

# Perturbation theory for the LDU factorization of diagonally dominant matrices and its application to accurate computation of singular values

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- 2 Perturbation theory for LDU factorization
- 3 Error analysis
- 4 Conclusions

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# Accurate LDU Rank Revealing Decompositions (RRD)

Let  $A = LDU$  and  $\widehat{L}\widehat{D}\widehat{U}$  be, respectively, the **exact** and **computed** LDU factorizations of a matrix  $A \in \mathbb{R}^{n \times n}$ .

**If** these factorizations satisfy

- $L$  and  $U$  are well-conditioned (this happens if complete pivoting is used),

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$$\frac{\|L - \widehat{L}\|}{\|L\|} = O(\epsilon), \quad \frac{\|U - \widehat{U}\|}{\|U\|} = O(\epsilon), \quad \frac{|d_{ii} - \widehat{d}_{ii}|}{|d_{ii}|} = O(\epsilon) \quad \forall i,$$

where  $\epsilon$  is machine precision (this can be guaranteed only for some types of matrices through special implementations of GECP),

**then** there are algorithms that use the factors  $\widehat{L}$ ,  $\widehat{D}$ ,  $\widehat{U}$  for

- **computing the SVD of  $A$  very accurately** (Demmel et al. 1999), and
- **computing very accurately the solution of  $Ax = b$  for almost every  $b$**  (D-Molera this conference).

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- Q. Ye, Math. Comp. (2008), developed a very ingenious algorithm for computing accurately in  $2n^3$  flops the LDU factorization with complete pivoting of **row diagonally dominant** matrices...
- that are parameterized in a particular way, but
- best error bounds that have been proved after considerable efforts are

$$\frac{\|L - \hat{L}\|_\infty}{\|L\|_\infty} \leq 6n8^{(n-1)}\epsilon, \quad \frac{\|U - \hat{U}\|_\infty}{\|U\|_\infty} \leq 6 \cdot 8^{(n-1)}\epsilon, \quad \frac{|d_{ii} - \hat{d}_{ii}|}{|d_{ii}|} \leq 5 \cdot 8^{(n-1)}\epsilon,$$

where  $n \times n$  is the size of the matrix.

- $\epsilon = 2^{-53}$  in double precision, **so the bounds are useless for  $n > 20$ ...**
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- Are accurate computations possible for diagonally dominant matrices?
- **I will prove sharper error bounds for Q. Ye's algorithm by using a new Perturbation Theory for the LDU of diagonally dominant matrices.**

$$\frac{\|L - \hat{L}\|}{\|L\|} \leq 14n^3\epsilon, \quad \frac{\|U - \hat{U}\|}{\|U\|} \leq 14n^3\epsilon, \quad \frac{|d_{ii} - \hat{d}_{ii}|}{|d_{ii}|} \leq 14n^3\epsilon \quad \forall i$$



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## Parameterizing row diagonally dominant matrices (Q. Ye)

- Assume  $A \in \mathbb{R}^{n \times n}$  satisfies  $a_{ii} \geq 0$  for all  $i$  (no restriction for SVD or linear systems).
- Define  $v = (v_1, v_2, \dots, v_n)$  where

$$v_i := a_{ii} - \sum_{j \neq i} |a_{ij}|$$

- $A$  is row diagonally dominant if and only if  $v_i \geq 0$  for all  $i$ .
- $A_D := \begin{cases} 0 & \text{for } i = j \\ a_{ij} & \text{for } i \neq j \end{cases}$
- The pair  $(A_D, v)$  allows us to recover the matrix  $A$  and we parameterize the set of  $n \times n$  matrices through pairs of this type. A matrix  $A$  parameterized in this way will be denoted as

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## Good perturbation properties of this parametrization

**Example:** Two types of small ( $\approx 10^{-3}$ ) **relative componentwise perturbations** of a **row diagonally dominant matrix**  $A$ :

$$A = \begin{bmatrix} 3 & -1.5 & 1.5 \\ -1 & 2.002 & 1 \\ 2 & 0.5 & 2.5 \end{bmatrix}, \quad v(A) = \begin{bmatrix} 0 \\ 0.002 \\ 0 \end{bmatrix}$$

$$B = \begin{bmatrix} 3 & -1.5 & 1.5 \\ -1 & \mathbf{2.001} & 1 \\ 2 & 0.5 & 2.5 \end{bmatrix}, \quad v(B) = \begin{bmatrix} 0 \\ 0.001 \\ 0 \end{bmatrix}$$

$$v(C) = \begin{bmatrix} 0 \\ \mathbf{0.002002} \\ 0 \end{bmatrix}, \quad c_{12} = \mathbf{-1.5015} \implies C = \begin{bmatrix} \mathbf{3.0015} & \mathbf{-1.5015} & 1.5 \\ -1 & \mathbf{2.002002} & 1 \\ 2 & 0.5 & 2.5 \end{bmatrix}$$

Singular values of  $A$ ,  $B$  and  $C$

	$A$	$B$	$C$
$\sigma_1$	4.641	4.640	4.642
$\sigma_2$	2.910	2.909	2.910
$\sigma_3$	$6.663 \cdot 10^{-4}$	$\mathbf{3.332 \cdot 10^{-4}}$	$\mathbf{6.673 \cdot 10^{-4}}$



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## Key features of Q. Ye's algorithm for LDU of diag. dominant

- **INPUT:**  $\mathcal{D}(A_D, v)$  with  $v \geq 0$  (not the matrix  $A$ ).
- It performs Gaussian elimination with complete (diagonal) pivoting.
- If we denote  $A^{(1)} := A$  and  $A^{(k)}$  is the matrix obtained after  $k - 1$  steps of Gaussian elimination are performed, then the algorithm iterates

$$\mathcal{D}(A_D^{(1)}, v^{(1)}) \rightarrow \mathcal{D}(A_D^{(2)}, v^{(2)}) \rightarrow \dots \rightarrow \mathcal{D}(A_D^{(k)}, v^{(k)}) \rightarrow \dots$$

- $v^{(k+1)}$  is obtained from  $\mathcal{D}(A_D^{(k)}, v^{(k)})$  as a sum of nonnegative terms. **There are no cancellation errors in this part!!**
- $A_D^{(k+1)}$  is computed from  $\mathcal{D}(A_D^{(k)}, v^{(k)})$  by applying the usual Gaussian elimination process. So cancellation errors may appear but they are bounded in an absolute sense.

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- $A_D^{(k+1)}$  is computed from  $\mathcal{D}(A_D^{(k)}, v^{(k)})$  by applying the usual Gaussian elimination process. So cancellation errors may appear but they are bounded in an absolute sense.

## Key features of Q. Ye's algorithm for LDU of diag. dominant

- **INPUT:**  $\mathcal{D}(A_D, v)$  with  $v \geq 0$  (not the matrix  $A$ ).
- It performs Gaussian elimination with complete (diagonal) pivoting.
- If we denote  $A^{(1)} := A$  and  $A^{(k)}$  is the matrix obtained after  $k - 1$  steps of Gaussian elimination are performed, then the algorithm iterates

$$\mathcal{D}(A_D^{(1)}, v^{(1)}) \rightarrow \mathcal{D}(A_D^{(2)}, v^{(2)}) \rightarrow \dots \rightarrow \mathcal{D}(A_D^{(k)}, v^{(k)}) \rightarrow \dots$$

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## What happens if the vector $v$ in $\mathcal{D}(A_D, v)$ is not known?

- If only the entries of the starting matrix  $A$  are known, then one can compute with the usual *recursive summation* method

$$v_i := a_{ii} - \sum_{j \neq i} |a_{ij}| \quad \text{for all } i,$$

but it may produce large relative cancellation errors if  $a_{ii} \approx \sum_{j \neq i} |a_{ij}|$  and this would spoil the accuracy of the whole computation.

- In case of severe cancellation, one can compute the  $v_i$  with *doubly compensated summation* (Priest, 1992) that computes the sum of  $n$  numbers with relative error  $2\epsilon$  with cost of  $10(n - 1)$  flops.

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# The absence of cancellation does not imply accuracy (I)

- Best available error bounds for Q. Ye's algorithm increase exponentially with the dimension  $6 \cdot n \cdot 8^{(n-1)} \epsilon$ .
- This algorithm avoids partially cancellation, but I will assume a much more favorable scenario to show why a *direct forward error analysis* produce exponential error bounds in the dimension.
- **Assumption: There is no cancellation at all in the whole process of Gaussian elimination**, so, in every step  $k \rightarrow k + 1$  and in every update

$$a_{ij}^{(k+1)} = a_{ij}^{(k)} - \frac{a_{ik}^{(k)} a_{kj}^{(k)}}{a_{kk}^{(k)}}, \quad (k+1) \leq i, j \leq n,$$

$a_{ij}^{(k+1)}$  is computed as a sum of two numbers with the same sign.

- Let the relative errors in the computed entries of iterate  $A^{(k)}$  be

$$\widehat{a}_{ij}^{(k)} = a_{ij}^{(k)} \langle p_k \rangle \quad k \leq i, j \leq n,$$

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$$\widehat{a}_{ij}^{(k+1)} = \left( a_{ij}^{(k)} - \frac{a_{ik}^{(k)} a_{kj}^{(k)}}{a_{kk}^{(k)}} \right) \langle 3 p_k + 3 \rangle = a_{ij}^{(k+1)} \langle 3 p_k + 3 \rangle$$

- We have proved that

$$p_{k+1} = 3 p_k + 3$$



$$p_1 = 0 \implies p_n = 3^n \left( \frac{3^n - 1}{2 \cdot 3^{n-1}} - 1 \right) \implies p_n \approx \frac{3^n}{2}$$

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1 Introduction

**2 Perturbation theory for LDU factorization**

3 Error analysis

4 Conclusions

## Theorem

Let  $A = \mathcal{D}(A_D, v) \in \mathbb{R}^{n \times n}$  and  $\tilde{A} = \mathcal{D}(\tilde{A}_D, \tilde{v}) \in \mathbb{R}^{n \times n}$  be row diagonally dominant matrices, and  $A = LDU$  and  $\tilde{A} = \tilde{L}\tilde{D}\tilde{U}$  be their factorizations. If

$$|\tilde{v} - v| \leq \delta v \quad \text{and} \quad |\tilde{A}_D - A_D| \leq \delta |A_D|, \quad \text{with } \delta < 1,$$

then

- For  $i = 1 : n$

$$\tilde{d}_{ii} = d_{ii} \frac{(1 + \eta_1) \cdots (1 + \eta_i)}{(1 + \alpha_1) \cdots (1 + \alpha_{i-1})} \quad |\eta_k| \leq \delta, \quad |\alpha_k| \leq \delta.$$

- For  $i < j$

$$|\tilde{u}_{ij} - u_{ij}| \leq 3i\delta$$

**Recall:**  $\max_{ij} |u_{ij}| = \max_{ii} |u_{ii}| = 1.$

## Theorem (continuation)

- For  $i > j$ ,

$$\begin{aligned} |\tilde{l}_{ij} - l_{ij}| &\leq |l_{ij}| \left( \frac{1}{(1-\delta)^j} - 1 \right) + 2 \frac{(1+\delta)^j - 1}{(1-\delta)^j} \left| \frac{a_{ii}^{(j)}}{a_{jj}^{(j)}} \right| \\ &= (j\delta + O(\delta^2)) \left( |l_{ij}| + 2 \left| \frac{a_{ii}^{(j)}}{a_{jj}^{(j)}} \right| \right), \end{aligned}$$

where  $A^{(j)}$  is the matrix obtained after  $(j-1)$  steps of Gaussian elimination.

- If the matrix  $A$  is ordered for complete pivoting, then  $|l_{ij}| \leq 1$ ,  $|a_{ii}^{(j)}| \leq |a_{jj}^{(j)}|$  and

$$|\tilde{l}_{ij} - l_{ij}| \leq 3j\delta + O(\delta^2)$$



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## Complete pivoting is essential for good behavior of $L$ : Example

Matrix ordered according to a pivoting strategy designed to make the factor  $L$  **column diagonally dominant** and as much as possible.

$$A = \begin{bmatrix} 1000 & 100 & 500 \\ 0 & 0.1 & 0.05 \\ 100 & 10 & 120 \end{bmatrix}, \quad v(A) = \begin{bmatrix} 400 \\ 0.05 \\ 10 \end{bmatrix}$$

$$A = \begin{bmatrix} 1 & & \\ 0 & 1 & \\ 0.1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1000 & & \\ & 0.1 & \\ & & 70 \end{bmatrix} \begin{bmatrix} 1 & 0.1 & 0.5 \\ & 1 & 0.5 \\ & & 1 \end{bmatrix}$$

**Example:**  $\delta \approx 10^{-2}$  perturbation in  $\mathcal{D}(A_D, v)$ .

$$\tilde{A} = \begin{bmatrix} 1000 & 101 & 500 \\ 0 & 0.1 & 0.05 \\ 100 & 10 & 120 \end{bmatrix}, \quad v(A) = \begin{bmatrix} 399 \\ 0.05 \\ 10 \end{bmatrix}$$

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# New error bounds for Q. Ye's algorithm

## Theorem

Let us apply Ye's algorithm with complete pivoting on  $A = \mathcal{D}(A_D, v) \in \mathbb{R}^{n \times n}$  row diagonally dominant matrix to compute  $\widehat{L}$ ,  $\widehat{D}$  and  $\widehat{U}$  with machine precision  $\epsilon$ . If  $L$ ,  $D$  and  $U$  are the exact factors then:

- For  $i > j$

$$|\widehat{\ell}_{ij} - \ell_{ij}| \leq 14 n j^2 \epsilon < 14 n^3 \epsilon.$$

- For  $i = 1, \dots, n$

$$|\widehat{d}_{ii} - d_{ii}| \leq |d_{ii}| \frac{6 n i^2 \epsilon}{1 - 6 n i^2 \epsilon} \leq |d_{ii}| \frac{6 n^3 \epsilon}{1 - 6 n^3 \epsilon}.$$

- For  $i < j$

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**Recall:**  $\max_{ij} |u_{ij}| = \max_{ij} |\ell_{ij}| = 1.$

$O(n^3 \epsilon)$  error bounds, no exponential growth with the dimension.



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# Two key facts on the error analysis (I)

- Delicate error analysis: inductive argument in the dimension  $n$ .
- **Fact 1.** If the first step of Gaussian Elimination is

$$A^{(1)} := \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} 1 & \\ \frac{A_{21}}{a_{11}} & I_{n-1} \end{bmatrix} \begin{bmatrix} a_{11} & A_{12} \\ & A^{(2)} \end{bmatrix}$$

and the LDU factorization of  $A^{(2)} = L_{22}D_{22}U_{22}$  then

$$A^{(1)} = \begin{bmatrix} 1 & \\ \frac{A_{21}}{a_{11}} & L_{22} \end{bmatrix} \begin{bmatrix} a_{11} & \\ & D_{22} \end{bmatrix} \begin{bmatrix} 1 & \frac{A_{12}}{a_{11}} \\ & U_{22} \end{bmatrix}.$$

is the LDU factorization of  $A = A^{(1)}$ .

- Let  $\mathcal{D}(\hat{A}_D^{(2)}, \hat{v}^{(2)})$  be the computed parametrization of  $A^{(2)}$ .

# Two key facts on the error analysis (I)

- Delicate error analysis: inductive argument in the dimension  $n$ .
- **Fact 1.** If the first step of Gaussian Elimination is

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# Two key facts on the error analysis (II)

- **Fact 2.** The computation of  $\mathcal{D}(\widehat{A}_D^{(2)}, \widehat{v}^{(2)})$  in Q. Ye's algorithm is equivalent to the following sequence:
  - 1 Make a **relative componentwise perturbation** of order  $n\epsilon$  in  $\mathcal{D}(A_D^{(1)}, v^{(1)})$ , getting  $\mathcal{D}(\widetilde{A}_D^{(1)}, \widetilde{v}^{(1)})$ .
  - 2 Apply **exactly** one step of GE to  $\mathcal{D}(\widetilde{A}_D^{(1)}, \widetilde{v}^{(1)})$ , getting  $\mathcal{D}(\widetilde{A}_D^{(2)}, \widetilde{v}^{(2)})$ .
  - 3 Make a **relative componentwise perturbation** of order  $n\epsilon$  in  $\mathcal{D}(\widetilde{A}_D^{(2)}, \widetilde{v}^{(2)})$ , getting  $\mathcal{D}(\widehat{A}_D^{(2)}, \widehat{v}^{(2)})$ .
- Let  $\Phi(n)$  be the error produced by Q. Ye's algorithm for LDU on a  $n \times n$  row diagonally dominant matrix. Then perturbation theory implies

$$\Phi(n) = \Phi(n-1) + C n^2 \epsilon, \quad \text{with } \Phi(1) = 0$$

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- 1 Introduction
- 2 Perturbation theory for LDU factorization
- 3 Error analysis
- 4 Conclusions**



# Conclusions

- The satisfactory **error analysis** that we have presented is possible because a **structured perturbation theory** has been developed.
- This error analysis proves rigorously that **for any diagonally dominant matrix  $A$** , there are algorithms that
  - **compute its SVD with high relative accuracy**, (Ye's + Demmel et al)
  - **compute accurately the solution of  $Ax = b$  for almost every  $b$** , (Ye's + D-Molera)

with cost  $O(n^3)$  and independently of the traditional condition number of  $A$ .