Accurate and Efficient Matrix Computations
with Totally Positive Generalized Vandermonde Matrices
Using Schur Functions

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GOALS

- **Accurate** (Small relative error) and **Efficient** \(O(n^3)\) or perhaps \(O(n^p)\), independent of condition number

Linear Algebra
  - \(A^{-1}\)
  - \(Ax = b\)
  - LDU from GENP, GEPP, GECP
  - SVD

- Can’t be done for general matrices, must be “structured”
  - Certain sparsity patterns
  - Cauchy
  - Vandermonde
  - ...

- Goal of this talk: Accurate and Efficient Linear Algebra for Generalized Vandermonde Matrices
<table>
<thead>
<tr>
<th>Type of Matrix</th>
<th>$\det(A)$</th>
<th>$A^{-1}$</th>
<th>Any minor</th>
<th>GENP</th>
<th>GEPP</th>
<th>GECP</th>
<th>SVD</th>
<th>Small Forward Error in $Ax = b$</th>
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**Totally Positive** = Matrix with all minors $> 0$
OUTLINE

• Model of arithmetic
• Classical method for achieving the goals for simple examples – The Björck-Pereyra Method for Vandermonde Matrices
• How and why it works?
• Application to TP Generalized Vandermonde matrices
How can we lose accuracy in computing in floating point?

- $\text{fl}(a \otimes b) = (a \otimes b)(1 + \delta)$ model of arithmetic with no over/underflow
- OK to multiply, divide, add positive numbers
  Proof: $1 + \delta$ factors can be factored out
- $x_i \pm x_j$, where $x_i$ and $x_j$ are initial data (so exact)
- $(x_i + y_j)(x_i - y_{j-1})x_{i+1}/(x_{i-1} - y_j)$ - OK
- Cancellation when subtracting approximate results dangerous:
  
  \[
  \begin{array}{c}
  \cdot 12345xxx \\
  - \cdot 12345yyy \\
  \hline
  \cdot 00000zzz
  \end{array}
  \]
- We will compute everything using only allowable expressions
Classical Example: A Vandermonde Linear System

• Solve $Vy = b$, where $V$ is Vandermonde:

$$
\begin{bmatrix}
1 & x_1 & \ldots & x_1^{n-1} \\
1 & x_2 & \ldots & x_2^{n-1} \\
1 & x_3 & \ldots & x_3^{n-1} \\
\vdots & \vdots & \ddots & \vdots \\
1 & x_n & \ldots & x_n^{n-1}
\end{bmatrix}
\begin{bmatrix}
y_1 \\
y_2 \\
y_3 \\
\vdots \\
y_n
\end{bmatrix}
= 
\begin{bmatrix}
+ \\
- \\
+ \\
\vdots \\
-
\end{bmatrix}
$$

and $0 < x_1 < \ldots < x_n$.

• Equivalent to interpolation

• The Björck-Pereyra method solves $Vy = b$
  
  – In $O(n^2)$ time
  
  – With small forward error: $|y_i - \hat{y}_i| \leq O(\epsilon)|y_i|$
  
  – With small backward error: If $\hat{V}\hat{y} = b$ then $|V_{ij} - \hat{V}_{ij}| \leq O(\epsilon)|V_{ij}|$.

• How does it work?
The Björck-Pereyra Method

• If \((x_1, x_2, x_3) = (1, 2, 3)\) and \(b = (2, -1, 14)^T\) then using BP to solve

\[
\begin{bmatrix}
1 & 1 & 1 \\
1 & 2 & 2^2 \\
1 & 3 & 3^2
\end{bmatrix}
\cdot y =
\begin{bmatrix}
2 \\
-1 \\
14
\end{bmatrix}
\]

means

\[
y = V^{-1}b = \begin{bmatrix}
1 & -1 & 1 \\
1 & -1 & 1 \\
1 & -1 & 1
\end{bmatrix}
\cdot \begin{bmatrix}
1 & 1 & 1 \\
1 & -2 & \frac{1}{2} \\
1 & -1 & \frac{1}{2}
\end{bmatrix}
\cdot \begin{bmatrix}
1 & -1 & 1 \\
-1 & 1 & -1 \\
-1 & 1 & 14
\end{bmatrix}
= \begin{bmatrix}
23 \\
-30 \\
9
\end{bmatrix}
\]

• Notice:
  – Bidiagonal Decomposition of \(V^{-1}\) (accurate)
  – Checkerboard sign pattern

\[\Rightarrow\] No subtractive cancellation
\[\Rightarrow\] High relative accuracy

• Questions:
  – Which matrices have bidiagonal decomposition of their inverses?
  – Checkerboard signs?
  – Accurate?
The Björck-Pereyra Method Dissected

• Questions:
  – Which matrices have bidiagonal decomposition of their inverses?
  – Checkerboard signs?
  – Accurate?

• Answers:
  – All nonsingular matrices do
    This is *Neville elimination* in matrix form:

\[
\begin{bmatrix}
1 & 1 \\
-1 & 1 \\
-1 & 1
\end{bmatrix}
\begin{bmatrix}
1 & 1 & 1 \\
1 & 2 & 4 \\
1 & 3 & 9
\end{bmatrix}
= 
\begin{bmatrix}
0 & 1 & 3 \\
0 & 1 & 5
\end{bmatrix};
\]

\[
\begin{bmatrix}
1 & -1 \\
1 & -1 \\
1
\end{bmatrix}
\begin{bmatrix}
1 & 1 & 1 \\
1 & 2 & 4 \\
1 & 3 & 9
\end{bmatrix}
= 
\begin{bmatrix}
1 \\
1
\end{bmatrix}
\]

– Checkerboard sign pattern \(\iff\) Total positivity
  \((A \text{ is TP }\iff \text{all minors } > 0)\)

– Accurate? Yes.
ACCURACY OF THE BJÖRCK-PEREYRA METHOD

\[
\begin{bmatrix}
1 & x_1 & x_1^2 & x_1^3 \\
x_2 & x_2^2 & x_2^3 \\
x_3 & x_3^2 & x_3^3 \\
x_4 & x_4^2 & x_4^3 \\
\end{bmatrix}^{-1} = \begin{bmatrix}
1 & -x_1 \\
1 & -x_1 & 1 \\
1 & -x_1 & 1 & 1 \\
\end{bmatrix} \times \begin{bmatrix}
1 & -x_2 & 1 \\
1 & -x_2 & 1 & 1 \\
\end{bmatrix}
\]

Other TP matrices? ... Yes
TP Cauchy matrices \(x_1 > \ldots > x_n > y_1 > \ldots > y_n\)

\[
\begin{bmatrix}
\frac{1}{x_1-y_1} & \frac{1}{x_1-y_2} & \frac{1}{x_1-y_3} \\
\frac{1}{x_2-y_1} & \frac{1}{x_2-y_2} & \frac{1}{x_2-y_3} \\
\frac{1}{x_3-y_1} & \frac{1}{x_3-y_2} & \frac{1}{x_3-y_3} \\
\end{bmatrix}^{-1} = \begin{bmatrix}
1 & \frac{y_1-y_1}{x_1-y_1} & 0 \\
0 & \frac{y_1-y_2}{x_1-y_2} & \frac{y_1-y_3}{x_1-y_3} \\
0 & 0 & \frac{y_1-y_3}{x_1-y_3} \\
\end{bmatrix} \times \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & \frac{y_2-y_1}{y_1-y_3} \\
0 & 0 & \frac{y_2-y_3}{y_1-y_3} \\
\end{bmatrix} \times \begin{bmatrix}
x_1 - y_1 \\
x_2 - y_2 \\
x_3 - y_3 \\
\end{bmatrix}
\]

Unifying Characteristic?
The Connection with Minors

- Which TP matrices permit \textit{accurate} bidiagonal decomposition?
- Each entry is \textit{product of quotients of minors}
  \[ L_{i+1,i}^{(k)} = -\frac{\det(A(i - k + 2 : i + 1, 1 : k))}{\det(A(i - k + 2 : i, 1 : k - 1))} \cdot \frac{\det(A(i - k + 1 : i - 1, 1 : k - 1))}{\det(A(i - k + 1 : i, 1 : k))} \]

- Specifically: Initial minors
  - Contiguous
  - Include first row and column
- Initial minors of Cauchy:
  \( \det(C) = \frac{\prod_{i<j}(x_j - x_i)(y_j - y_i)}{\prod_{i,j}(x_i + y_j)} \)
- Initial minors of Vandermonde:
  \( \det V = \prod_{i>j}(x_i - x_j) \)
- How did we think of minors?
- Gaussian Elimination and Neville Elimination
  Each entry of \( V = LDU \) is a quotient of minors, so not surprising
New results: Generalized Vandermonde Matrices

- TP Matrices with initial minors that are easy to compute accurately

\[
V = \begin{bmatrix}
1 & x_1 & \cdots & x_1^{n-1} \\
1 & x_2 & \cdots & x_2^{n-1} \\
\vdots & & & \vdots \\
1 & x_n & \cdots & x_n^{n-1}
\end{bmatrix}, \quad G_\lambda = \begin{bmatrix}
x_1^{\lambda_1} & x_1^{1+\lambda_2} & \cdots & x_1^{n-1+\lambda_n} \\
x_2^{\lambda_1} & x_2^{1+\lambda_2} & \cdots & x_2^{n-1+\lambda_n} \\
\vdots & & & \vdots \\
x_n^{\lambda_1} & x_n^{1+\lambda_2} & \cdots & x_n^{n-1+\lambda_n}
\end{bmatrix},
\]

where \( x_1 > x_2 > \cdots > x_n > 0, \lambda_n \geq \lambda_{n-1} \geq \cdots \geq \lambda_1 \geq 0, |\lambda| = \lambda_1 + \ldots + \lambda_n \)

- Initial Minors for \( G_\lambda \)?

\[
\det(G_\lambda) = \det(V) \cdot s_\lambda(x_1, x_2, \ldots, x_n)
\]

- \( s_\lambda \) - called Schur function

  - Polynomial with positive integer coefficients
  - Widely studied in combinatorics [MacDonald], group representation theory

- Example:

\[
\det \begin{bmatrix}
1 & x_1^2 & x_1^4 \\
1 & x_2^2 & x_2^4 \\
1 & x_3^2 & x_3^4
\end{bmatrix} = \det \begin{bmatrix}
1 & x_1^2 \\
1 & x_2^2 \\
1 & x_3^2
\end{bmatrix} \cdot (2x_1x_2x_3 + x_1^2x_2^2 + x_1x_2^2x_3 + x_1x_2^2x_3 + x_2^2x_3 + x_2x_3^2)
\]
Accuracy and Efficiency for Generalized Vandermonde Matrices

• Example:
  \[
  \det \begin{pmatrix}
  1 & x_1^2 & x_1^4 \\
  1 & x_2^2 & x_2^4 \\
  1 & x_3^2 & x_3^4
  \end{pmatrix} = \det \begin{pmatrix}
  1 & x_1 & x_1^2 \\
  1 & x_2 & x_2^2 \\
  1 & x_3 & x_3^2
  \end{pmatrix} \cdot (2x_1x_2x_3 + x_1^2x_2 + x_1x_2^2 + x_1x_3^2 + x_2x_3 + x_2x_3^2)
  \]

• Accuracy?
  - \( \det(V) = \prod_{i>j} (x_i - x_j) \) - YES.
  - \( s_\lambda \) - polynomials with \( > 0 \) coefficients - YES.

• Efficiency?
  - \( \det(V) = \prod_{i>j} (x_i - x_j) \) - OK.
  - \( s_\lambda(x_1, x_2, \ldots, x_n) \)?
    * Traditional algorithm - exponential - \( n^{\vert \lambda \vert} \)
    * Now exponential speedup: Linear complexity in \( n \). Idea:
      \[
      s_2(x_1, \ldots, x_n) = \sum_{i \leq j} x_i x_j = (x_1 + \ldots + x_n)x_1 + (x_2 + \ldots + x_n)x_2 + \ldots + (x_{n-1} + x_n)x_{n-1} + x_n x_n
      \]
      cost: \( 3n \), although \( n^2 \) terms.
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<th>SVD</th>
<th>NENP</th>
<th>Frwrd*</th>
<th>Bckwrd*</th>
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<td>Cauchy</td>
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Big-O sense

*FORWARD BOUND: $|x - \hat{x}| \leq O(\epsilon) |A^{-1}| |b|$, implying $|x - \hat{x}| \leq O(\epsilon) |x|$ for $x$ checkerboard

BACKWARD BOUND: $|A - \hat{A}| \leq O(\epsilon) |A|$, where $\hat{A} \hat{x} = b.$

$1) +$ Other conditions on the signs of the three-term recurrence

$\Lambda \leq (\lambda_1 + 1)(\lambda_2 + 1)^2 \ldots (\lambda_p + 1)^2 p$, where $\lambda = (\lambda_1, \ldots, \lambda_p).$
Conclusions

• TP Structured linear systems can be solved very accurately, if initial minors factor
• Implies accurate $A^{-1}$
• New application: Generalized Vandermonde Matrices
• Accurate SVD of some Polynomial Vandermonde Matrices
• Sometimes the SVD is easier than the inverse

Open Problems

• Totally Positive Matrices in general appear impossible. Proof?
• Characterize which structured matrices permit accurate and efficient linear algebra
Resources

- These slides: www.math.berkeley.edu/~plamen/bascd02.pdf
- Reports: