Accurate Eigenvalues and SVDs of Totally Nonnegative Matrices

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Motivation

- ▶ Def: A matrix is Totally Nonnegative (TN) if all minors ≥ 0
- This talk: All matrix computations with TN matrices possible:
 - to high relative accuracy
 - in floating point arithmetic
 - at no extra cost

Connection to computed-aided geometric design, e.g.,

"When converting a curve expressed in a B-spline expansion into its Bézier form, corner cutting of the Bspline control polygon leads to the Bézier points exactly when the Bézier matrix is totally positive."

Ref: Corner cutting algorithms for the Bézier representation of free form curves, Goodman, Micchelli, Linear Algebra Appl. 1998.

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Examples of TN matrices

Vandermonde, Hilbert, Pascal:

$$V = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2^2 & 2^3 \\ 1 & 3 & 3^2 & 3^3 \\ 1 & 5 & 5^2 & 5^3 \end{bmatrix} \quad H = \begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix}$$
$$P = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \\ 1 & 3 & 6 & 10 \\ 1 & 4 & 10 & 20 \end{bmatrix}$$

Also Cauchy, Said–Ball, etc.

 Ubiquitous in practice: Occupy an octant in n² space when properly parameterized (as will see)

The matrix eigenvalue problem

- Goal: compute all eigenvalues of a TN matrix in floating point arithmetic
- Including the zero Jordan structure!
- Very hard in general (per higher powers):

"The Jordan form is useful theoretically but is very hard to compute in a numerically stable fashion..."

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James Demmel, Applied Numerical Linear Algebra.

Why is that?

Floating point arithmetic

- ► Finite, countably many floating point numbers representing the infinite, uncountable R
- Roundoff errors could make equal eigenvalues different and *destroy* the Jordan structure!
- Even accurate eigenvalues alone are problematic
- The determinant and eigenvalues of $\begin{bmatrix} 1 & 3 \\ 3 & 9 \end{bmatrix}$.

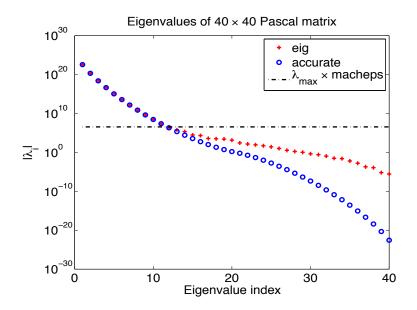
```
>> det([1 3; 3 9])
ans =
-4.9960e-16
>> eig([1 3; 3 9])
ans =
1.1102e-16
1.0000e+01
```

Eigenvalues of Pascal Matrix (which is TN)

$$P_n = \begin{bmatrix} 1 & 1 & 1 & 1 & \cdots \\ 1 & 2 & 3 & 4 & \cdots \\ 1 & 3 & 6 & 10 & \cdots \\ 1 & 4 & 10 & 20 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

 $cond(P_{40}) = 6 \times 10^{44}$

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Absolute vs. Relative Accuracy

Absolute accuracy

$$|\boldsymbol{x} - \hat{\boldsymbol{x}}| \leq \varepsilon$$

- Depends on the magnitude of x
- \triangleright $\varepsilon = 10^{-4}$ means what?
- Does x equal distance between planets or between molecules?
- Relative accuracy

$$|\boldsymbol{x} - \hat{\boldsymbol{x}}| \le \varepsilon |\boldsymbol{x}|$$

Works fine regardless of magnitude of *x* ε = 10⁻⁴ means *x̂* has 4 correct decimal digits!
 What if *x* = 0?

Reason accuracy is lost in floating point arithmetic

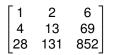
- ► fl($a \odot b$) = ($a \odot b$)(1 + δ), $\odot \in \{+, -, \times, /\}$
- Relative accuracy preserved in ×,+, / Proof: (1 + δ) factors accumulate multiplicatively
- Subtractions of approximate quantities dangerous:

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- subtraction of exact initial data is OK!
- if all other subtractions avoided, we get accuracy
- Exactly what we do with TN matrices

How do we know if a matrix is TN?

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How do we know if a matrix is TN?

$$\begin{bmatrix} 1 & 2 & 6 \\ 4 & 13 & 69 \\ 28 & 131 & 852 \end{bmatrix} = \begin{bmatrix} 1 & & \\ 1 & & \\ & 7 & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ 4 & 1 & \\ & 8 & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 5 & \\ & & 9 \end{bmatrix} \begin{bmatrix} 1 & 2 & \\ & 1 & 6 \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & 3 \\ & & 1 \end{bmatrix}$$

Product of TN bidiagonals

How do we know if a matrix is TN?

$$\begin{bmatrix} 1 & 2 & 6 \\ 4 & 13 & 69 \\ 28 & 131 & 852 \end{bmatrix} = \begin{bmatrix} 1 & & \\ & 1 & \\ & 7 & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ 4 & 1 & \\ & 8 & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 5 & \\ & & 9 \end{bmatrix} \begin{bmatrix} 1 & 2 & \\ & 1 & 6 \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & 3 \\ & & 1 \end{bmatrix}$$

Product of TN bidiagonals

In general:

$$A = L_1 \cdots L_{n-1} \cdot D \cdot U_{n-1} \cdots U_1,$$

where L_i lower bidiagonal, D diagonal, U_i upper bidiagonal

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- Cauchy–Binet: TN × TN = TN
- Each red entry = $\frac{\min_{1}(A)}{\min_{2}(A)} \cdot \frac{\min_{3}(A)}{\min_{4}(A)}$

How do we know if a matrix is TN?

$$\begin{bmatrix} 1 & 2 & 6 \\ 4 & 13 & 69 \\ 28 & 131 & 852 \end{bmatrix} = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 7 & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 4 & 1 \\ & & 8 & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 5 & \\ & & 9 \end{bmatrix} \begin{bmatrix} 1 & 2 & & \\ & 1 & 6 \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & 3 \\ & & 1 \end{bmatrix}$$

$$\downarrow$$

$$\mathcal{BD}(A) = \begin{cases} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{cases}$$

The n^2 nontrivial entries of $\mathcal{BD}(A)$:

- parameterize class of nonsingular TN matrices
- ▶ allow for highly accurate computations: If $A \rightarrow B$, then $\mathcal{BD}(A) \rightarrow \mathcal{BD}(B)$ accurate

Starting point is the bidiagonal decomposition

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

These are parameters the user must deliver

• Readily available for Vandermonde $A = \left[x_i^{j-1}\right]_{i=1}^n$

$$d_i = \prod_{j=1}^{i-1} (x_i - x_j), \quad l_{ik} = \prod_{j=n-k}^{i-1} \frac{x_{i+1} - x_{j+1}}{x_i - x_j}, \quad u_{ik} = x_{i+n-k}$$

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Starting point is the bidiagonal decomposition

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

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

$$I_{ik} = \frac{x_{n-k} + y_{i-n+k+1}}{x_i + y_{i-n+k+1}} \prod_{l=n-k}^{i-1} \frac{x_{l+1} - x_{l+1}}{x_i - x_l} \prod_{l=1}^{i-n+k-1} \frac{x_i + y_l}{x_{i+1} + y_l}$$

$$u_{ik} = \frac{y_{n-k} + x_{i-n+k+1}}{y_i + x_{i-n+k+1}} \prod_{l=n-k}^{i-1} \frac{y_{i+1} - y_{l+1}}{y_i - y_l} \prod_{l=1}^{i-n+k-1} \frac{y_i + x_l}{y_{i+1} + x_l}$$

Starting point is the bidiagonal decomposition

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

► Pascal: $d_i = l_{ij} = u_{ij} = 1$

- Reasonable requirement: Show me that your matrix is TN!
- Critical observation: BD(A) determines all eigenvalues accurately! (matrix entries do not!)
- I.e., small relative perturbations in BD(A) cause small relative perturbations to eigenvalues
- Eigenvalues "deserve" to be computed accurately
- The logic: The computed eigenvalues are rational functions of entries of BD(A)
- So those rational functions must have only positive coefficients (intuition, not proof)

Eigenvalue algorithm

- Reduction to tridiagonal form (Cryer '76)
- Using only one operation: Addition/subtraction of one row to the next/previous

• $\lambda_i = \sigma_i^2$, $\sigma_i = \text{singular values of bidiagonal Cholesky factor}$

- Solved accurately by Demmel and Kahan in 1989
- We implement on $\mathcal{BD}(A)$ and not on A!

Cryer's algorithm applied to A

► To create a 0 in position (3,1) of

we use similarity

$$\begin{bmatrix} 1 & & \\ & 1 & \\ & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 4 & 16 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & 1 \\ & 1 & 1 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & 2 & 4 \\ 1 & 3 & 9 \\ 0 & 1 & 7 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & 1 \\ & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 6 & 4 \\ 1 & 12 & 9 \\ 0 & 8 & 7 \end{bmatrix}$$

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Now, Cryer's applied to $\mathcal{BD}(A)$

Subtracting a multiple of one row from next to create a 0 is equivalent to setting an entry of the BD to 0

$$\begin{bmatrix} 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 4 & 16 \end{bmatrix} = \begin{bmatrix} 1 & & \\ & 1 & 1 \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & 1 \\ & & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & \\ & 1 & 2 \\ & & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 & & \\ & 1 & 3 \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & 2 \\ & & 1 \end{bmatrix} \downarrow$$
$$\downarrow$$
$$\begin{bmatrix} 1 & 2 & & \\ & 1 & 3 \\ & 0 & 1 & 7 \end{bmatrix} = \begin{bmatrix} 1 & & \\ & 1 & & \\ & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & 1 \\ & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & 2 \\ & & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 & & \\ & 1 & 3 \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & 2 \\ & & 1 \end{bmatrix}$$

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- No arithmetic performed!
- New matrix still TN

Next: Completing the similarity

Adding a multiple of one row/col to next/previous is done by changing the entries of the BD only

- New entries are rational functions with > 0 coefficients
- No subtractions \Rightarrow accuracy
- New matrix is still TN (Cauchy–Binet)

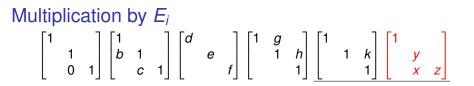
Elementary bidiagonal matrix

The only operation we need to compute everything TN

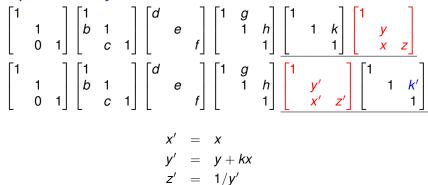
$$E_i(b,c) = egin{bmatrix} 1 & & & & \ & \ddots & & \ & & b & 1 & \ & & & \ddots & \ & & & & 1 \end{bmatrix}$$

an "elementary bidiagonal matrix", $b \ge 0, c \ge 0$

- Differs from I in two entries only
- Building block of $\mathcal{BD}(A)$: $A = (\prod E_i) \cdot (\prod E_i^T)$
- E_i = addition/subtraction of multiple of one row/column from next previous



Multiplication by E_i

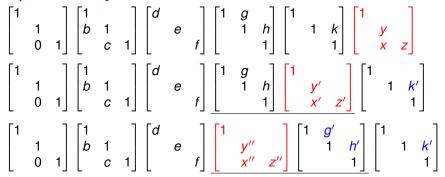


 $k' = kz/y_1$

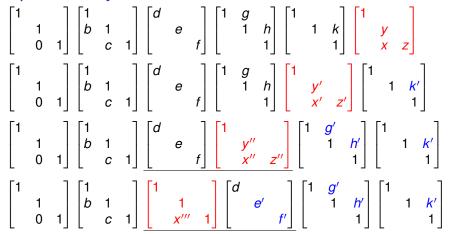
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This is the LR algorithm, implemented as dqd

Multiplication by E_i

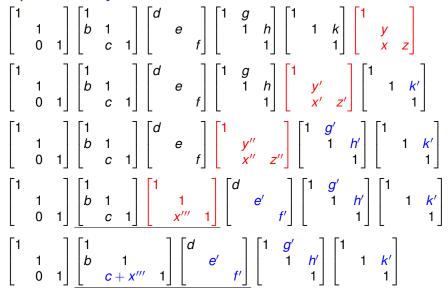


Multiplication by E_i



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Multiplication by E_i



Jordan blocks corresponding to zero eigenvalues

- OK, we get accurate eigenvalues
- Zero eigenvalues are exact!
- How about Jordan blocks?
 - $n \operatorname{rank}(A) = #$ Jordan blocks
 - ▶ $rank(A) rank(A^2) = #$ of Jordan blocks of size ≥ 2
 - ► ...
 - rank(A), rank(A²), ... readily obtainable from its BD
 - A² is TN (as a product of TN) and its BD is a TN-preserving op, thus BD accurate

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• need to form BD of A^2, \ldots, A^n

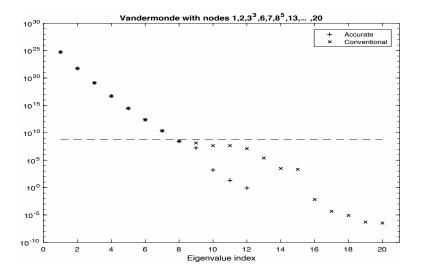
Example

A = 3 3 2 1 2 2 3 2 1 1 2 3 1 1 2 3 >> eig(A) ans = 7.828427124746188e+00 2.171572875253811e+00 5.247731480861326e-16 -1.110223024625157e-16 >> [B,C]=STNBD(A); [e,jb]=STNEigenValues(B,C) e = 7.8284 2.1716 0 0

jb =

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Conclusions

- First example of a Jordan structure being computed to high relative accuracy
- Complete Jordan structure of *Irreducible* TN matrices (Nonzero eigenvalues are distinct per Fallat–Gekhtman.)
- Future work: Get formulas for non-unique BD of singular Vandermonde, etc.

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Software, paper:

http://www.math.sjsu.edu/~koev