

Implicit Standard Jacobi Gives High Relative Accuracy on Rank Revealing Decompositions

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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

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

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- **Algorithm stops** when the **off diagonal part** of $A_f = X_f D X_f^T$ is small enough.
- **OUTPUT:**
 - The eigenvalues of A are the **computed diagonal entries** of $X_f D X_f^T$.
 - 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

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

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- This implicit Jacobi algorithm is mathematically equivalent to the standard one.
- This is the first algorithm that
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- 3 The rigorous roundoff error result
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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

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and, in addition,

- HRA is only possible for **special types of matrices**.

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HRA is not obtained from standard algorithms

EXAMPLE: Symmetric INDEFINITE 100×100 Cauchy matrix A

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

- $\kappa(A) = 3.5 \cdot 10^{147}$
- **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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- Improved Convergence analysis of Jacobi Algorithms (Drmač, Hari, Matejas).
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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 **hrra** from the **factors** X and D with a **Jacobi-type** method.

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Classes of symmetric matrices with accurate RRDs algorithms

- 1 Well Scaled Symmetric Positive Definite (Demmel and Veselić).
- 2 Scaled diagonally dominant (Barlow and Demmel)
- 3 Symmetric Cauchy and Scaled-Cauchy (D and Koev).
- 4 Symmetric Vandermonde (D and Koev).
- 5 Symmetric Totally nonnegative (D and Koev).
- 6 Symmetric Graded Matrices (D and Molera).
- 7 Symmetric DSTU and TSC (Peláez and Moro).
- 8 Symmetric diagonally dominant M-matrices (Demmel and Koev), (Peña).
- 9 Symmetric diagonally dominant (Ye)....

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

Theorem (D., Koev (2006))

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 $D = \text{diag}(d_1, \dots, d_r) \in \mathbb{R}^{r \times r}$. Let \hat{X} and $\hat{D} = \text{diag}(\hat{d}_1, \dots, \hat{d}_r)$ be perturbations of X and D , respectively, that satisfy

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

where $\delta < 1$. Then

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

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



$$|\tilde{\lambda}_i - \lambda_i| \leq (2\|F\|_2 + \|F\|_2^2) |\lambda_i|, \quad \text{for } i = 1, \dots, n$$

- For the corresponding eigenvectors, v_i and \tilde{v}_i ,

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

A symmetric RRD determines accurately its eigenvalues and eigenvectors (III): Final Result

Corollary (D., Koev (2006))

Let $A = A^T = XDX^T$ be an RRD. Let \hat{X} and $\hat{D} = \text{diag}(\hat{d}_1, \dots, \hat{d}_r)$ be perturbations of X and D such that

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

where $\delta < 1$. Then, for all i , the e-values, $\hat{\lambda}_i$, and e-vectors, \hat{v}_i , of $\hat{X}\hat{D}\hat{X}^T$ satisfy

$$\left| \frac{\lambda_i - \hat{\lambda}_i}{\lambda_i} \right| \leq \kappa(X) \left(4\delta + 2\delta^2 + \kappa(X) (2\delta + \delta^2)^2 \right) \approx 4\delta \kappa(X) + O(\delta^2)$$

$$\frac{1}{2} \sin 2\theta(v_i, \hat{v}_i) \leq \frac{8\delta \kappa(X) + O(\delta^2)}{\min_{j \neq i} \left| \frac{\lambda_i - \lambda_j}{\lambda_i} \right|}$$

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

$$A = X\sqrt{D}(X\sqrt{D})^T = U\Sigma^2U^T.$$

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

Comments on Algorithm by Demmel and Veselić

Fully satisfactory algorithm because:

- The symmetry is preserved.
- Only orthogonal transformations are used.

Remarks

- If the Jacobi rotations are applied on $X\sqrt{D}$ from the **right** then the algorithm is faster but it is not possible to prove that the error bounds are small.
- If the rotations are applied on $X\sqrt{D}$ on the **left** then it is mathematically equivalent to apply the standard Jacobi algorithm to $XDXT$.

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Accurate e-values and e-vectors from X and D (3): General case

Hyperbolic Algorithm (Veselić (1993), Slapničar (1992, 2003))

Given RRD $A = XDX^T$ possibly indefinite:

- 1 Write

$$A = X\sqrt{|D|} J \left(X\sqrt{|D|} \right)^T,$$

with $J = \text{diag}\{\pm 1\}$.

- 2 Compute **Hyperbolic SVD** of

$$X\sqrt{|D|} = U\Sigma H^T \text{ where } U^T U = I, H^T J H = J$$

with **hyperbolic one-sided Jacobi** on the right.

- 3 The spectral decomposition is

$$A = U (\Sigma^2 J) U^T$$

Comments on Hyperbolic Algorithm

Not fully satisfactory algorithm because:

- **Hyperbolic rotations are used.**
- Symmetric matrices are diagonalizable by orthogonal similarity.
- It is not possible to prove that the error bounds are small.
- It works well in practice.

Accurate e-values and e-vectors from X and D (5): General case

SSVD Algorithm (D, Molera, Moro (2003), D, Molera (2008))

Given RRD $A = XDX^T$ possibly indefinite:

- 1 Compute SVD of $A = U\Sigma V^T$ from RRD using a **nonsymmetric** algorithm by Demmel et al. (1999) that uses one-sided Jacobi.
- 2 Compute eigenvalues and eigenvectors from SVD by using $A = A^T$.

Comments on SSVD Algorithm

Not fully satisfactory algorithm because:

- The symmetry is not respected. (It allows us flexibility by using nonsymmetric RRDs).
- HRA error bounds are perfect for eigenvalues and eigenvectors,
- but to get accurate e-vectors requires a delicate process.

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To prove that the standard Jacobi algorithm **implicitly** applied on the factor X of a given RRD

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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 Singular matrices $A = XDX^T$
- 5 Numerical Experiments
- 6 Conclusions

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 $A = XDX^T$

$U = I_n$

repeat

for $i < j$

compute a_{ii}, a_{ij}, a_{jj} of $A = XDX^T$ and $T = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$, such that

$$T^T \begin{bmatrix} a_{ii} & a_{ij} \\ a_{ij} & a_{jj} \end{bmatrix} T = \begin{bmatrix} \mu_1 & \\ & \mu_2 \end{bmatrix}$$

$$X = R(i, j, c, s)^T X$$

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until convergence $\left(\frac{|a_{ij}|}{\sqrt{|a_{ii}a_{jj}|}} \leq \text{tol} = O(\epsilon) \text{ for all } i > j \right)$

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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

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$$\widehat{X}_N \equiv \text{fl}(\widehat{R}_N^T \cdots \widehat{R}_1^T X) = (I + F)R_N^T \cdots R_1^T X,$$

where $\|F\|_2 = O(N \epsilon \kappa(X))$, and

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$$\widehat{X}_N D \widehat{X}_N^T = (I + F)(R_1 \cdots R_N)^T X D X^T (R_1 \cdots R_N)(I + F)^T$$

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Proof of Rounding Errors in Jacobi rotations

Proof.

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

- $\mathbf{fl}(\widehat{R}_N^T \cdots \widehat{R}_1^T X) = R_N^T \cdots R_1^T (X + E)$ with $\|E\|_2 = O(N\epsilon\|X\|_2)$.
- $\mathbf{fl}(\widehat{R}_N^T \cdots \widehat{R}_1^T X) = U^T (I + EX^{-1})X = (I + U^T EX^{-1}U)U^T X$.
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Errors on diagonal entries of almost diagonal RRDs (I)

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

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$$\left| \frac{\text{fl}(a_{ii}) - a_{ii}}{a_{ii}} \right| \leq \frac{(n+1)\epsilon}{1 - (n+1)\epsilon} \frac{\sum_{k=1}^n x_{ik}^2 |d_k|}{\left| \sum_{k=1}^n x_{ik}^2 d_k \right|}$$

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

INPUT: $\kappa(X) = 7.21$

$$XDX^T = \begin{bmatrix} 1 & 1 & 1 \\ -1 & -1 & 1 \\ 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} 10^{50} & & \\ & 1 & \\ & & -10^{50} \end{bmatrix} X^T$$

RUNNING IMPLICIT JACOBI UNTIL CONVERGENCE

$$\begin{aligned} X_f D X_f^T &= \begin{bmatrix} 4.79 \cdot 10^{-48} & 5.35 \cdot 10^{-1} & 2.04 \cdot 10^{-47} \\ 3.8 \cdot 10^{-1} & 4.03 \cdot 10^{-2} & 1.64 \\ 2.42 & 1.65 & 5.67 \cdot 10^{-1} \end{bmatrix} \begin{bmatrix} 10^{50} & & \\ & 1 & \\ & & -10^{50} \end{bmatrix} X_f^T \\ &= \begin{bmatrix} 2.86 \cdot 10^{-1} & -3.16 \cdot 10^3 & 2.39 \cdot 10^{-3} \\ -3.16 \cdot 10^3 & -2.53 \cdot 10^{50} & 1.04 \cdot 10^{34} \\ 2.39 \cdot 10^{-3} & 2.08 \cdot 10^{34} & 5.53 \cdot 10^{50} \end{bmatrix} \\ &= (4.79 \cdot 10^{-48})^2 \times 10^{50} + (5.35 \cdot 10^{-1})^2 \times 1 + (2.04 \cdot 10^{-47})^2 \times (-10^{50}) \\ &= 2.29 \cdot 10^{-45} + 2.86 \cdot 10^{-1} - 4.18 \cdot 10^{-44} \end{aligned}$$

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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 $D = \text{diag}(d_1, \dots, d_n)$ 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

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

$$\frac{\sum_{k=1}^n x_{ik}^2 |d_k|}{|a_{ii}|} \leq \frac{\kappa(X)}{1 - 2n\delta} \left(1 + \frac{2n^{5/2}\delta}{1 - n\delta} + n^2 \left(\frac{n\delta}{1 - n\delta} \right)^2 \right), \quad i = 1, \dots, n.$$

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

Corollary

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

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

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

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

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

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

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

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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 $\hat{\Lambda}$ and \hat{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

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

with

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

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

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

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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.,

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

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

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

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

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Rectangular RRDs

- So far we have considered $A = XDX^T$ with **square and nonsingular** X and D , which excludes singular matrices A .
- If we insist on X being nonsingular, then A is singular if and only if D is singular.
- The zero eigenvalues of A are revealed by the zero diagonal entries of D
- Discarding these entries we get

$$A = XDX^T \in \mathbb{R}^{n \times n} \quad \text{where} \quad X \in \mathbb{R}^{n \times r} \quad D \in \mathbb{R}^{r \times r},$$

with $n > r$, X with full rank, and D nonsingular.

- Implicit Jacobi converges to an $n \times n$ diagonal matrix with zero entries and cancellation is unavoidable.

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Algorithm for rectangular RRD $A = XDX^T$

$$A = XDX^T \in \mathbb{R}^{n \times n} \quad \text{with} \quad X \in \mathbb{R}^{n \times r}, \quad D \in \mathbb{R}^{r \times r},$$

- 1 Compute full QR factorization of X

$$Q \begin{bmatrix} R \\ 0 \end{bmatrix} = X \quad \text{where} \quad Q \in \mathbb{R}^{n \times n}, \quad R \in \mathbb{R}^{r \times r}$$

- 2 Note that

$$A = Q \begin{bmatrix} RDR^T & 0 \\ 0 & 0 \end{bmatrix} Q^T$$

- 3 Apply Implicit Jacobi on RDR^T (**with factors square and nonsingular**) to compute

- 1 Nonzero eigenvalues of A : $\lambda_1, \dots, \lambda_r$.
- 2 Eigenvector matrix of RDR^T : U_R

- 4 $[Q(:, 1:r)U_R \mid Q(:, r+1:n)]$ is the eigenvector matrix of A .

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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-l** (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-I	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

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

Number of sweeps: Increasing the dimension of the RRD (I)

In all of these tests $\kappa(X) = 100$, $\kappa(D) = 10^{40}$, and X, D are $n \times n$.

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

n	Imp. Jac.	Hyp. Jac.	SSVD-l	SSVD-r
100	11	11.4	10.2	15.8
500	13	13.4	14	18
1000	13	14	15	19
2000	14	15	16	20

Number of sweeps: Increasing the dimension of the RRD (II)

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n	Imp. Jac.	Hyp. Jac.	SSVD-l	SSVD-r
100	28.8	10	4.6	44.6
500	46	11	6	87
1000	58	11	7	> 100
2000	68	11	7	> 100

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-I, 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**.
 - The implicit Jacobi algorithm is **backward stable** in a strong **multiplicative** sense.
 - More research to speed up the algorithm is needed.

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