Structured perturbation theory of diagonally dominant matrices and numerical applications

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Outline

Motivation (I)

- Diagonally dominant matrices appear in many applications.
- Q. Ye, *Math. Comp. (2008)*, developed a very ingenuous algorithm for **computing accurately?** in $2n^3$ flops the LDU factorization with complete pivoting of row diagonally dominant **(rDD)** matrices
- that are parameterized in a particular way, but
- best error bounds that Q. Ye proved after a direct error analysis that requires considerable efforts are

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

  where $n\times n$ is the size of the matrix and ϵ the unit roundoff.
- $\epsilon = 2^{-53}$ in double precision, **so the bounds are** >1 **for** $n>20$...
- However, numerical experiments indicated accuracy.

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- **Using a structured perturbation theory of LDU of DD matrices** and intricate error analysis, we proved *(D. and Koev, Numer. Math, to appear)*

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

for the errors of Q. Ye's algorithm (here $\|A\|_M = \max_{ij} |a_{ij}|$).

- **Fundamental consequences:** Q. Ye's algorithm + other existing implicit algorithms for factorized matrices allow **for DD matrices to compute with guaranteed high relative accuracy**

1. solutions of linear systems and least square probs. for most rhs *(D. and Molera, IMAJNA, to appear), (Molera et al., this conference)*,
2. SVDs and eigenval-vec of positive definite matrices *(Demmel et al, SIMAX 1992, LAA 1999)*,
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Goal of the talk

- To revise published perturbation bounds *(D. and Koev, Numer. Math, to appear)* for the LDU factorization of DD matrices under structured perturbations.
- **To present a family of new perturbation bounds under structured perturbations** for several magnitudes corresponding to **DD matrices**: inverses, solutions of linear systems, singular values, eigenvalues.
- Common key point in (almost all) these perturbation bounds: they are always tiny for tiny structured perturbations, even for extremely ill conditioned matrices (independent of traditional condition numbers).
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Parameterizing row diagonally dominant matrices (Q. Ye)

- We will assume that $A \in \mathbb{R}^{n\times n}$ satisfies $a_{ii} \geq 0$ for all i, unless otherwise stated (**no restriction** for linear systems, least squares, SVD, but **yes** for eigenvalues).
- Define $v = (v_1, v_2, \ldots, v_n)$ 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 is this way will be denoted as

$$A = \mathcal{D}(A_D, v)$$

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Example: Good perturbation properties of this parametrization

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

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

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

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

Singular values of A, B and C

	A	B	C
σ_1	4.641	4.640	4.642
σ_2	2.910	2.909	2.910
σ_3	$6.663 \cdot 10^{-4}$	$3.332 \cdot 10^{-4}$	$6.673 \cdot 10^{-4}$

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Bounds for the LDU factors under structured perturbations

Theorem (D. and Koev, Numer. Math. to appear)

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

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

then

- For $i = 1 : n$

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

- For $i < j$

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

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

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- $$\frac{\|\widetilde{U} - U\|_M}{\|U\|_M} \leq 3n\delta$$

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Bounds for the L factor

Theorem (continuation)

- For $i > j$,

$$|\widetilde{\ell}_{ij} - \ell_{ij}| \leq |\ell_{ij}| \left(\frac{1}{(1-\delta)^j} - 1 \right) + 2\, \frac{(1+\delta)^j - 1}{(1-\delta)^j} \left| \frac{a_{ii}^{(j)}}{a_{jj}^{(j)}} \right|$$
$$= (\, j\delta + O(\delta^2)\,) \left(|\ell_{ij}| + 2 \left| \frac{a_{ii}^{(j)}}{a_{jj}^{(j)}} \right| \right),$$

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

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

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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.

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

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

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

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

$$\widetilde{A} = \begin{bmatrix} 1 & & \\ 0 & 1 & \\ 0.1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1000 & & \\ & 0.1 & \\ & & 70.05 \end{bmatrix} \begin{bmatrix} 1 & 0.101 & 0.5 \\ & 1 & 0.5 \\ & & 1 \end{bmatrix}$$

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

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

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

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

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

Then

- A *is nonsingular if and only if* $\widetilde{A}$ *is nonsingular.*
- $(\widetilde{A}^{-1})_{ii} = (A^{-1})_{ii} \dfrac{(1+\eta_1)\cdots(1+\eta_{n-1})}{(1+\alpha_1)\cdots(1+\alpha_n)} \qquad |\eta_k| \leq \delta,\ |\alpha_k| \leq \delta.$
- $|(\widetilde{A}^{-1})_{ij} - (A^{-1})_{ij}| \leq \dfrac{(3n-2)\delta}{1-2n\delta} |(A^{-1})_{jj}|, \quad i \neq j$ *and* $2n\delta < 1$
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Bounds for the inverse under structured perturbations

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Consider the systems

$$A\, x = b \quad \text{and} \quad \widetilde{A}\,\widetilde{x} = \widetilde{b}$$

with $\|b - \widetilde{b}\|_\infty \leq \mu \|b\|_\infty$*. If* $2n\delta < 1$*, then*

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For most vectors b, $\|A^{-1}\|_\infty \|b\|_\infty / \|x\|_\infty$ is a moderate number and for A ill-conditioned, $\|A^{-1}\|_\infty \|b\|_\infty / \|x\|_\infty \ll \kappa_\infty(A)$

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Example: Good perturbation properties for linear systems

Two types of small ($\approx 10^{-3}$) relative componentwise perturbations of a rDD matrix A:

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

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

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

Solutions of $Ax = b$, $Bx = b$ and $Cx = b$ for $b = [1, 1, -1]^T$:

	$Ax_A = b$	$Bx_B = b$	$Cx_C = b$
x_1	$1.5009 \cdot 10^3$	$3.0009 \cdot 10^3$	$1.4987 \cdot 10^3$
x_2	$1.5000 \cdot 10^3$	$3.0000 \cdot 10^3$	$1.4978 \cdot 10^3$
x_3	$-1.5011 \cdot 10^3$	$-3.0011 \cdot 10^3$	$-1.4989 \cdot 10^3$

$$\frac{\|x_A - x_B\|_\infty}{\|x_A\|_\infty} = 0.999 \qquad \frac{\|x_A - x_C\|_\infty}{\|x_A\|_\infty} = 1.44 \cdot 10^{-3}$$

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Theorem (Q. Ye, SIMAX 2009)

Let $A = \mathcal{D}(A_D, v) \in \mathbb{R}^{n \times n}$ *and* $\widetilde{A} = \mathcal{D}(\widetilde{A}_D, \widetilde{v}) \in \mathbb{R}^{n \times n}$ *be diagonally dominant symmetric matrices with nonnegative diagonal entries such that*

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

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Parameterizing rDD matrices with diagonal entries of any sign

- Let $A \in \mathbb{R}^{n\times n}$.
- Define $v = (v_1, v_2, \ldots, v_n)$ 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.
- $A_D := \begin{cases} 0 & \text{for } i = j \\ a_{ij} & \text{for } i \neq j \end{cases}$
- Define $\boxed{S = \text{diag}(\text{sign}(a_{11}), \ldots, \text{sign}(a_{nn}))}$ $(\text{sign}(0) := 1)$.
- The triplet (A_D, v, S) allows us to recover the matrix A and we parameterize the set of $n \times n$ matrices through triplets of this type. Any matrix A parameterized is this way will be denoted as

$$\boxed{A = \mathcal{D}(A_D, v, S)}$$

Theorem

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Assume $n^3\delta < 1/5$ and define $\quad \nu := \dfrac{4n^3\delta}{1 - n\delta}.$

Then

$$\begin{aligned} |\widetilde{\lambda}_i - \lambda_i| &\leq (2\nu + \nu^2)\, |\lambda_i| \\ &= (\, 8n^3\delta + O(\delta^2)\,)\, |\lambda_i|, \qquad i = 1, \ldots, n \end{aligned}$$

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Define

$$\nu_1 := \frac{n^2\delta}{1-n\delta}\left(3 + \frac{2n\delta}{1-n\delta}\right)\|L^{-1}\|_2 \quad \text{and} \quad \nu_2 = \frac{5n^3\delta}{1-2n\delta},$$

where L *is the* LDU *factor corresponding to complete (diagonal) pivoting. If* $n\delta < 1$ *and* $\nu := \max\{\nu_1\,,\,\nu_2\} < 1$*, then*

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$$y^* A = \lambda y^* \qquad \text{and} \qquad Ax = \lambda x$$

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If $s_{ij} = sign(a_{ij})$, then

$$\operatorname{relcond}(\lambda; A_D, v) = \frac{1}{|\lambda|\,|y^* x|} \sum_{i=1}^{n} |y_i| \left(v_i\,|x_i| + \sum_{j\neq i} |a_{ij}|\,|x_i + s_{ij} x_j| \right)$$

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Example: Good perturbation properties of eigenvalues of nonsymmetric row diagonally dominant matrices

Two types of small ($\approx 10^{-3}$) relative componentwise perturbations of a rDD matrix A:

$$A = \begin{bmatrix} 3 & -1.5 & 1.5 \\ -1 & 2.002 & 1 \\ 3 & 1.5 & 4.5 \end{bmatrix}, \qquad v(A) = \begin{bmatrix} 0 \\ 0.002 \\ 0 \end{bmatrix}$$

$$B = \begin{bmatrix} 3 & -1.5 & 1.5 \\ -1 & 2.001 & 1 \\ 3 & 1.5 & 4.5 \end{bmatrix}, \qquad v(B) = \begin{bmatrix} 0 \\ 0.001 \\ 0 \end{bmatrix}$$

$$v(C) = \begin{bmatrix} 0 \\ 0.002002 \\ 0 \end{bmatrix}, \quad c_{12} = -1.5015 \Longrightarrow C = \begin{bmatrix} 3.0015 & -1.5015 & 1.5 \\ -1 & 2.002002 & 1 \\ 3 & 1.5 & 4.5 \end{bmatrix}$$

Eigenvalues and condition numbers:

	A	B	C	$\frac{\lvert y\rvert^T \lvert A\rvert \lvert x\rvert}{\lvert\lambda\rvert \lvert y^* x\rvert}$	relcond$(\lambda; A_D, v)$
λ_1	$8.5686 \cdot 10^{-4}$	$4.2850 \cdot 10^{-4}$	$8.5803 \cdot 10^{-4}$	$6.75 \cdot 10^3$	2.14
λ_2	3.5011	3.5006	3.5023	1.44	1.00
λ_3	6.0000	6.0000	6.0003	1.05	1.00

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Conclusions and open problems

- We have presented structured perturbation results of rDD matrices for all basic problems in Numerical Linear Algebra, **except least square problems**.

- Except in the case of eigenvalues of nonsymmetric matrices, **the perturbation bounds that we have obtained are rigorous and we have proved that are always tiny for tiny perturbations**.

- **Numerical methods to perform accurate and efficient dense Numerical Linear Algebra with parameterized rDD matrices are available**, **except in the case of eigenvalues of nonsymmetric matrices (open problem!!)**.

- We believe that some of the presented bounds can be improved, in particular the one for singular values.