Accurate Computations with Totally Nonnegative Matrices

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Can we perform accurate computations with $n \times n$ structured matrices in $O(n^3)$ time?

GOAL

- **Conventional: Abs error bounds:**

$$|\hat{\lambda}_i - \lambda_i| \leq O(\epsilon)\frac{||A||}{|y^* x|} \qquad |\hat{\sigma}_i - \sigma_i| \leq O(\epsilon)\sigma_1$$

- **New: Relative error bounds:**

$$|\hat{\lambda}_i - \lambda_i| \leq O(\epsilon)|\lambda_i| \qquad |\hat{\sigma}_i - \sigma_i| \leq O(\epsilon)\sigma_i$$

- **Similarly for A^{-1}_{ij}, LDU, etc.**

THIS TALK

Positive answer for Totally Nonnegative matrices

OUTLINE

- **TN matrices**
  - **Definition**
  - **Examples**
  - **Properties**
- **Tricks for performing accurate computations**
  - **No subtractions**
  - **Use structure-revealing representation**
- **New results:**
  - **Can perform virtually all numerical linear algebra in the class of TN matrices to high relative accuracy**
  - **Accurate eigenvectors (with correct sign pattern)**
  - **TN toolbox available**

DEFINITION OF A TN MATRIX

$$\boldsymbol{A} \textbf{ is TN} \iff \textbf{All minors} \geq \mathbf{0}$$

SOME APPLICATIONS OF TN MATRICES

- **Vibrations of mechanical systems (Gantmacher, Krein)**
- **Corner cutting algorithms (Cutting corners from polytopes)**
- **Electrical Impedance Tomography (Y. Chen)**
- **Stochastic analysis**

- **Books by Karlin, Gantmacher–Krein, Gasca–Micchelli**
- **Motivated by work of Whitney, Björck, Pereyra, Higham, Gasca, Peña, Kahan, C. Johnson, Fallat**

EXAMPLES OF TN MATRICES

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2^2 & 2^3 \\ 1 & 3 & 3^2 & 3^3 \\ 1 & 4 & 4^2 & 4^3 \end{bmatrix}$$

Vandermonde

$$\begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix}$$

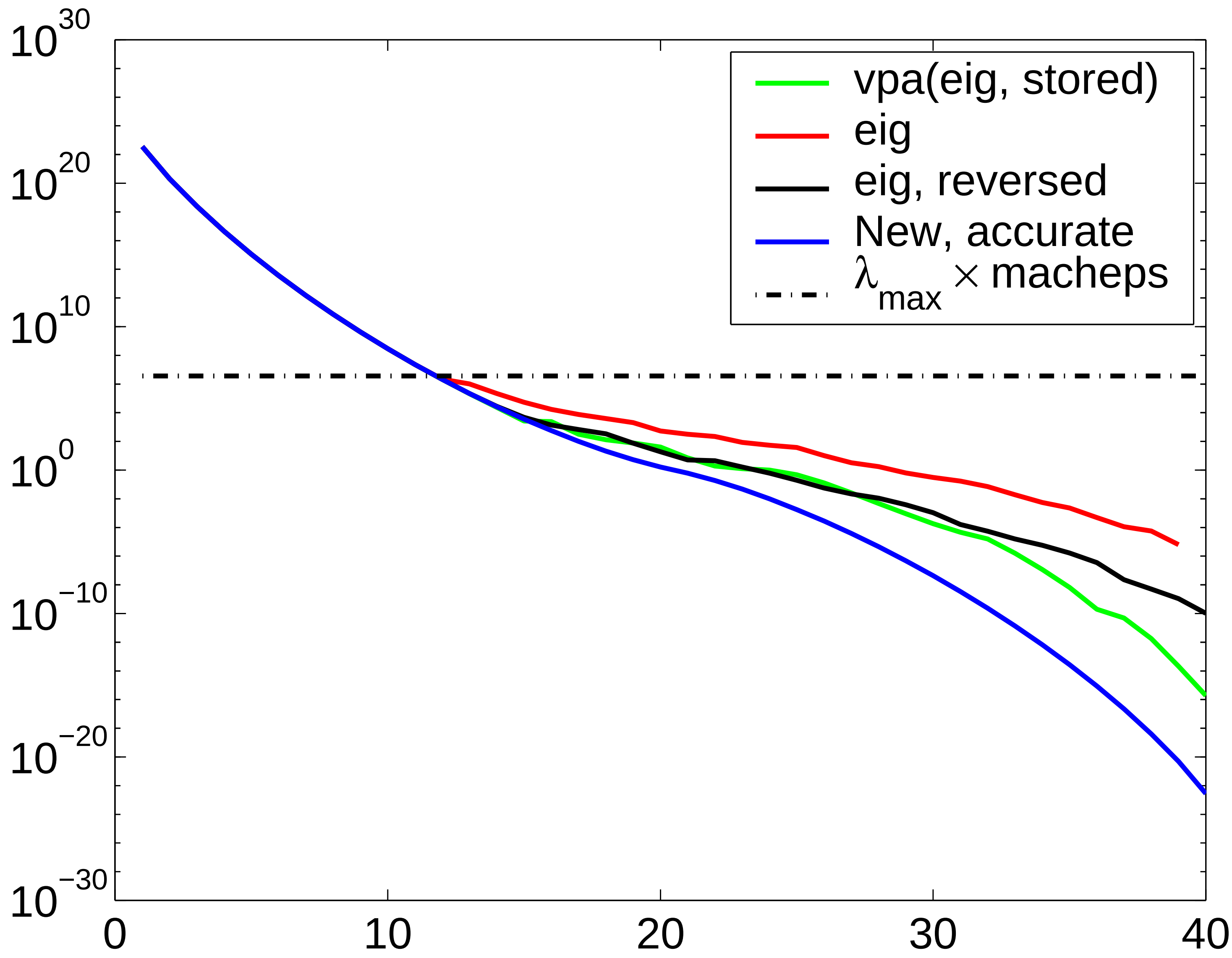
Hilbert (Cauchy)

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \\ 1 & 3 & 6 & 10 \\ 1 & 4 & 10 & 20 \end{bmatrix}$$

Pascal

Notoriously ill conditioned $\Longrightarrow$ conventional algorithms fail

Computed Eigenvalues of Pascal(40)

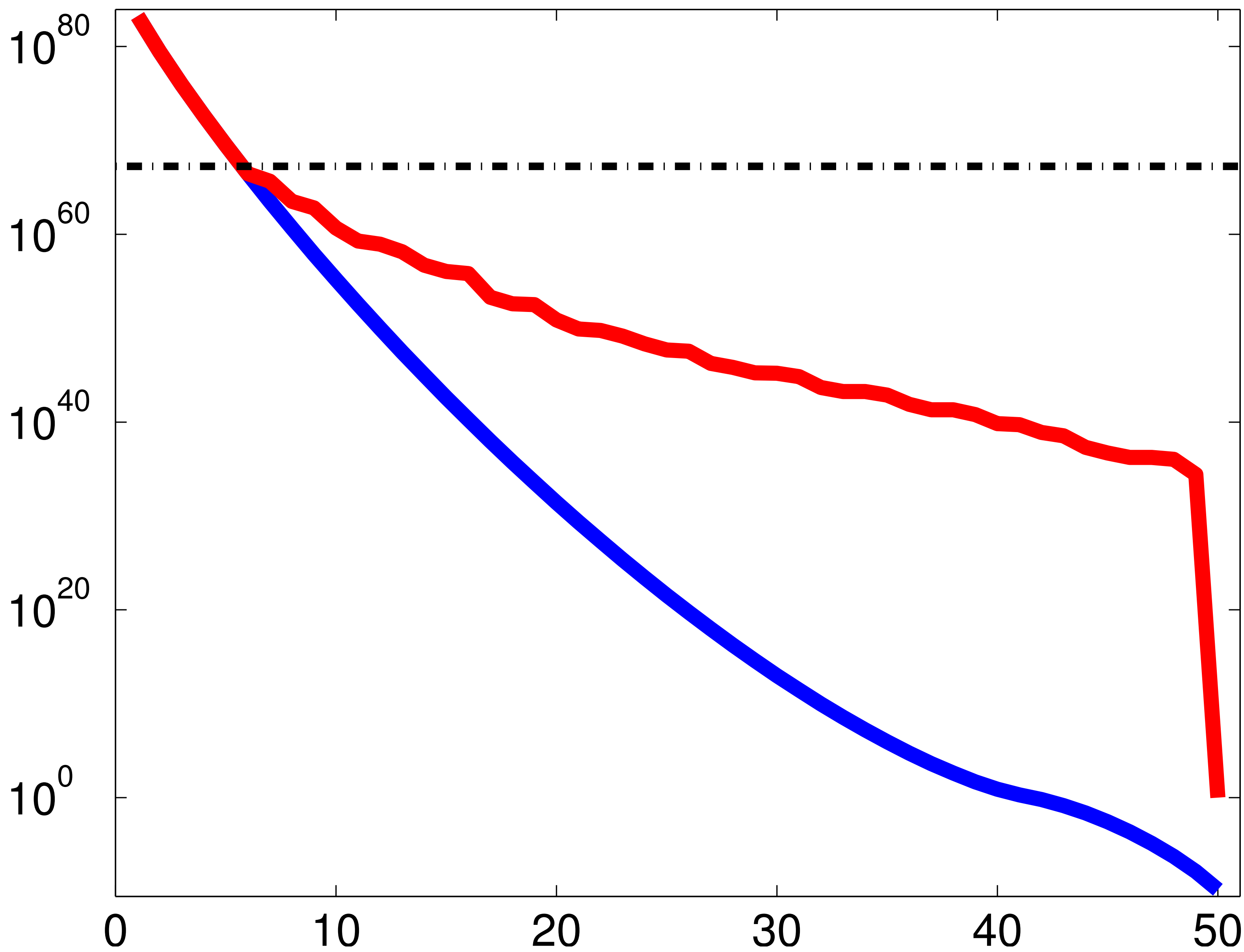


EXAMPLE: PASCAL(5)

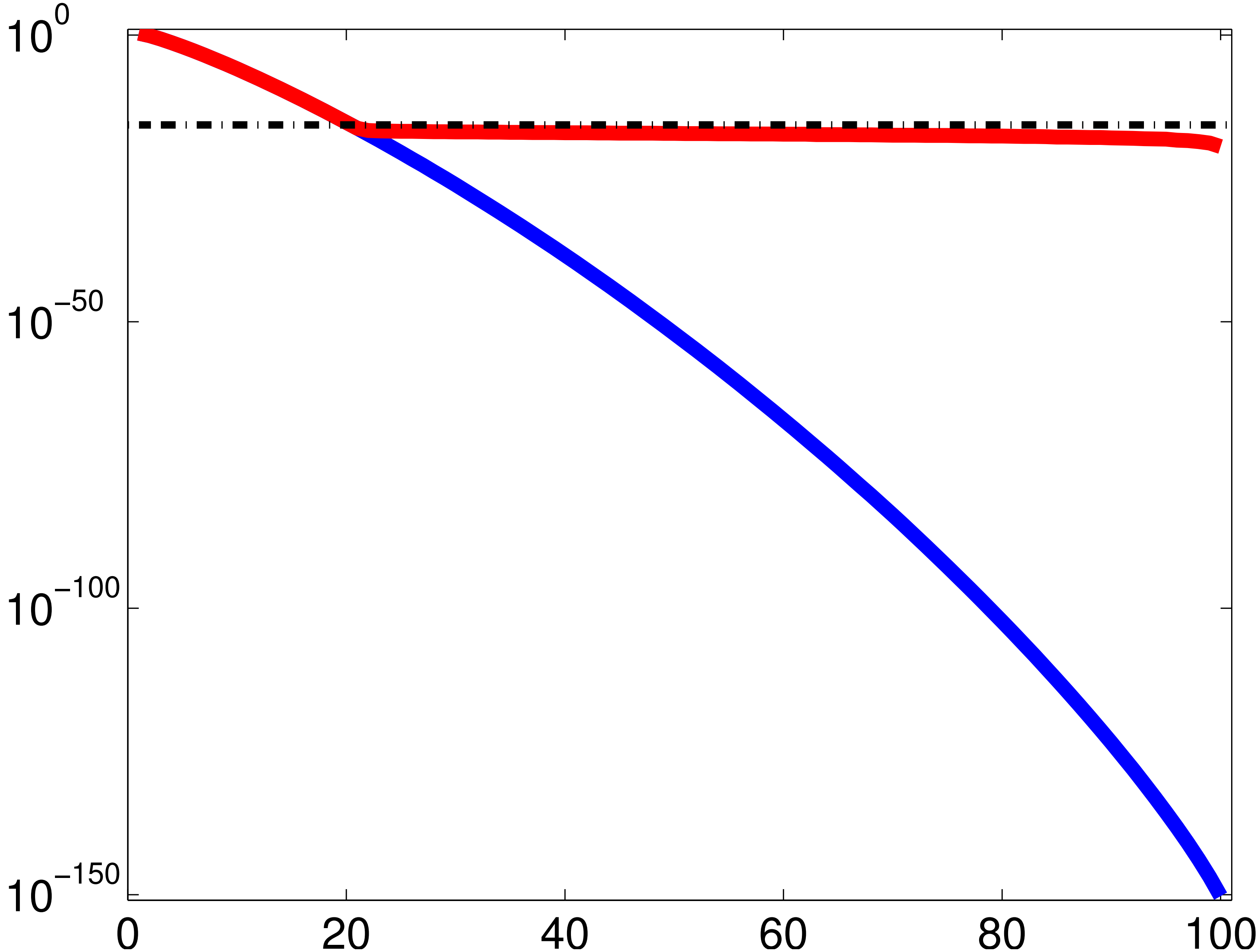
$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 & 5 \\ 1 & 3 & 6 & 10 & 15 \\ 1 & 4 & 10 & 20 & 35 \\ 1 & 5 & 15 & 35 & 70 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & -1 & 1 & -1 & 1 \\ -1 & 2 & -3 & 4 & -5 \\ 1 & -3 & 6 & -10 & 15 \\ -1 & 4 & -10 & 20 & -35 \\ 1 & -5 & 15 & -35 & 70 \end{bmatrix}$$

$$P_n^{-1} = \mathrm{diag}(\pm 1) \cdot P_n \cdot \mathrm{diag}(\pm 1)$$

Eigenvalues of 50 × 50 Vandermonde Matrix $V_{ij} = i^{j-1}$



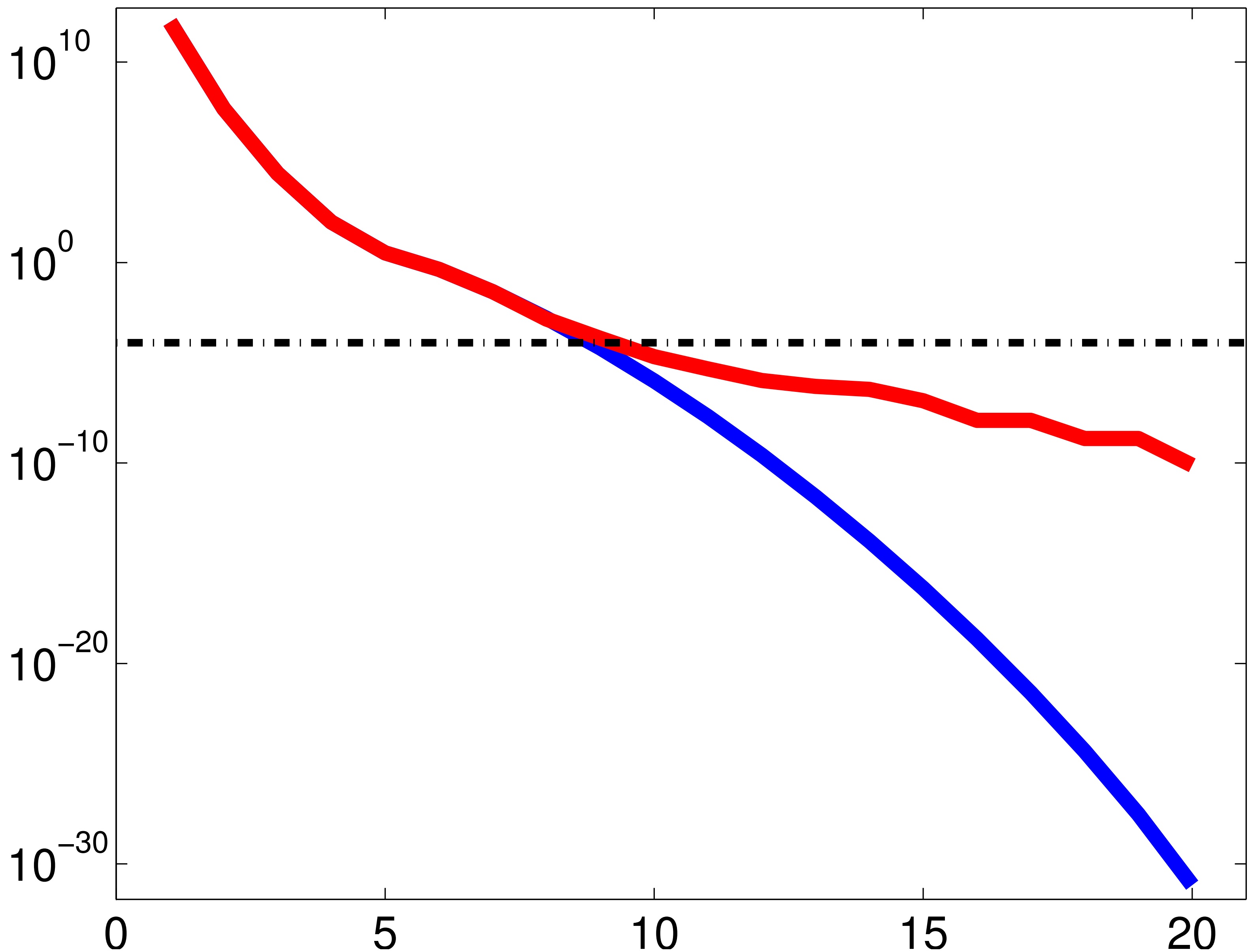
Eigenvalues of 100 × 100 Hilbert Matrix $H_{ij} = 1/(i + j - 1)$



MATHEMATICAL PROPERTIES OF TN MATRICES

- $\lambda_i > 0$ (even when A is nonsymmetric)
- The set of TN matrices closed under:
  - Multiplication
  - Schur Complementation
  - Taking a converse $A^{\#} = (a_{n-j+1,n-i+1})_{i,j=1}^{n}$
  - Taking a J-Inverse: $JA^{-1}J = \left((-1)^{i+j}(A^{-1})_{ij}\right)$ (= abs(A^{-1}))
  - Taking a submatrix
- Goal: Accurate computations within the class of TN matrices
- Consider only irreducible TN matrices

New: Eigenvalues of 20-by-30 Hilbert × 30-by-20 Pascal



EIGENVECTORS ARE OSCILLATING

```
>> [U,S]=svd(pascal(4))

U =
   -0.0602   -0.5304    0.7873   -0.3087
   -0.2012   -0.6403   -0.1632    0.7231
   -0.4581   -0.3918   -0.5321   -0.5946
   -0.8638    0.3939    0.2654    0.1684

S =
   26.3047         0         0         0
         0    2.2034         0         0
         0         0    0.4538         0
         0         0         0    0.0380
```

jth eigenvector has $j-1$ changes of sign

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```

jth eigenvector has $j-1$ changes of sign

This statement fails numerically for large sizes

TWO TRICKS FOR ACCURATE COMPUTATIONS

- **No subtractions!**
- **Use structure-revealing representation**

WHY CAN SUBTRACTIONS BE BAD?

- if $\hat{a} \approx a > 0$ and $\hat{b} \approx b > 0$ to (say) 9 digits, then

$$\left.\begin{aligned} \hat{a} \cdot \hat{b} &\approx a \cdot b \\ \hat{a} + \hat{b} &\approx a + b \\ \hat{a}/\hat{b} &\approx a/b \end{aligned}\right\} \quad \text{to about 9 digits}$$

BUT

$$\hat{a} - \hat{b}$$

may have no correct digits if $a \approx b$, e.g.,

$$\begin{array}{rl} & .123456789xxx \\ - & .123456789yyy \\ \hline & .000000000zzz \end{array}$$

- Some subtractions are OK, e.g.,

$$x_i - x_j$$

where x_i are initial data.

NO SUBTRACTIONS

$\Downarrow$ **Error Analysis**

$1 + \varepsilon$ errors accumulate multiplicatively

$\Downarrow$ $\boldsymbol{O(n^3)}$ **factors**

ACCURACY

No Subtractions $\not\Rightarrow$ Accuracy

Ref: Prof. Kahan's talk and paper, §10

REPRESENTING TN MATRICES

$$\mathbf{PASCAL(4)} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \\ 1 & 3 & 6 & 10 \\ 1 & 4 & 10 & 20 \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & 1 & 1 & \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ & 1 & 1 & \\ & & 1 & 1 \end{bmatrix}}_{\boldsymbol{L}} \underbrace{\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}}_{\boldsymbol{D}} \underbrace{\begin{bmatrix} 1 & 1 & & \\ & 1 & 1 & \\ & & 1 & 1 \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & 1 & \\ & & 1 & 1 \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & 1 \\ & & & 1 \end{bmatrix}}_{\boldsymbol{U}}$$

- **Reveals TN structure**
- **Obtained by elimination using adjacent rows**

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$$= \underbrace{\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & 1 & 1 & \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ & 1 & 1 & \\ & & 1 & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}}_{D} \underbrace{\begin{bmatrix} 1 & 1 & & \\ & 1 & 1 & \\ & & 1 & 1 \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & 1 & \\ & & 1 & 1 \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & 1 \\ & & & 1 \end{bmatrix}}_{U}$$

- **Reveals TN structure**
- **Obtained by elimination using adjacent rows**

$$\textbf{Vandermonde} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2^2 & 2^3 \\ 1 & 3 & 3^2 & 3^3 \\ 1 & 4 & 4^2 & 4^3 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & 1 & 1 & \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ & 1 & 1 & \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 2 & \\ & & & 6 \end{bmatrix} \begin{bmatrix} 1 & 1 & & \\ & 1 & 2 & \\ & & 1 & 3 \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & 1 & \\ & & 1 & 2 \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & 1 \\ & & & 1 \end{bmatrix}$$

ANY TN = PRODUCT OF NONNEGATIVE BIDIAGONALS

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & l_{41} & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & l_{31} & 1 & \\ & & l_{42} & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ l_{21} & 1 & & \\ & l_{32} & 1 & \\ & & l_{43} & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & d_3 & \\ & & & d_4 \end{bmatrix}}_{D} \underbrace{\begin{bmatrix} 1 & u_{12} & & \\ & 1 & u_{23} & \\ & & 1 & u_{34} \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & u_{13} & \\ & & 1 & u_{24} \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & u_{14} \\ & & & 1 \end{bmatrix}}_{U}$$

Theorem: A is TN $\iff l_{ij}, d_i, u_{ij} \geq 0$

Proof:

$\Leftarrow$ (TN)×(TN) = TN (Cauchy–Binet)

$\Rightarrow$ Red entries $= \dfrac{\det A(1{:}k, i-k+2{:}i+1)}{\det A(1{:}k-1, i-k+2{:}i)} \cdot \dfrac{\det A(1{:}k-1, i-k+1{:}i-1)}{\det A(1{:}k, i-k+1{:}i)}$

ANY TN = PRODUCT OF NONNEGATIVE BIDIAGONALS

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

$$= \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & l_{41} & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & l_{31} & 1 & \\ & & l_{42} & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ l_{21} & 1 & & \\ & l_{32} & 1 & \\ & & l_{43} & 1 \end{bmatrix} \begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & d_3 & \\ & & & d_4 \end{bmatrix} \begin{bmatrix} 1 & u_{12} & & \\ & 1 & u_{23} & \\ & & 1 & u_{34} \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & u_{13} & \\ & & 1 & u_{24} \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & u_{14} \\ & & & 1 \end{bmatrix}$$

$\downarrow$ (nontrivial entries)

$$\mathcal{BD}(A) = \begin{Bmatrix} d_1 & u_{12} & u_{13} & u_{14} \\ l_{21} & d_2 & u_{23} & u_{24} \\ l_{31} & l_{32} & d_3 & u_{34} \\ l_{41} & l_{42} & l_{43} & d_4 \end{Bmatrix}$$

- An octant in n^2 space
- $\mathcal{BD}(A)$ reveals A is TN !!!
- Thm (K.): Determines λ_i, σ_i, A^{-1}_{ij}, etc., to high relative accuracy

EXAMPLE

- Say A', A'' – TN, and $A' \times A'' = A$

$$\begin{bmatrix} 1 & & \\ & 1 & \\ & l'_{31} & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ l'_{21} & 1 & \\ & l'_{32} & 1 \end{bmatrix} \begin{bmatrix} d'_1 & & \\ & d'_2 & \\ & & d'_3 \end{bmatrix} \begin{bmatrix} 1 & u'_{12} & \\ & 1 & u'_{23} \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & u'_{13} \\ & & 1 \end{bmatrix}$$

$$\times \begin{bmatrix} 1 & & \\ & 1 & \\ & l''_{31} & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ l''_{21} & 1 & \\ & l''_{32} & 1 \end{bmatrix} \begin{bmatrix} d''_1 & & \\ & d''_2 & \\ & & d''_3 \end{bmatrix} \begin{bmatrix} 1 & u''_{12} & \\ & 1 & u''_{23} \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & u''_{13} \\ & & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & & \\ & 1 & \\ & l_{31} & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ l_{21} & 1 & \\ & l_{32} & 1 \end{bmatrix} \begin{bmatrix} d_1 & & \\ & d_2 & \\ & & d_3 \end{bmatrix} \begin{bmatrix} 1 & u_{12} & \\ & 1 & u_{23} \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & u_{13} \\ & & 1 \end{bmatrix}$$

- $\mathcal{BD}(A)$ obtained from $\mathcal{BD}(A'), \mathcal{BD}(A'')$ using only $\times, /, +$
  $\Rightarrow$ rel. error in l_{ij}, d_i, u_{ij} bounded by $O(n^3\varepsilon)$
- Virtually all LA with TN matrices can be done analogously

Accurate Computations with TN Matrices

- Discard A, work with $\mathcal{BD}(A)$
- Transforming TN matrices happens to not involve subtractions (subtractions when working with matrix entries are equivalent to setting entries of $\mathcal{BD}(A)$ to zero exactly)
- Need bidiagonal SVD alg for eigenvalues, SVD
- Challenge: Eigenvectors such that

$$\#\text{ sign changes in } v_j \equiv S(v_j) = j - 1$$

EIGENVECTORS

```
>> [V,S]=svd(pascal(4))

V =  -0.0602   -0.5304    0.7873   -0.3087
     -0.2012   -0.6403   -0.1632    0.7231
     -0.4581   -0.3918   -0.5321   -0.5946
     -0.8638    0.3939    0.2654    0.1684
```

$S(v_j) = j - 1$, but $S(\hat{v}_j) = j - 1$ fails for larger sizes

- Eigenvectors computed accurately in norm:

$$\|v_j - \hat{v}_j\| = \frac{O(\varepsilon)}{\text{relgap}_i}$$

- But (tiny) v_{ij} and sign(v_{ij}) may NOT BE
- New: We compute v_j such that $S(v_j) = j - 1$!
- Trick: If A is TN, then $A = \Pi$ Bidiagonals $\Rightarrow$

$$S(Ax) \leq S(x) \qquad S(A^{-1}x) \geq j - 1$$

Both analytically and numerically!

- Structure-preserving reduction $\Rightarrow S(\hat{v}_j) = j - 1$

QR DECOMPOSITION

```
[Q,R]=qr(pascal(4))

Q = -0.5000    0.6708    0.5000    0.2236
    -0.5000    0.2236   -0.5000   -0.6708
    -0.5000   -0.2236   -0.5000    0.6708
    -0.5000   -0.6708    0.5000   -0.2236
```

- **Theorem (K.):** $S(q_j) = j - 1$
- **Analogously computable so that** $S(\hat{q}_j) = j - 1$**.**

CONCLUSIONS

- **Accurate computations in the class of TN matrices**
- $\boldsymbol{O(n^3)}$
- **TNPACK toolbox available**
- **Paper to appear in SIMAX**
- **All available from:** `math.mit.edu/~plamen`

- **TN Vandermonde** $(0 < x_1 < x_2 < \cdots < x_n)$

$$V = \left[x_i^{j-1}\right]_{i,j=1}^{n}$$

$$D_{ii} = \prod_{j=1}^{i-1}(x_i - x_j), \quad L^{(k)}_{i+1,i} = \prod_{j=n-k}^{i-1}\frac{x_{i+1}-x_{j+1}}{x_i - x_j}, \quad U^{(k)}_{i,i+1} = x_{i+n-k}$$

- **TN Cauchy** $(x_1 < \cdots < x_n,\ y_1 < \cdots < y_n\ , x_1 + y_1 > 0)$

$$C = \left[\frac{1}{x_i + y_j}\right]_{i,j=1}^{n}$$

$$D_{ii} = \prod_{k=1}^{i-1}\frac{(x_i - x_k)(y_i - y_k)}{(x_i + y_k)(y_i + x_k)}$$

$$L^{(k)}_{i,i+1} = \frac{x_{n-k} + y_{i-n+k+1}}{x_i + y_{i-n+k+1}}\prod_{l=n-k}^{i-1}\frac{x_{i+1}-x_{l+1}}{x_i - x_l}\cdot\prod_{l=1}^{i-n+k-1}\frac{x_i + y_l}{x_{i+1}+y_l}$$

$$U^{(k)}_{i+1,i} = \frac{y_{n-k} + x_{i-n+k+1}}{y_i + x_{i-n+k+1}}\prod_{l=n-k}^{i-1}\frac{y_{i+1}-y_{l+1}}{y_i - y_l}\cdot\prod_{l=1}^{i-n+k-1}\frac{y_i + x_l}{y_{i+1}+x_l}$$

Building Block of TN Matrices – Elementary Bidiagonal Matrices

$$\boldsymbol{E}_i(\boldsymbol{x}) \equiv \begin{bmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & \ddots & & & & & \\ & & & 1 & & & & \\ & & & \boldsymbol{x} & 1 & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix}, \qquad \boldsymbol{E}_i^{-1}(\boldsymbol{x}) = \boldsymbol{E}_i(-\boldsymbol{x})$$

Building Block of TN Matrices – Elementary Bidiagonal Matrices

$$E_i(x) \equiv \begin{bmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & \ddots & & & & & \\ & & & 1 & & & & \\ & & & x & 1 & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{bmatrix}, \qquad E_i^{-1}(x) = E_i(-x)$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

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$$= \quad \Pi \; E_i(l_{ij}) \quad \cdot D \cdot \quad \Pi \; E_i^T(u_{ij})$$

VARIATION DIMINISHING PROPERTY

$$E_i(x) \cdot \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 1 & & \\ x & 1 & \\ & & 1 \end{bmatrix} \cdot \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} a \\ b + ax \\ c \end{bmatrix}, x > 0$$

$$\begin{matrix} + & & + \\ + & \longrightarrow & + \\ + & & + \end{matrix} \qquad \begin{matrix} + & & + \\ * & \longrightarrow & * \\ - & & - \end{matrix} \qquad \begin{matrix} + & & + \\ - & \longrightarrow & ? \\ + & & + \end{matrix}$$

$$\begin{matrix} - & & - \\ - & \longrightarrow & - \\ - & & - \end{matrix} \qquad \begin{matrix} - & & - \\ * & \longrightarrow & * \\ + & & + \end{matrix} \qquad \begin{matrix} - & & - \\ + & \longrightarrow & ? \\ - & & - \end{matrix}$$

$$0 \longrightarrow 0 \qquad 1 \longrightarrow 1 \qquad 2 \longrightarrow 0, 2$$

Therefore: #Sign Changes$(Az) \leq$ #Sign Changes(z)

Analogously: #Sign Changes$(A^{-1}z) \geq$ #Sign Changes(z)

EIGENVECTORS WITH CORRECT SIGN PATTERN

- $A = V\Lambda V^T$ symmetric TN $\Rightarrow$

$$V = \Pi \text{ Givens} = \Pi \begin{bmatrix} + & - \\ + & + \end{bmatrix} = \begin{bmatrix} 1 & \\ + & 1 \end{bmatrix} \begin{bmatrix} + & \\ & + \end{bmatrix} \begin{bmatrix} 1 & - \\ & 1 \end{bmatrix}$$

- Variation (non) diminishing $\Rightarrow$ $S(v_j) \leq j-1$
- Also numerically $\Rightarrow$ $S(\hat{v}_j) \leq j-1$
- Need equality!
- Next: Eigenvectors of $A^{-1} = V\Lambda^{-1}V^T$
- Analogously, $S(\tilde{v}_j) \geq j-1$
- Combine leading entries of $\hat{v}_j$ and trailing ones of $\tilde{v}_j$ to obtain w_j:

$$S(w_j) = j-1$$

- w_j also accurate on norm
- Works in the nonsymmetric case, thought notion of accuracy elusive ...