Triple dqds for Real Unsymmetric Tridiagonals

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The problem

Find the eigenvalues of C

$$C = \begin{bmatrix} \alpha_1 & \gamma_1 & & & \\ \beta_1 & \alpha_2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{n-2} & \alpha_{n-1} & \gamma_{n-1} \\ & & & \beta_{n-1} & \alpha_n \end{bmatrix} \in \mathbb{R}^{n \times n}$$

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- Unreduced C ($\beta_i\gamma_i \neq 0$) is diagonally similar to a J matrix

$$J = \begin{bmatrix} \alpha_1 & 1 & & & \\ \beta_1\gamma_1 & \alpha_2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{n-2}\gamma_{n-2} & \alpha_{n-1} & 1 \\ & & & \beta_{n-1}\alpha_{n-1} & \alpha_n \end{bmatrix}$$

Two algorithms

- Shifted QR algorithm [Francis,1959/1960]

$$A_i - \sigma_i I = Q_i R_i \qquad (\text{QR factorization})$$
$$A_{i+1} = R_i Q_i + \sigma_i I \quad \text{so} \quad A_{i+1} = Q_i^{-1} A_i Q_i$$

  - destroys tridiagonal form in unsymmetric case
  - does not breakdown

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  - destroys tridiagonal form in unsymmetric case
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- Shifted LR algorithm [Rutishauser, 1957]

$$A_i - \sigma_i I = L_i R_i \qquad \text{(LU factorization)}$$
$$A_{i+1} = R_i L_i + \sigma_i I \quad \text{so} \quad A_{i+1} = L_i^{-1} A_i L_i$$

  - preserves bandwith
  - can breakdown

LU factorization of a J matrix

$$J - \sigma I = LU$$

$$L = \begin{bmatrix} 1 & & & & \\ l_1 & 1 & & & \\ & l_2 & 1 & & \\ & & \ddots & \ddots & \\ & & & l_{n-1} & 1 \end{bmatrix}, \qquad U = \begin{bmatrix} u_1 & 1 & & & \\ & u_2 & 1 & & \\ & & u_3 & \ddots & \\ & & & \ddots & 1 \\ & & & & u_n \end{bmatrix}$$

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$$UL = \begin{bmatrix} l_1 + u_1 & 1 & & & \\ l_1 u_2 & l_2 + u_2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & l_{n-2}u_{n-1} & l_{n-1} + u_{n-1} & 1 \\ & & & l_{n-1}u_n & u_n \end{bmatrix}$$

Equivalence of LR for J matrix and dqds

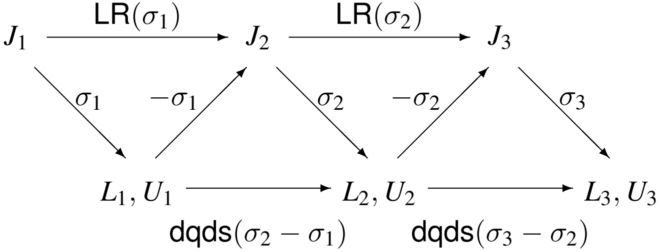

Figure: Relation of LR to dqds

$$J_i - \sigma_i I = L_i U_i$$

$$\begin{aligned} J_{i+1} - \sigma_{i+1} I &= U_i L_i + \sigma_i I - \sigma_{i+1} I \\ &= U_i L_i - (\sigma_{i+1} - \sigma_i) I = L_{i+1} U_{i+1} \end{aligned}$$

Why dqds instead of LR?

- L and U define the small eigenvalues better than J does (usually)
- dqds has *high mixed relative stability* (even with element growth)

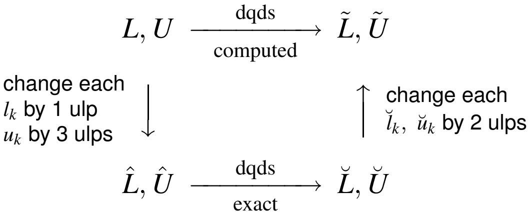

Figure: Effects of roundoff for dqds

- LU reveals singularity, J does not

Choosing a shift

- Ideally we would want to shift by the smallest eigenvalue
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- Complex shifts for complex eigenvalues

Choosing a shift

- Ideally we would want to shift by the smallest eigenvalue
- Shifts σ_i close to eigenvalues hasten convergence
- Complex shifts for complex eigenvalues
- Complex arithmetic increases the cost by a factor of about 4 when J is real
- Retain real arithmetic using complex shifts σ and $\overline{\sigma}$ combined (**double shift**)

Double shifted LR algorithm

- Double shifted LR algorithm similar to Francis double shifted QR algorithm [Francis, 1959/1960]

Successive σ and $\overline{\sigma}$ yields

$$\begin{aligned} J_i - \sigma I &= L_i R_i \\ J_{i+1} &= R_i L_i + \sigma I \\ J_{i+1} - \overline{\sigma} I &= L_{i+1} R_{i+1} \\ J_{i+2} &= R_{i+1} L_{i+1} + \overline{\sigma} I \end{aligned}$$

So

$$J_{i+2} = \mathcal{L}^{-1} J_i \mathcal{L}$$

where $\mathcal{L} \equiv L_i L_{i+1}$ (real)

Double shifted LR and triple dqds

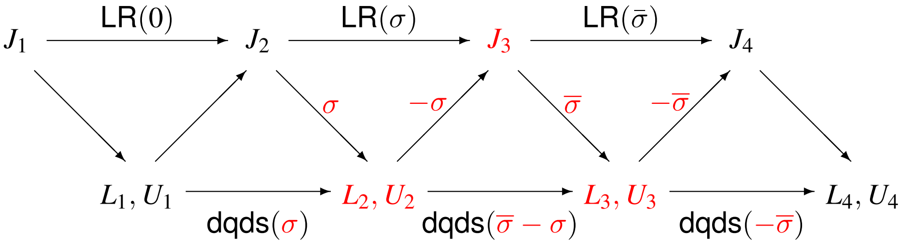

Figure: Double shifted LR and three steps of dqds

$$
\begin{aligned}
U_1L_1 - \sigma I &= L_2U_2 \\
U_2L_2 - (-2(\Im\sigma)i) &= L_3U_3 \\
U_3L_3 - (-\overline{\sigma}I) &= L_4U_4
\end{aligned}
$$

Implicit triple dqds algorithm

- For $\mathcal{L} = L_2 L_3$ and $\mathcal{U} = U_3 U_2$

$$M \equiv (U_1 L_1)^2 - 2(\Re\sigma) U_1 L_1 + |\sigma|^2 I = \mathcal{L}\mathcal{U}$$

- $L_4 U_4 = \mathcal{L}^{-1} U_1 L_1 \mathcal{L}$

Implicit triple dqds algorithm

- For $\mathcal{L} = L_2 L_3$ and $\mathcal{U} = U_3 U_2$

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- $L_4 U_4 = \mathcal{L}^{-1} U_1 L_1 \mathcal{L}$
- L_4, U_4 from L_1,U_1 using *Bulge Chasing*

$$\underbrace{\mathcal{L}_1^{-1} U_1}\,\underbrace{L_1 \mathcal{L}_1} \qquad \text{[spoils the bidiagonal form]}$$

$$L' U' = \underbrace{\mathcal{L}_{n-1}^{-1} \ldots \mathcal{L}_2^{-1} \mathcal{L}_1^{-1} U_1}\,\underbrace{L_1 \mathcal{L}_1 \mathcal{L}_2 \ldots \mathcal{L}_{n-1}}.$$

- IMPLICIT L THEOREM ensures that

$$\mathcal{L} = \mathcal{L}_1 \mathcal{L}_2 \ldots \mathcal{L}_{n-1} \qquad \text{and} \qquad L_4 = L',\ U_4 = U'$$

Derivation of implicit triple dqds

- Get $\mathcal{L}_i$ and find unique X such that

$$L_4 = \mathcal{L}_n^{-1}\mathcal{L}_{n-1}^{-1}\dots\mathcal{L}_2^{-1}\mathcal{L}_1^{-1}U_1X^{-1} \qquad [U_1 \longrightarrow L_4]$$

$$U_4 = XL_1\mathcal{L}_1\mathcal{L}_2\dots\mathcal{L}_{n-1}\mathcal{L}_n \qquad [L_1 \longrightarrow U_4]$$

$$L_4U_4 = \underbrace{\mathcal{L}^{-1}U_1X^{-1}}\underbrace{XL_1\mathcal{L}}$$

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$$L_4U_4 = \underbrace{\mathcal{L}^{-1}U_1X^{-1}}\underbrace{XL_1\mathcal{L}}$$

- X will be best written as

$$X = X_nX_2\cdots X_1$$

where

$$X_i = Y_iZ_i$$

Some detail

- Start

$$U_1 = \begin{bmatrix} u_1 & 1 & & & \\ & u_2 & 1 & & \\ & & u_3 & \ddots & \\ & & & \ddots & 1 \\ & & & & u_n \end{bmatrix}, \quad L_1 = \begin{bmatrix} 1 & & & & \\ l_1 & 1 & & & \\ & l_2 & 1 & & \\ & & \ddots & \ddots & \\ & & & l_{n-1} & 1 \end{bmatrix}$$

Some detail

- Start

$$U_1 = \begin{bmatrix} u_1 & 1 & & & \\ & u_2 & 1 & & \\ & & u_3 & \ddots & \\ & & & \ddots & 1 \\ & & & & u_n \end{bmatrix}, \quad L_1 = \begin{bmatrix} 1 & & & & \\ l_1 & 1 & & & \\ & l_2 & 1 & & \\ & & \ddots & \ddots & \\ & & & l_{n-1} & 1 \end{bmatrix}$$

- End

$$L_4 = \begin{bmatrix} 1 & & & & \\ \hat{l}_1 & 1 & & & \\ & \hat{l}_2 & 1 & & \\ & & \ddots & \ddots & \\ & & & \hat{l}_{n-1} & 1 \end{bmatrix}, \quad U_4 = \begin{bmatrix} \hat{u}_1 & 1 & & & \\ & \hat{u}_2 & 1 & & \\ & & \hat{u}_3 & \ddots & \\ & & & \ddots & 1 \\ & & & & \hat{u}_n \end{bmatrix}$$

- *Active* part of F and active part of G

$$\mathcal{L}_i^{-1} F Z_i^{-1} Y_i^{-1} = \begin{bmatrix} \ddots & & & & & & \\ \ddots & 1 & & & & & \\ & \hat{l}_{i-1} & 1 & & & & \\ & & \hat{l}_i & u_{i+1} & 1 & & \\ & & + & & u_{i+2} & 1 & \\ & & + & & & u_{i+3} & \ddots \\ & & & & & & \ddots \end{bmatrix}$$

$$Y_i Z_i G \mathcal{L}_i = \begin{bmatrix} \ddots & \ddots & & & & & \\ & \hat{u}_{i-1} & 1 & & & & \\ & & \hat{u}_i & 1 & & & \\ & & & * & & & \\ & & & + & 1 & & \\ & & & + & l_{i+2} & 1 & \\ & & & & & \ddots & \ddots \end{bmatrix}$$

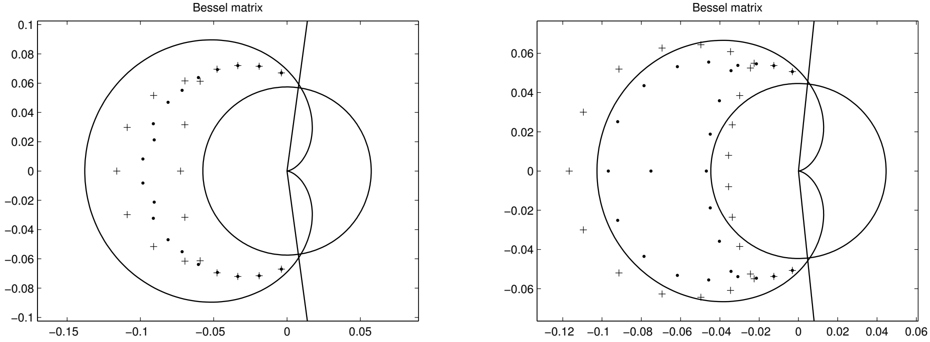
The 3dqds algorithm

for $i = 2, \ldots, n-3$

$$
\begin{aligned}
&x_l = x_l * aux_1 \\
&y_l = y_l * aux_1 \\
&\hat{u}_i = t + y_r + x_l \\
&aux_1 = 1/\hat{u}_i \\
&aux = (l_{i+1} * x_l + y_l + z_r) * aux_1 \\
&y_r = l_{i+1} - aux \\
&t = u_{i+1} * t * aux_1 \\
&\hat{l}_i = u_{i+1} - t + aux - x_l \\
&z_r = -l_{i+2} * y_l * aux_1 \\
&x_l = u_{i+2} * aux - z_r - y_l \\
&y_l = -u_{i+3} * z_r \\
&aux_1 = 1/\hat{l}_i
\end{aligned}
$$

end for

Numerical examples
1. Bessel matrices

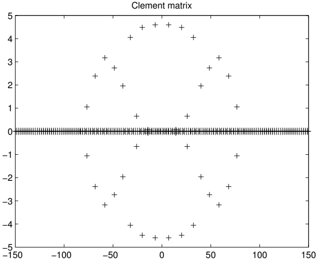


(a) $n = 20$

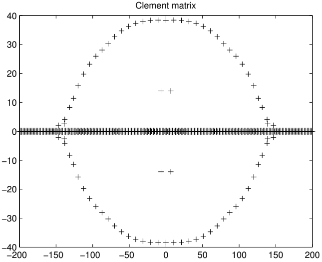
(b) $n = 25$

Figure: *Bessel matrix* $B_n^{(-4.5,2)}$

2. Clement matrices



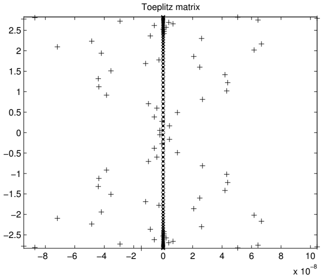
(a) $n = 150$



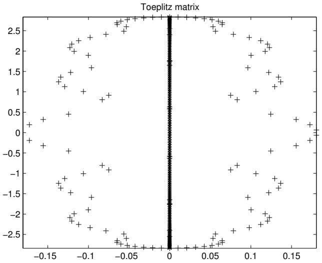
(b) $n = 200$

	3dqds		eig	
n	rel_{min}	rel_{max}	rel_{min}	rel_{max}
300	$3.6\ 10^{-11}$	$1.1\ 10^{-8}$	$6.6\ 10^{-3}$	$1.7\ 10^{2}$
450	$4.5\ 10^{-12}$	$1.8\ 10^{-8}$	$4.5\ 10^{-3}$	$2.6\ 10^{2}$

Table: *Relative errors for the Clement matrix*



(c) $n = 80$

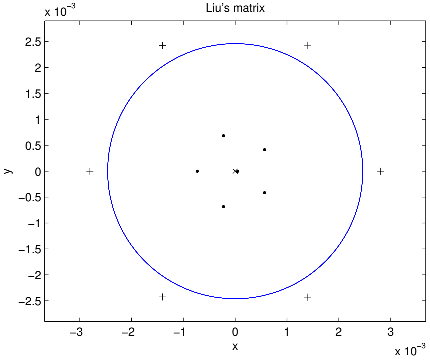


(d) $n = 150$

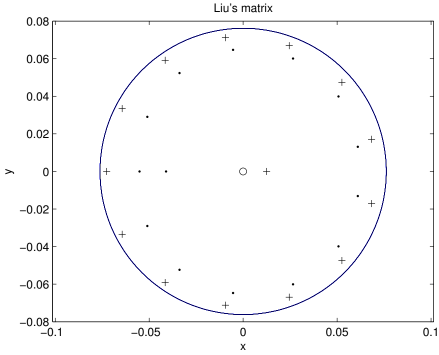
	3dqds		eig	
n	rel_{min}	rel_{max}	rel_{min}	rel_{max}
80	$5.4\ 10^{-14}$	$3.5\ 10^{-10}$	$5.0\ 10^{-9}$	$1.2\ 10^{-6}$
150	$1.2\ 10^{-13}$	$4.3\ 10^{-5}$	$3.2\ 10^{-3}$	$1.8\ 10^{-1}$

Table: *Relative errors for Toeplitz matrix* $T_n^{(1,2,-1)}$

4. One-point spectrum Liu matrices



(e) $n = 6$



(f) $n = 14$

Figure: *Liu matrices*

- Approximations inside the circle $|z| = \sqrt[n]{\varepsilon}$ ($\varepsilon \approx 1.1\ 10^{-16}$)

Liu matrices (cont.)

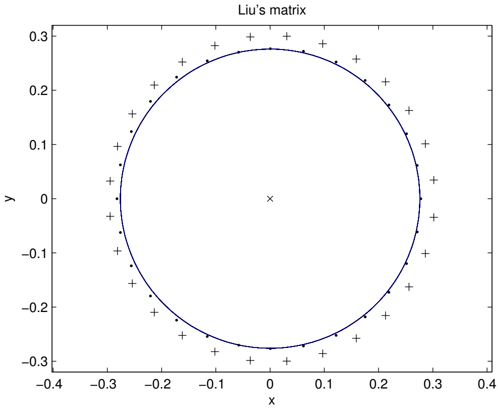


Figure: *Liu matrix* $(n = 28)$

Work in progress

- Develop a more sophisticated version of 3dqds
- Develop realistic condition numbers
- Error analysis

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- Develop realistic condition numbers
- Error analysis

- Explore properties of different representations of tridiagonals
- How well can we define the spectrum?

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Connection of double shift LR to dqds

Double shifted LR algorithm dqds

$$\begin{cases} J_1 = & L_1 U_1 \\ J_2 = & U_1 L_1 \end{cases}$$

Connection of double shift LR to dqds

Double shifted LR algorithm   dqds

$$\begin{cases} J_1 = & L_1 U_1 \\ J_2 = & U_1 L_1 \end{cases}$$

$$\begin{cases} J_2 - \sigma I = & L_2 U_2 \\ J_3 = & U_2 L_2 + \sigma I \end{cases}$$

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$$U_1 L_1 - \sigma I = L_2 U_2$$

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$$U_1 L_1 - \sigma I = L_2 U_2$$

$$\begin{cases} J_3 - \overline{\sigma} I = & L_3 U_3 \\ J_4 = & U_3 L_3 + \overline{\sigma} I \end{cases}$$

Connection of double shift LR to dqds

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$$\begin{cases} J_3 - \overline{\sigma} I = & L_3U_3 \\ J_4 = & U_3L_3 + \overline{\sigma} I \end{cases} \qquad (U_2L_2 + \sigma I) - \overline{\sigma} I = L_3U_3$$

Connection of double shift LR to dqds

Double shifted LR algorithm | dqds

$$\begin{cases} J_1 = & L_1U_1 \\ J_2 = & U_1L_1 \end{cases}$$

$$\begin{cases} J_2 - \sigma I = & L_2U_2 \\ J_3 = & U_2L_2 + \sigma I \end{cases} \qquad U_1L_1 - \sigma I = L_2U_2$$

$$\begin{cases} J_3 - \overline{\sigma} I = & L_3U_3 \\ J_4 = & U_3L_3 + \overline{\sigma} I \end{cases} \qquad (U_2L_2 + \sigma I) - \overline{\sigma} I = L_3U_3$$

$$\begin{cases} J_4 = & L_4U_4 \\ \dots \end{cases}$$

Connection of double shift LR to dqds

Double shifted LR algorithm   dqds

$$\begin{cases} J_1 = & L_1 U_1 \\ J_2 = & U_1 L_1 \end{cases}$$

$$\begin{cases} J_2 - \sigma I = & L_2 U_2 \\ J_3 = & U_2 L_2 + \sigma I \end{cases} \qquad U_1 L_1 - \sigma I = L_2 U_2$$

$$\begin{cases} J_3 - \overline{\sigma} I = & L_3 U_3 \\ J_4 = & U_3 L_3 + \overline{\sigma} I \end{cases} \qquad (U_2 L_2 + \sigma I) - \overline{\sigma} I = L_3 U_3$$

$$\begin{cases} J_4 = & L_4 U_4 \\ \quad \ldots \end{cases} \qquad (U_3 L_3 + \overline{\sigma} I) - 0I = L_4 U_4$$

Bessel matrix $B_{20}^{(-4.5,2)}$

λ	$\kappa_\lambda(B)$	$\kappa_\lambda(J)$	$\text{relcond}_1(\lambda; LU)$	$\text{relcond}_2(\lambda; LU)$
$-3.8\ 10^{-3}\ -6.7\ 10^{-2}\mathbf{i}$	$6\ 10^{8}$	$3\ 10^{22}$	$3\ 10^{5}$	$6\ 10^{5}$
$-3.8\ 10^{-3}\ +6.7\ 10^{-2}\mathbf{i}$	$6\ 10^{8}$	$4\ 10^{22}$	$5\ 10^{5}$	$9\ 10^{5}$
$-7.1\ 10^{-2}\ -1.6\ 10^{-2}\mathbf{i}$	$5\ 10^{10}$	$4\ 10^{25}$	$5\ 10^{5}$	$10\ 10^{5}$
$-7.1\ 10^{-2}\ +1.6\ 10^{-2}\mathbf{i}$	$5\ 10^{10}$	$4\ 10^{25}$	$3\ 10^{6}$	$10\ 10^{6}$
$-1.9\ 10^{-2}\ -7.2\ 10^{-2}\mathbf{i}$	$1\ 10^{14}$	$3\ 10^{23}$	$3\ 10^{6}$	$2\ 10^{6}$
$-1.9\ 10^{-2}\ +7.2\ 10^{-2}\mathbf{i}$	$1\ 10^{14}$	$3\ 10^{23}$	$9\ 10^{8}$	$1\ 10^{8}$
$-3.4\ 10^{-2}\ -7.2\ 10^{-2}\mathbf{i}$	$1\ 10^{14}$	$2\ 10^{24}$	$8\ 10^{8}$	$1\ 10^{8}$
$-3.4\ 10^{-2}\ +7.2\ 10^{-2}\mathbf{i}$	$1\ 10^{12}$	$2\ 10^{24}$	$3\ 10^{10}$	$3\ 10^{9}$
$-6.5\ 10^{-2}\ -4.6\ 10^{-2}\mathbf{i}$	$1\ 10^{12}$	$3\ 10^{25}$	$3\ 10^{10}$	$2\ 10^{9}$
$-6.5\ 10^{-2}\ +4.6\ 10^{-2}\mathbf{i}$	$1\ 10^{14}$	$3\ 10^{25}$	$10\ 10^{10}$	$6\ 10^{9}$
$-4.7\ 10^{-2}\ -6.9\ 10^{-2}\mathbf{i}$	$1\ 10^{14}$	$6\ 10^{24}$	$10\ 10^{10}$	$7\ 10^{9}$
$-4.7\ 10^{-2}\ +6.9\ 10^{-2}\mathbf{i}$	$1\ 10^{13}$	$6\ 10^{24}$	$5\ 10^{11}$	$3\ 10^{10}$
$-6.0\ 10^{-2}\ -6.6\ 10^{-2}\mathbf{i}$	$1\ 10^{13}$	$9\ 10^{24}$	$4\ 10^{11}$	$3\ 10^{10}$
$-6.0\ 10^{-2}\ +6.6\ 10^{-2}\mathbf{i}$	$1\ 10^{14}$	$9\ 10^{24}$	$1\ 10^{12}$	$9\ 10^{10}$
$-8.0\ 10^{-2}\ -5.9\ 10^{-2}\mathbf{i}$	$1\ 10^{14}$	$4\ 10^{24}$	$1\ 10^{12}$	$8\ 10^{10}$
$-8.0\ 10^{-2}\ +5.9\ 10^{-2}\mathbf{i}$	$1\ 10^{14}$	$4\ 10^{24}$	$3\ 10^{12}$	$2\ 10^{11}$
$-1.0\ 10^{-1}\ -4.3\ 10^{-2}\mathbf{i}$	$1\ 10^{14}$	$1\ 10^{24}$	$2\ 10^{12}$	$1\ 10^{11}$
$-1.0\ 10^{-1}\ +4.3\ 10^{-2}\mathbf{i}$	$2\ 10^{14}$	$1\ 10^{24}$	$3\ 10^{12}$	$2\ 10^{11}$
$-1.2\ 10^{-1}\ -1.6\ 10^{-2}\mathbf{i}$	$2\ 10^{14}$	$5\ 10^{23}$	$2\ 10^{12}$	$2\ 10^{11}$
$-1.2\ 10^{-1}\ +1.6\ 10^{-2}\mathbf{i}$	$2\ 10^{14}$	$5\ 10^{23}$	$2\ 10^{12}$	$1\ 10^{11}$

Table: *Relative condition numbers for* $B_{20}^{(-4.5,2)}$

Toeplitz matrix $T_{80}^{(1,2,-1)}$

λ	$\kappa_\lambda(T)$	$\kappa_\lambda(J)$	$\text{relcond}_1(\lambda; LU)$	$\text{relcond}_2(\lambda; LU)$
$1.0 - 5.4\ 10^{-2}\mathbf{i}$	$1\ 10^{8}$	$2\ 10^{10}$	4.7	4.7
$1.0 + 5.4\ 10^{-2}\mathbf{i}$	$1\ 10^{8}$	$2\ 10^{10}$	4.7	4.7
...	...	...	...	...
$1.0 - 3.8\ 10^{-1}\mathbf{i}$	$1\ 10^{9}$	$2\ 10^{10}$	4.4	4.6
$1.0 + 3.8\ 10^{-1}\mathbf{i}$	$1\ 10^{9}$	$2\ 10^{10}$	4.4	4.6
...	...	...	...	...
$1.0 - 1.6\mathbf{i}$	$9\ 10^{9}$	$1\ 10^{10}$	2.6	4.6
$1.0 + 1.6\mathbf{i}$	$9\ 10^{9}$	$1\ 10^{10}$	2.6	4.6
$1.0 - 2.1\mathbf{i}$	$1\ 10^{10}$	$9\ 10^{9}$	2.2	4.5
$1.0 + 2.1\mathbf{i}$	$1\ 10^{10}$	$9\ 10^{9}$	2.2	4.5
...	...	...	...	...
$1.0 - 2.7\mathbf{i}$	$2\ 10^{10}$	$1\ 10^{9}$	1.9	5.2
$1.0 + 2.7\mathbf{i}$	$2\ 10^{10}$	$1\ 10^{9}$	1.9	5.2
$1.0 - 2.8\mathbf{i}$	$7\ 10^{9}$	$9\ 10^{8}$	1.9	5.4
$1.0 + 2.8\mathbf{i}$	$7\ 10^{9}$	$9\ 10^{8}$	1.9	5.4
$1.0 - 2.8\mathbf{i}$	$2\ 10^{10}$	$4\ 10^{8}$	1.9	5.6
$1.0 + 2.8\mathbf{i}$	$2\ 10^{10}$	$4\ 10^{8}$	1.9	5.6
$1.0 - 2.8\mathbf{i}$	$1\ 10^{10}$	$1\ 10^{8}$	1.9	5.7
$1.0 + 2.8\mathbf{i}$	$1\ 10^{10}$	$1\ 10^{8}$	1.9	5.7

Table: *Relative condition numbers*

Summary of contributions

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$$J \qquad L_1, U_1 \qquad L, D, \Delta$$

  - superdiagonal of 1's

$$J = L_1 U_1$$

  - if balanced $(|\beta_j| = |\gamma_j|)$

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- Convergence of LR for one-point spectrum matrix
- Triple dqds algorithm
  - complex eigenvalues from real arithmetic
  - preserves tridiagonal structure