Accurate Eigenvectors and QR decompositions of Totally Positive Matrices

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$$\boldsymbol{A} \textbf{ is TP} \iff \textbf{All minors} > \mathbf{0}$$

Some Applications of TP 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

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

Vandermonde

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

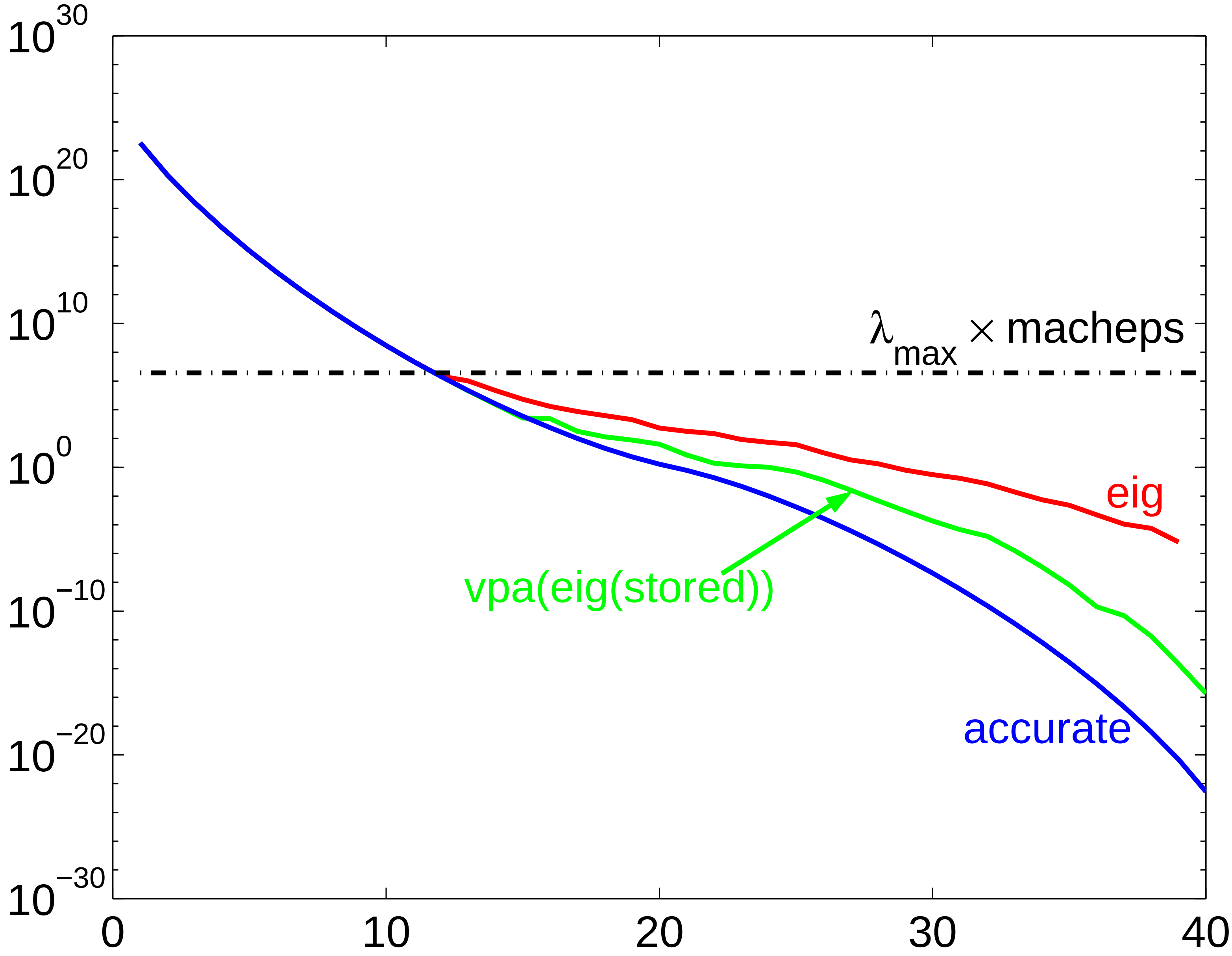
Hilbert
(Cauchy)

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

Pascal

Notoriously illconditioned $\Rightarrow$ conventional algorithms fail

Computed Eigenvalues of Pascal(40)



Goal: Numerically Respect the TP Structure

- $\lambda_i > 0$ (real!)
- Determined to high relative accuracy
- (TP)×(TP)=(TP)
  $\Rightarrow$ eig(Pascal × Hilbert) > 0, real
- Schur Complement is TP
- Re-signed inverse is TP (abs(A^{-1}))
- *Oscillating* properties:
  - jth eigenvector has $j-1$ changes of sign
  - New result: q_j in $A = QR$ has $j-1$ changes of sign
- We *guarantee* these numerically
- MATLAB Example for the sign changes

Virtually all TP linear algebra possible accurately

Approach:

- **Use a *structure-relealing* representation!**
- **Perturbation theory (K.) – $\boldsymbol{\lambda}_i, \boldsymbol{\sigma}_i$, etc., determined accurately**
- **Computations can be arranged so no subtractive cancellation is encountered**

$\Rightarrow$ High relative accuracy

Why Can Subtractions be Bad?

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

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

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.

Bidiagonal Decompositions of TP 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 (Neville)**

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

Any TP = 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 TP $\iff l_{ij}, d_i, u_{ij} > 0$
- This representation reveals the TP structure
- Thm (K.): $\mathcal{BD}(A)$ determines $\lambda_i, \sigma_i, A^{-1}_{ij}, \ldots$ accurately
- Red entries $= \frac{\det A(1:k, i-k+2:i+1)}{\det A(1:k-1, i-k+2:i)} \cdot \frac{\det A(1:k-1, i-k+1:i-1)}{\det A(1:k, i-k+1:i)}$

  $\Rightarrow$ Formulas

Accurate $\mathcal{BD}$ of Vandermonde and Cauchy

- $V = \left[x_i^{j-1}\right]_{i,j=1}^{n}$ (TP if $0 < x_1 < x_2 < \cdots < x_n$)

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

- $C = \left[\dfrac{1}{x_i + y_j}\right]_{i,j=1}^{n}$ (TP if $0 < x_1 < \cdots < x_n,\ 0 < y_1 < \cdots < y_n$)

$$\begin{aligned} D_{ii} &= \prod_{k=1}^{i-1} \frac{(x_i - x_k)(y_i - y_k)}{(x_i + y_k)(y_i + x_k)} \\ L^{(k)}_{i,i+1} &= \frac{x_{n-k} + y_{i-n+k+1}}{x_i + y_{i-n+k+1}} \prod_{l=n-k}^{i-1} \frac{x_{i+1} - x_{l+1}}{x_i - x_l} \cdot \prod_{l=1}^{i-n+k-1} \frac{x_i + y_l}{x_{i+1} + y_l} \\ U^{(k)}_{i+1,i} &= \frac{y_{n-k} + x_{i-n+k+1}}{y_i + x_{i-n+k+1}} \prod_{l=n-k}^{i-1} \frac{y_{i+1} - y_{l+1}}{y_i - y_l} \cdot \prod_{l=1}^{i-n+k-1} \frac{y_i + x_l}{y_{i+1} + x_l} \end{aligned}$$

- No subtractive cancellation $\Rightarrow$ accurate

Idea in Accurate Eigenvalue Computations

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

$$\downarrow \quad \text{(Well known similarity)}$$

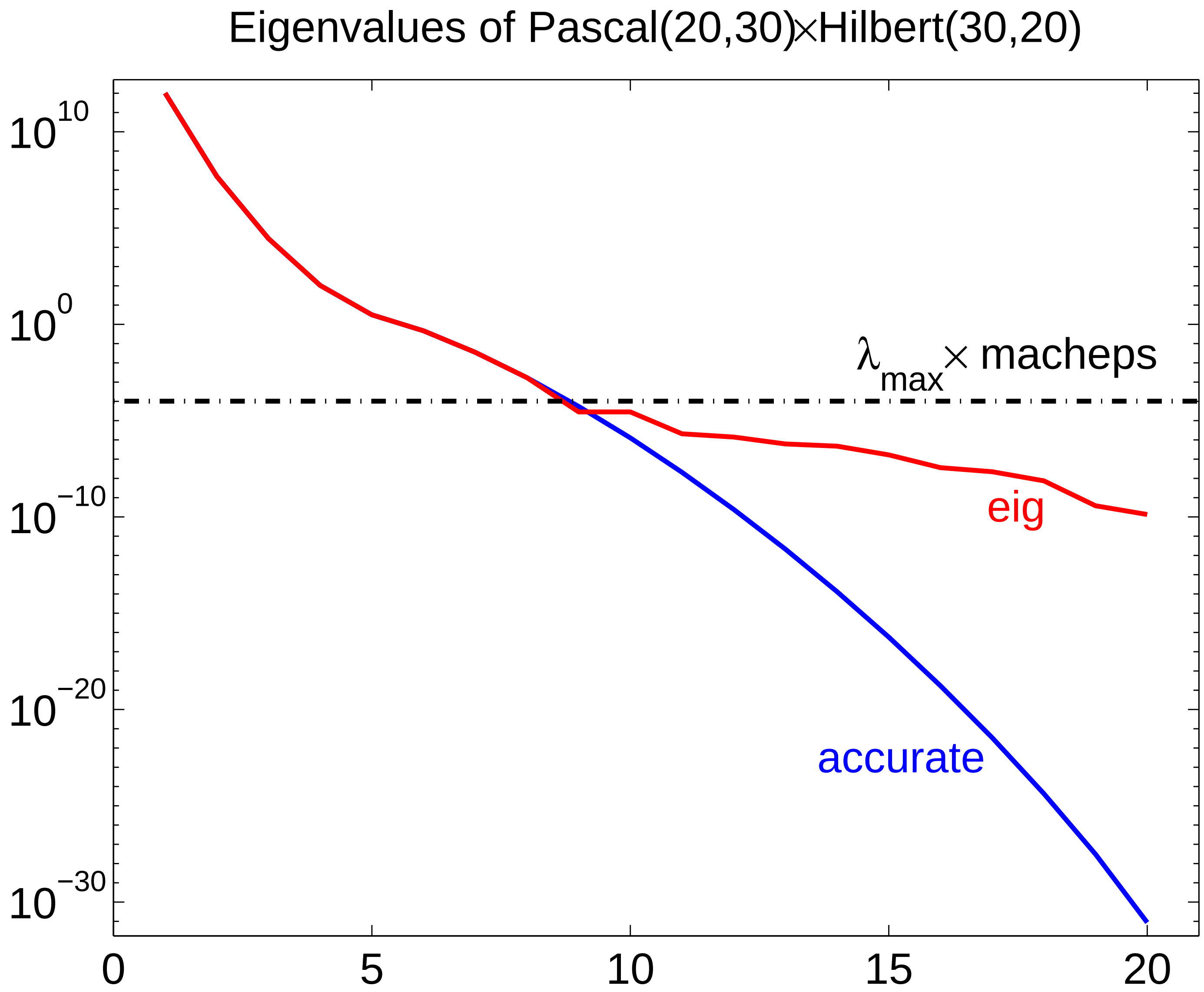
$$\begin{bmatrix} 1 &&& \\ l_1 & 1 && \\ & l_2 & 1 & \\ && l_3 & 1 \end{bmatrix}\begin{bmatrix} d_1 &&& \\ & d_2 && \\ && d_3 & \\ &&& d_4 \end{bmatrix}\begin{bmatrix} 1 & l_1 && \\ & 1 & l_2 & \\ && 1 & l_3 \\ &&& 1 \end{bmatrix}$$

$$\left(\begin{array}{c} \text{Blue} = \text{Rational\_Function(Red) using ONLY } +, \times, / \\ \Rightarrow \text{accurate! and } > 0 \end{array} \right)$$

$$\downarrow$$

$$\text{SVD}\left(\begin{bmatrix} d_1 &&& \\ & d_2 && \\ && d_3 & \\ &&& d_4 \end{bmatrix}^{\frac{1}{2}}\begin{bmatrix} 1 & l_1 && \\ & 1 & l_2 & \\ && 1 & l_3 \\ &&& 1 \end{bmatrix}\right)$$

Virtually all Linear Algebra with TP Analogous



Oscillating Vectors and TP Matrices

Let A be TP, $A = V \cdot \Lambda \cdot V^{-1}$, then

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

- Lowerly Totally Positive (LTP) matrix
- Variation Diminishing Property $\Rightarrow S(v_j) \leq j-1$
- V^{-T} eigenvecs of A^T $\Rightarrow V^{-T}$ LTP $\Rightarrow S(v_j) \geq j-1$

- Call these LTP^2 matrices (V *and* V^{-T} are LTP)
- Thm (Dopico, K.): LTP^2 $\Leftrightarrow S(v_j) = j-1$
- Cor: Q in $A = QR$ is LTP; $Q = Q^{-T}$ $\Rightarrow S(q_j) = j-1$
- Numerically?

- **Multiplication by a bidiagonal matrix**

$$\begin{bmatrix} 1 & & & \\ b_1 & 1 & & \\ & \ddots & \ddots & \\ & & b_{n-1} & 1 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 + b_1 x_1 \\ \vdots \\ x_n + b_{n-1} x_{n-1} \end{bmatrix}$$

—**all ops are** $ax + b$

- **Fused Multiply-Add,** $\mathrm{fl}(ax + b) = (ax + b)(1 + \delta)$
- **Use it to form** v_j **from** $\mathcal{BD}(V)$
- $\hat{v}_j$**—exact for** $\widehat{\mathcal{BD}}(V)$**—*still LTP!***

$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & \widehat{+} & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & \widehat{+} & 1 & \\ & & \widehat{+} & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ \widehat{+} & 1 & & \\ & \widehat{+} & 1 & \\ & & \widehat{+} & 1 \end{bmatrix} \begin{bmatrix} \widehat{+} & & & \\ & \widehat{+} & & \\ & & \widehat{+} & \\ & & & \widehat{+} \end{bmatrix} \begin{bmatrix} 1 & \widehat{-} & & \\ & 1 & \widehat{-} & \\ & & 1 & \widehat{-} \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & \widehat{-} & \\ & & 1 & \widehat{-} \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \widehat{-} \\ & & & 1 \end{bmatrix} \cdot e_j = \hat{v}_j$$

$\Rightarrow S(\hat{v}_j) \le j - 1$

- $\hat{v}'_j$ **from** $\mathcal{BD}(V^{-T})$
- **Combine** $\hat{v}_j, \hat{v}'_j$ **to obtain** w_j**, s.t.** $S(w_j) = j - 1$

Conclusions

- **Virtually all linear algebra with TN matrices done to high relative accuracy in $O(n^3)$ time**
- **New: Understanding of oscillating properties of TP matrices**
- **Key: Bidiagonal Decompositions**
- **Slides, papers, software:**

  `http://math.mit.edu/~plamen` **(= Google(Plamen Koev))**