Structured perturbation theory for diagonally dominant matrices and numerical applications

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Outline

1. Introduction
2. Perturbation theory for LDU factorization
3. Perturbation theory for the inverse
4. Perturbation theory for linear systems
5. Perturbation theory for eigenvalues of symmetric matrices
6. Perturbation theory for singular values
7. Structured condition numbers for eigenvalues of nonsymmetric matrices
8. Conclusions and open problems

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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** $n > 20$...
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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, 2011)*

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

  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)*,
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- To revise published perturbation bounds *(D. and Koev, Numer. Math, 2011)* 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., 2011)

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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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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$$\frac{\|\widetilde{L} - L\|_M}{\|L\|_M} \leq 3\, n\delta + O(\delta^2)$$

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.

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

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

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Bounds for the inverse under structured perturbations

Theorem

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 such that*

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

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

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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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

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

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

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

$$\boxed{|\widetilde{\sigma}_i - \sigma_i| \leq (2\nu + \nu^2)\,\sigma_i, \qquad i = 1, \ldots, n.}$$

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2. Perturbation theory for LDU factorization
3. Perturbation theory for the inverse
4. Perturbation theory for linear systems
5. Perturbation theory for eigenvalues of symmetric matrices
6. Perturbation theory for singular values
7. **Structured condition numbers for eigenvalues of nonsymmetric matrices**
8. Conclusions and open problems

Theorem

Let $A = \mathcal{D}(A_D, v) \in \mathbb{R}^{n\times n}$ *be a rDD matrix with nonnegative diagonal entries and* λ *a simple eigenvalue of* A. *Consider left and right eigenvectors*

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

and define

$$\operatorname{relcond}(\lambda; A_D, v) := \lim_{\delta\to 0} \sup \left\{ \frac{|\widetilde{\lambda} - \lambda|}{\delta\,|\lambda|} \;:\; \widetilde{\lambda} \text{ eigenvalue of } \widetilde{A} = \mathcal{D}(\widetilde{A}_D, \widetilde{v}), \right.$$
$$\left. |\widetilde{v} - v| \le \delta\, v,\; |\widetilde{A}_D - A_D| \le \delta |A_D| \right\}.$$

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

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

Structured condition numbers for eigenvalues of nonsymmetric matrices

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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.