Accurate and Efficient Matrix Computations with Vandermonde Matrices Using Schur Functions

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- 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

							Small	Small
							Forward	Backward
Type of			Any	GENP			Error in	Error in
Matrix	$\det(A)$	A^{-1}	minor	GEPP	GECP	SVD	Ax = b	Ax = b
Cauchy								
Totally Positive								
Cauchy								
Vandermonde								
Totally positive								
Vandermonde								
Polynomial								
Vandermonde								
Poly. Vand.								
Orth. poly.								
Generalized								
Vandermonde								
TP Generalized								
Vandermonde								

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?

- $f(a \otimes b) = (a \otimes b)(1 + \delta)$ 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:

.12345xxx - .12345yyy .00000zzz

- We will compute everything using only allowable expressions
- Explains our interest in TP matrices, minors > 0

• Solve Vy = b, where V is Vandermonde:

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

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

- Equivalent to interpolation
 - Lagrange
 - Newton
- The Björck-Pereyra method solves Vy = b, by doing Newton interpolation
 - In $O(n^2)$ time
 - With small forward error: $|y_i \hat{y}_i| \le O(\epsilon)|y_i|$
 - 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?

 $2 - (x - 1)[3 - 9(x - 2)] = 2 - (x - 1)(21 - 9x) = 2 + 21 - (9 + 21)x + 9x^2 = 23 - 30x + 9x^2$

x	f(x)	$f[\cdot, \cdot]$	$f[\cdot,\cdot,\cdot]$
1	2	2	2
2	-1	-3	-3
3	14	15	9

Matrix version:
$$\begin{bmatrix} 1 \\ -1 & 1 \\ & -1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ -1 \\ 14 \end{bmatrix} = \begin{bmatrix} 2 \\ -3 \\ 15 \end{bmatrix}; \begin{bmatrix} 1 \\ 1 \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \cdot \begin{bmatrix} 2 \\ -3 \\ 15 \end{bmatrix} = \begin{bmatrix} 2 \\ -3 \\ 9 \end{bmatrix}$$

yielding $f(x) = 2 - 3(x - 1) + 9(x - 1)(x - 2)$

yreiding f(x) = 2 - 5(x - 1) + 9(x - 1)(x - 2)Now going back to the solution:

$$\begin{bmatrix} 1 \\ 1 \\ -2 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ -3 \\ 9 \end{bmatrix} = \begin{bmatrix} 1 \\ -21 \\ 9 \end{bmatrix}; \qquad \begin{bmatrix} 1 & -1 \\ 1 & -1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -21 \\ 9 \end{bmatrix} = \begin{bmatrix} 23 \\ -30 \\ 9 \end{bmatrix}$$

yielding $f(x) = 23 - 30x + 9x^2$

• Putting it all together

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

- 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?

- Questions:
 - Which matrices have bidiagonal decomposition of their inverses?
 - Checkerboard signs?
 - Accurate?
- Answers:
 - All nonsingular matrices do

This is *Neville elimination* in matrix form:

$$\begin{bmatrix} 1 \\ -1 & 1 \\ 1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 1 & 5 \end{bmatrix}; \qquad \begin{bmatrix} 1 \\ 1 \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 1 & 5 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 1 & -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \cdot \begin{bmatrix} 1 \\ -1 & 1 \\ -1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

- Checkerboard sign pattern \iff Total positivity

(A is TP \iff all minors > 0)

– Accurate? Yes.



Accuracy ... OK

Other TP matrices? ... Yes. Cauchy

• *Cauchy* matrices

$$C = \frac{1}{x_i - y_j}$$

• **TP**, if $x_1 > ... > x_n > y_1 > ... > y_n$

$$\begin{pmatrix} \left[\begin{array}{cccc} \frac{1}{x_1 - y_1} & \frac{1}{x_1 - y_2} & \frac{1}{x_1 - y_3} \\ \frac{1}{x_2 - y_1} & \frac{1}{x_2 - y_2} & \frac{1}{x_2 - y_3} \\ \frac{1}{x_3 - y_1} & \frac{1}{x_3 - y_2} & \frac{1}{x_3 - y_3} \end{array} \right] \end{pmatrix}^{-1} = \begin{bmatrix} 1 & \frac{-(x_1 - y_1)}{y_1 - y_2} & 0 \\ 0 & \frac{x_1 - y_2}{y_1 - y_2} & \frac{-(x_1 - y_2)}{y_2 - y_3} \\ 0 & 0 & \frac{x_1 - y_3}{y_2 - y_3} \end{array} \right] \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{x_2 - y_3}{y_1 - y_3} \end{bmatrix} \\ \\ \begin{bmatrix} x_1 - y_1 \\ x_2 - y_2 \\ x_3 - y_3 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \frac{-(x_1 - y_2)}{x_3 - x_1} & \frac{x_3 - y_2}{x_3 - x_1} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ \frac{-(x_1 - y_1)}{x_2 - x_1} & \frac{x_2 - y_1}{x_3 - x_2} & 0 \\ 0 & \frac{-(x_2 - y_1)}{x_3 - x_2} & \frac{x_3 - y_1}{x_3 - x_2} \end{bmatrix}$$

• Unifying Characteristic?

- Which TP matrices permit *accurate* bidiagonal decomposition?
- Each entry is *product of quotients of initial minors*

$$L_{i+1,i}^{(k)} = -\frac{\det(A(i-k+2:i+1,1:k))}{\det(A(i-k+2:i,1:k-1))} \cdot \frac{\det(A(i-k+1:i-1,1:k-1))}{\det(A(i-k+1:i,1:k))}$$



• Initial minors of:

Cauchy
$$\frac{\prod_{i < j} (x_j - x_i)(y_j - y_i)}{\prod_{i,j} (x_i + y_j)}$$
; Vandermonde $\prod_{i > j} (x_i - x_j)$

- How did we think of minors?
- Gaussian Elimination and Neville Elimination Each entry of V = LDU is a quotient of minors, so not surprising

• TP Matrices with initial minors that are easy to compute accurately Vandermonde and Generalized Vandermonde

$$V = \begin{bmatrix} 1 & x_1 & \dots & x_1^{n-1} \\ 1 & x_2 & \dots & x_2^{n-1} \\ & \ddots & \\ 1 & x_n & \dots & x_n^{n-1} \end{bmatrix}, \qquad G_{\lambda} = \begin{bmatrix} x_1^{\lambda_n} & x_1^{1+\lambda_{n-1}} & \dots & x_1^{n-1+\lambda_1} \\ x_2^{\lambda_n} & x_2^{1+\lambda_{n-1}} & \dots & x_2^{n-1+\lambda_1} \\ & & \ddots & \\ x_n^{\lambda_n} & x_n^{1+\lambda_{n-1}} & \dots & x_n^{n-1+\lambda_1} \end{bmatrix},$$

where $x_1 > x_2 > \cdots > x_n > 0$, $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n \ge 0$, $|\lambda| = \lambda_1 + \ldots + \lambda_n$

• Initial Minors for G_{λ} ?

$$\det(G_{\lambda}) = \det(V) \cdot s_{\lambda}(x_1, x_2, \dots, x_n)$$

- s_{λ} called Schur function
 - Polynomial with positive integer coefficients
 - Widely studied in combinatorics [MacDonald], group representation theory
- Example:

$$\det \left(\begin{bmatrix} 1 & x_1^2 & x_1^4 \\ 1 & x_2^2 & x_2^4 \\ 1 & x_3^2 & x_3^4 \end{bmatrix} \right) = \det \left(\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix} \right) \cdot (2x_1x_2x_3 + x_1^2x_2 + x_1x_2^2 + x_1x_3^2 + x_1x_3^2 + x_2x_3 + x_2x_3^2)$$

• Example:

$$\det \left(\begin{bmatrix} 1 & x_1^2 & x_1^4 \\ 1 & x_2^2 & x_2^4 \\ 1 & x_3^2 & x_3^4 \end{bmatrix} \right) = \det \left(\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix} \right) \cdot (2x_1x_2x_3 + x_1^2x_2 + x_1x_2^2 + x_1x_3^2 + x_1x_3^2 + x_2x_3 + x_2x_3^2)$$

• Accuracy?

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

$$-\det(V) = \prod_{i>j}(x_i - x_j) - \mathbf{OK}.$$

$$-s_{\lambda}(x_1,x_2,\ldots,x_n)$$
?

* Has exponentially many terms $-n^{|\lambda|}$, we'll look in detail

- We are only interested in subtraction-free algorithms, thus
 - * $s_{\lambda} = f(\text{elementary symmetric polynomials})$ useless
 - * Same for the Jacobi-Trudi identity

- Def: $\lambda = (\lambda_1, \lambda_2, ..., \lambda_n)$ is a partition of $|\lambda| = \lambda_1 + \lambda_2 + \cdots + \lambda_n$
- Def: Young Diagrams \equiv partitions:

Partition: 7 = 4 + 2 + 1, Young diagram: $\lambda = (4, 2, 1) =$



• Def: Semistandard Young Tableau T_{λ} :

1	1	2	3
2	3		
4			

• **Def:**
$$x^{T_{\lambda}} = x_1^2 x_2^2 x_3^2 x_4$$

ullet

$$s_{\lambda} = \sum_{\substack{T_{\lambda} \\ ext{semi-std}}} x^{T_{\lambda}}$$

$$s_{\lambda} = \sum_{\substack{T_{\lambda} \\ \text{semi-std}}} x^{T_{\lambda}}$$

• Example:

$$\det\left(\begin{bmatrix}1 & x_1^2 & x_1^4\\ 1 & x_2^2 & x_2^4\\ 1 & x_3^2 & x_3^4\end{bmatrix}\right) = \det\left(\begin{bmatrix}1 & x_1 & x_1^2\\ 1 & x_2 & x_2^2\\ 1 & x_3 & x_3^2\end{bmatrix}\right) \underbrace{(2x_1x_2x_3 + x_1^2x_2 + x_1x_2^2 + x_1x_3^2 + x_1x_3^2 + x_2x_3 + x_2x_3^2)}_{s_\lambda}$$

•
$$\lambda = (2, 1)$$
, Young diagram:





$$s_{\lambda}(x_1, x_2, x_3) = 2x_1x_2x_3 + x_1^2x_2 + x_1x_2^2 + x_1^2x_3 + x_1x_3^2 + x_2^2x_3 + x_2x_3^2$$

• Exponentially many non-zero terms, need a more efficient approach

- Lexicographic ordering of partitions
- If $\mu < \lambda$, then λ/μ skew partition
- Young diagram (4, 2, 1)/(2, 1):



• Macdonald:

$$s_{\lambda}(x,y) = \sum_{\mu < \lambda} s_{\mu}(x) s_{\lambda/\mu}(y),$$

- $\boldsymbol{x},\boldsymbol{y}$ sets of indices
- Corollary:

$$s_{\lambda}(x_1, x_2, ..., x_n) = \sum_{\mu} s_{\mu}(x_1, x_2, ..., x_{n-1}) x_n^{|\lambda| - |\mu|},$$

summation over λ/μ - horizontal strip.

• Example:

$$s_{(2)}(x_1, \dots, x_n) = \sum_{i \le j} x_i x_j = x_1 x_1 + (x_1 + x_2) x_2 + (x_1 + x_2 + x_3) x_3 + \dots + (x_1 + \dots + x_n) x_n$$

Cost: 3n, although $s_{(2)}$ has n^2 terms.

$$s_{\lambda}(x_1, x_2, ..., x_n) = \sum_{\mu} s_{\mu}(x_1, x_2, ..., x_{n-1}) x_n^{|\lambda| - |\mu|},$$

summation over λ/μ - horizontal strip.

- Allows us to compute s_{λ} efficiently in many cases
- \bullet Exponentially faster than traditional $O(n^{|\lambda|})$ algorithm

n/μ	(0)	(1)	•••	λ
1	1	x_1	•••	$s_\lambda(x_1)$
2	1	$x_1 + x_2$	•••	$s_\lambda(x_1,x_2)$
:	:	:	:	:
n	1	$x_1 + x_2 + \ldots + x_n$	•••	$s_\lambda(x_1,x_2,\ldots,x_n)$

Table entries are $s_{\mu}(x_1, ..., x_i)$. Cost per entry:

 $F(\mu, i) = \#\{\nu < \mu | \mu / \nu - \text{horizonal strip}\}$... independent of n

• Total cost:

$$G(\lambda, n) = \sum_{i=1}^{n} \sum_{\mu < \lambda} F(\mu, i)$$

• Bound on total cost: If $\lambda_1 \ge \lambda_2 \ge \ldots \lambda_p \ge 0 = \lambda_{p+1} = \ldots = \lambda_n$ then

$$G(\lambda, n) \leq (\lambda_1 + 1)(\lambda_2 + 1)^2 \dots (\lambda_p + 1)^2 pn$$

Type of			Any	GENP				Ax = b	Ax = b
Matrix	$\det(A)$	A^{-1}	minor	GEPP	GECP	SVD	NENP	Frwrd*	Bckwrd*
Cauchy	n^2	n^2	n^2	n^3	n^3	n^3	n^2	n^2	
TP Cauchy	n^2	n^2	n^2	n^3	n^3	n^3	n^2	n^2	n^2
Vandermonde	n^2					n^3	n^2	n^2	
TP Vandermonde	n^2	n^3	Exp	n^3	Exp	n^3	n^2	n^2	n^2
Polynomial Vandermonde	n^2			n^3		n^3			
Orth. Poly.									
Orth. $poly.^{1)}$	n^2	n^3		n^3		n^3			
$0 < x_1 < \ldots < x_n$									
Generalized									
Vandermonde									
TP Generalized Vandermonde	$ \Lambda n + n^2 $	$ \Lambda n^3 $	Exp	Λn^2	Exp	Exp	Λn^2	Λn^2	Λn^2

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

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

- TP Structured linear systems can be solved very accurately, if initial minors factor
- Implies accurate A^{-1}
- New application: Generalized Vandermonde Matrices
- New algorithm for computing the Schur function
- Not in this talk:
 - 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

• These slides: www.math.berkeley.edu/~plamen/mit02.pdf

• Reports:

- J. Demmel and P. Koev, Necessary and sufficient conditions for accurate and efficient rational function evaluation and factorizations of rational matrices. In Structured matrices in mathematics, computer science, and engineering. II (Boulder, CO, 1999), pages 117–143. Amer. Math. Soc., Providence, RI, 2001.
- J. Demmel and P. Koev, Accurate and Efficient Matrix Computations with Totally Positive Generalized Vandermonde Matrices Using Schur Functions, www.math.berkeley.edu/~plamen/hagen.ps
- J. Demmel, M. Gu, S. Eisenstat, I. Slapničar, K. Veselić, and Z. Drmač. Computing the singular value decomposition with high relative accuracy. *Lin. Alg. Appl.*, 299(1-3):21-80, 1999.
 www.cs.berkeley.edu/~demmel/DGESVD.ps
- J. Demmel, Accurate SVDs for Structured Matrices, Accurate SVDs of structured matrices. SIAM J. Mat. Anal. Appl., 21(2):562-580, 1999. www.netlib.org/lapack/lawns/lawn130.ps