

# Implicit Jacobi Algorithm for the SVD with High Relative Accuracy

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# Outline

- 1 Objectives of this work
- 2 Jacobi methods for the SVD
- 3 Implicit Jacobi SVD
- 4 Error Analysis
- 5 Numerical Experiments
- 6 Conclusions



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  - ④ Alg. 3.2, Two applications of one-sided Jacobi. It does not have the previous factor.
- The implicit Jacobi SVD algorithm gets hra, starting from an RRD, with error bounds that reflect the sensitivity of the problem, with only one run of Jacobi.





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- Errors in MATLAB's svd function: double precision,  $u \approx 10^{-16}$ , compared to “exact” 200-decimal digits,

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- Errors in accurate algorithm (Factorization + Imp. SVD Jacobi)

$$\max_i \frac{|\hat{\sigma}_i - \sigma_i|}{|\sigma_i|} = 2.9 \cdot 10^{-14} \quad \text{and} \quad \max_i \|\hat{v}_i - v_i\|_2 = 6.1 \cdot 10^{-13}$$



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## Accurate Rank Revealing Decomposition

- Given  $A \in \mathbb{R}^{m \times n}$ , with  $\text{rank}(A) = r$ ,

$$A = XDY^T,$$

with  $X \in \mathbb{R}^{m \times r}$ ,  $Y \in \mathbb{R}^{n \times r}$  and  $D \in \mathbb{R}^{r \times r}$  diagonal invertible, it is called a **Rank Revealing Decomposition (RRD)** of  $A$  if

$$\kappa(X), \kappa(Y) \gtrsim 1 \quad \text{and} \quad \kappa(D) \approx \kappa(A).$$



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- We say that an RRD,  $A = XDY^T$ , is **accurate** if the computed factors ( $u$ , the unit roundoff)  $\hat{X}$ ,  $\hat{Y}$  and  $\hat{D}$  obey

$$\frac{\|\hat{X} - X\|}{\|X\|} = O(u), \quad \frac{\|\hat{Y} - Y\|}{\|Y\|} = O(u) \quad \text{and} \quad \frac{|\hat{D} - D|}{|D|} = O(u)$$



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Accurate RRDs are only possible for special types of matrices through structured implementations of Gaussian elimination with complete pivoting (**GECP**), or variations of GECP.

- (Scaled-)Cauchy, (Polynomial) Vandermonde (DFT + GECP). [Demmel, Koev]
- Diagonally Dominant M-Matrices. [Demmel and Koev, Peña]
- Polynomial Vandermonde. [Demmel and Koev]
- Well Scaled Positive Definite. [Demmel and Veselić]
- Acyclic Matrices (include bidiagonal). [Demmel and Gragg]
- Diagonally Dominant. [Qiang Ye, Dopico and Koev]
- DSTU. [Demmel]
- Graded matrices, Total signed compound, [Demmel et al.]
- Positive definite [Demmel, Veselić, Mathias]
- Symmetric and diagonally scaled Cauchy, Vandermonde [Dopico, Koev]
- Symmetric DSTU and TSC [Peláez, Moro]





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$$X = Q_X \begin{bmatrix} X_0 \\ 0 \end{bmatrix} \quad Y = Q_Y \begin{bmatrix} Y_0 \\ 0 \end{bmatrix}$$

$X_0, Y_0^T \in \mathbb{R}^{r \times r}$  upper triangular invertible matrices  
 $D \in \mathbb{R}^{r \times r}$  diagonal and invertible.



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- Compute

$$A_{(i,j)} = \sum_{k=1}^r (X_0)_{(i,k)} D_{(k,k)} (Y_0)_{(j,k)}$$

- Apply the rotations only on

$$X_0 \rightarrow J X_0, \quad \text{and} \quad Y_0^T \rightarrow Y_0^T \bar{J}$$



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$$\sigma_i = \sum_{k=1}^r (X_f)_{(i,k)} D_{(k,k)} (Y_f)_{(i,k)}$$

$$(J_M \dots J_2 J_1 X_0) D (Y_0^T \bar{J}_1 \bar{J}_2 \dots \bar{J}_N) = \Sigma$$

and

$$U_0 = J_1^T J_2^T \dots J_M^T \quad V_0 = \bar{J}_1 \bar{J}_2 \dots \bar{J}_N$$



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$$\Sigma = \text{diag}[\sigma_1, \dots, \sigma_r]$$

$$U = Q_X \begin{bmatrix} U_0 & 0 \\ 0 & \mathbb{I}_{m-r} \end{bmatrix}, \quad V = Q_Y \begin{bmatrix} V_0 & 0 \\ 0 & \mathbb{I}_{n-r} \end{bmatrix}$$



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The **errors** in the computed singular values and singular vectors are,

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Depend on  $\bar{\kappa} = \max\{\kappa(X), \kappa(Y)\}$ , independent of  $\kappa(A), \kappa(D)$ .



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## Implicit Jacobi SVD for square factors $A = XDY^T$

input:  $X, Y \in \mathbb{R}^{n \times n}$  and  $D \in \mathbb{R}^{n \times n}$  diag., all nonsingular

output: sing-values,  $\sigma_i$ , and matrices of sing-vectors,  $U, V$

$$U = V = I_n$$

repeat

for  $i, j$

compute  $a_{ii}, a_{ij}, a_{ji}, a_{jj}$  of  $A = XDY^T$  and  $J, \bar{J}$  Jacobi rotations:

$$J \begin{bmatrix} a_{ii} & a_{ij} \\ a_{ji} & a_{jj} \end{bmatrix} \bar{J} = \begin{bmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{bmatrix}$$

$$X = JX, \quad Y^T = Y^T \bar{J}$$

$$U = UJ^T, \quad V = V\bar{J}$$

endfor

until convergence  $\frac{|a_{ij}|}{\sqrt{|a_{ii}a_{jj}|}} \leq \text{tol}$  for all  $i, j$

$$\text{tol} = O(u)$$

compute  $\sigma_k = a_{kk}$  for  $k = 1, 2, \dots, n$ .





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Theorem (Eisenstat-Ipsen 1995, R-C Li 1998)

Let  $\tilde{A}, A \in \mathbb{C}^{n \times n}$  and

$$\tilde{A} = (I + E)A(I + F).$$

*Singular values:*

$$|\tilde{\sigma}_i - \sigma_i| \leq (2\eta + \eta^2)\sigma_i \quad 1 \leq i \leq n$$

$$\eta = \max\{\|E\|_2, \|F\|_2\} < 1, \eta' = 2\eta + \eta^2$$



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- 2 Multiplicative perturbation theory

Theorem (Eisenstat-Ipsen 1995, R-C Li 1998)

Let  $\tilde{A}, A \in \mathbb{C}^{n \times n}$  and

$$\tilde{A} = (I + E)A(I + F).$$

Singular vectors:

$$\max\{\theta(u_i, \hat{u}_i), \theta(v_i, \hat{v}_i)\} \leq 2\sqrt{n} \left[ \eta + \frac{\eta'}{1 - \eta} \frac{1}{\min_{j \neq i} \left| \frac{\sigma_i - \sigma_j}{\sigma_i} \right|} \right] \quad 1 \leq i \leq n$$

$$\eta = \max\{\|E\|_2, \|F\|_2\} < 1, \quad \eta' = 2\eta + \eta^2$$



## Key (well known) Facts

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### Theorem (Demmel et al. 1999)

Let  $A = XDY^T \in \mathbb{R}^{m \times n}$  be an RRD, and  $\tilde{A} = \tilde{X}\tilde{D}\tilde{Y}^T$  perturbations, that satisfy, with  $\epsilon < 1$ ,

$$\frac{\|\tilde{X} - X\|_2}{\|X\|_2}, \frac{\|\tilde{Y} - Y\|_2}{\|Y\|_2} \leq \epsilon \quad \text{and} \quad \frac{|\tilde{d}_i - d_i|}{|d_i|} \leq \epsilon \quad \text{for } i = 1, \dots, r.$$

Then

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

with  $\|E\|_2 \leq \epsilon\kappa(X)$  and  $\|F\|_2 \leq (2\epsilon + \epsilon^2)\kappa(Y)$ .



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### Theorem

Let  $\hat{Q}$  and  $\hat{R}$  be the *computed* factors (with Householder reflections) of the full QR decomposition of  $X = QR \in \mathbb{R}^{m \times r}$ , then there exists an exact orthogonal matrix  $Q \in \mathbb{R}^{m \times m}$  such that

$$Q\hat{R} = (I + E)X$$

where  $\|E\|_F \leq O(mr^{3/2}u) \kappa(X)$  and

$$\|\hat{Q} - Q\|_F \leq O(m^{3/2}ru)$$



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### Lemma (Small multiplicative backward errors of Jacobi rotations)

Let  $J_i$  be *exact* Jacobi rotations and  $\hat{J}_i$  their *floating point* approximations. Then

$$\hat{X}_M \equiv \text{fl}(\hat{J}_M^T \cdots \hat{J}_1^T X) = (I + F) J_M^T \cdots J_1^T X$$

where  $\|F\|_2 = O(M u \kappa(X))$ , and



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# Key (new) Facts

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$$\sigma_i = \sum_{j=1}^r x_{ij} d_j y_{ij} \quad \text{for all } i$$



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# Diagonally dominant matrices

## Theorem

Let  $A \in \mathbb{R}^{n \times n}$   $a_{ii} \neq 0$ , with for all  $i$ , and

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

where  $\delta \leq \frac{1}{5n}$ , then

$$\text{diag}(a_{11}, \dots, a_{nn}) = (I + F_1)A(I + F_2)$$

with  $\|F_1\|_F, \|F_2\|_F \leq n\delta + O(\delta^2)$ .





# Key Facts (New)

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## Errors in the diagonal entries

$$a_{ii} = \sum_{k=1}^n x_{ik} d_k y_{ik}$$

$$\left| \frac{fl(a_{ii}) - a_{ii}}{a_{ii}} \right| \leq \frac{3(n-1)u}{1 - 3(n-1)u} \frac{\sum_{k=1}^n |x_{ik}| |d_k| |y_{ik}|}{\left| \sum_{k=1}^n x_{ik} d_k y_{ik} \right|}$$



## Errors in the diagonal entries of almost diagonal RRDs

Input:  $\kappa(X) = 7.21$ ,  $\kappa(Y) = 8.29$

$$XDY^T = \begin{bmatrix} 1 & 1 & 1 \\ -1 & -1 & 1 \\ 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} 10^{50} & & \\ & 1 & \\ & & -10^{50} \end{bmatrix} \begin{bmatrix} 2 & -3 & 1 \\ 0 & 1 & 0 \\ 1 & 1 & -1 \end{bmatrix}$$



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$$\begin{bmatrix} -2.4 & -1.6 & -1.0 \\ -8.4 \cdot 10^{-85} & 0.53 & 5.9 \cdot 10^{-84} \\ 0.31 & 0.42 & -1.4 \end{bmatrix} \begin{bmatrix} 10^{50} & & \\ & 1 & \\ & & -10^{50} \end{bmatrix} \begin{bmatrix} 3.7 & 3.4 \cdot 10^{-49} & -0.63 \\ -0.89 & -0.49 & -0.21 \\ -0.81 & -2.6 \cdot 10^{-49} & -1.5 \end{bmatrix}$$



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There is no cancellation

$$-0.26 = (-8.4 \cdot 10^{-85})(10^{50})(3.4 \cdot 10^{-49}) + 0.53(-0.49) + (5.9 \cdot 10^{-84})(-10^{50})(-2.6 \cdot 10^{-49})$$





## Absence of cancellation in the diagonal

### Theorem

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

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$$\frac{\sum_{k=1}^n |x_{ik}| |d_k| |y_{ik}|}{|a_{ii}|} \leq (1 + O(n^2\delta)) \bar{\kappa}, \quad i = 1, \dots, n.$$

with  $\bar{\kappa} = \max\{\kappa(X), \kappa(Y)\}$



## Implicit Jacobi is multiplicative backward stable

### Theorem

Let  $M$  and  $N$  be resp. the number of left and right rotations applied by implicit Jacobi on  $A = XDY^T \in \mathbb{R}^{m \times n}$  until convergence, and  $\hat{\Sigma}$  and  $\hat{U}, \hat{V}$  be the computed matrices of singular values and left/right singular vectors. Then there exists two exact orthogonal matrices  $U \in \mathbb{R}^{m \times m}, V \in \mathbb{R}^{n \times n}$  such that

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$$\|F\|_F = O(u) (N \kappa(Y) + n^2 \bar{\kappa}) \quad \text{and} \quad \|\hat{V} - V\|_F = O(N u).$$

with  $\bar{\kappa} = \max\{\kappa(X), \kappa(Y)\}$



# Implicit Jacobi is multiplicative backward stable

Corollary (Forward errors in singular values and vectors)

$$\frac{|\hat{\sigma}_i - \sigma_i|}{|\sigma_i|} \leq O(u)\bar{\kappa}$$

and

$$\max\{\theta(u_i, \hat{u}_i), \theta(v_i, \hat{v}_i)\} \leq \frac{O(u)\bar{\kappa}}{\min_{j \neq i} \left| \frac{\sigma_i - \sigma_j}{\sigma_i} \right|} \quad \text{for all } i,$$

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- 1 Objectives of this work
- 2 Jacobi methods for the SVD
- 3 Implicit Jacobi SVD
- 4 Error Analysis
- 5 Numerical Experiments**
- 6 Conclusions



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- We have used `gallery('randsvd', ...)` by N. Higham in MATLAB to generate random RRDs with  $X$  well-conditioned and  $D$  and **extremely** ill-conditioned.



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

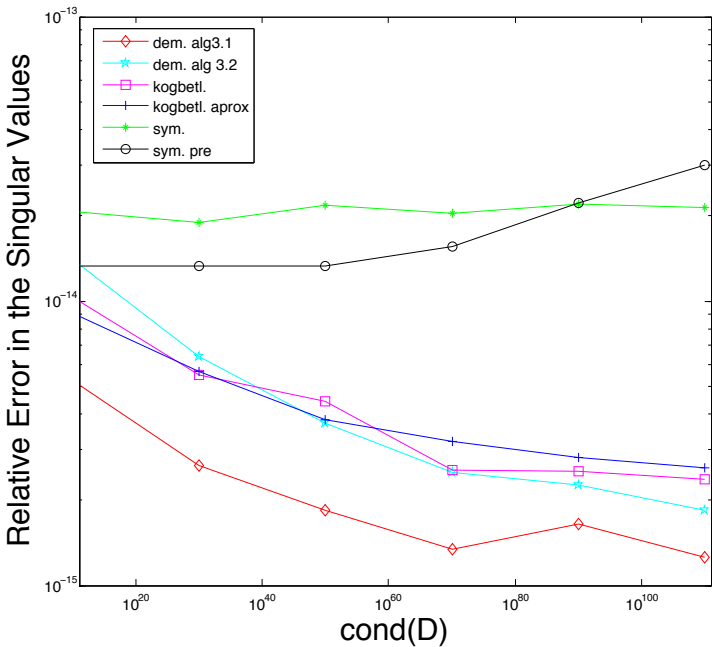
In all these tests  $\kappa(X) = \kappa(Y) = 30$  and  $X, D$  are  $100 \times 100$ .

$D$  has entries with magnitudes geometrically distributed

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

$\kappa(D)$	sym	sym pre	kogb	kogb aprox	dem-3.1	dem-3.2
$10^{10}$	16.2	6	6.2	6.2	5.2	10.2
$10^{30}$	22.8	6.4	5	5	4	8.2
$10^{50}$	26.6	13.8	6	6	3.6	7.4
$10^{70}$	29.2	20.4	4	4	3	6
$10^{90}$	31.6	24.4	4	4	3	6
$10^{110}$	32	28	4	4	3	6





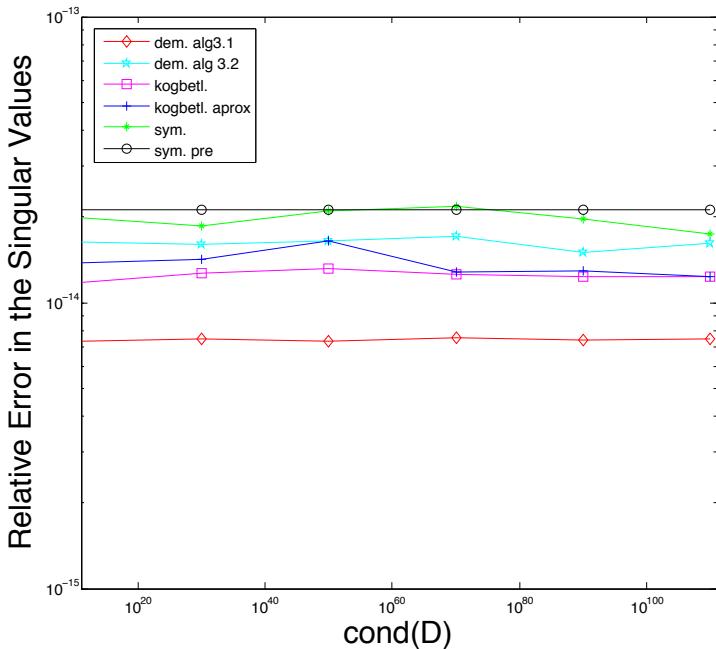
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In all of these tests  $\kappa(X) = \kappa(Y) = 30$  and  $X, D$  are  $100 \times 100$ .

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

$\kappa(D)$	sym	sym pre	kogb	kogb aprox	dem-3.1	dem-3.2
$10^{10}$	10	9	9	9.2	9.2	18.8
$10^{30}$	10.2	9	9	9.4	9.2	18.6
$10^{50}$	11.2	10.8	9.6	9.4	8.8	18.6
$10^{70}$	11.4	11.2	9.2	9.4	9	18.6
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## Number of sweeps: Increasing the dimension

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

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$n$	sym	sym pre	kogb	kogb aprox	dem-3.1	dem-3.2
100	34	16	6	6	4	9
500	58	20	7	7	6	12
1000	68	22	7	8	7	13
2000	76	24	9	9	7	14



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100	12	12	10	10	10	21
500	13	12	12	12	14	25
1000	14	13	13	13	15	28
2000	14	13	14	15	17	30





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- computes the singular values and vectors of  $A$  to high relative accuracy,
- the error bounds are the best possible ones from the sensitivity of the problem,
- is backward stable in a strong multiplicative sense.
- the number of Jacobi sweeps is comparable to other algorithms.
- More research to speed up the algorithm is needed [as is Drmac's works for SVD one-sided Jacobi].

