the **best possible ones** from the sensitivity of the problem.
- The implicit Jacobi algorithm is **very simple and natural**.
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