# Accurate symmetric rank revealing factorizations of some structured matrices

Froilán M. Dopico

Universidad Carlos III de Madrid (Spain)

joint work with
Plamen Koev and Juan M. Molera

# Rank Revealing Decompositions (RRD)

$A$ $m \times n$ matrix.

$$A = XDY^T$$

$X$ $m \times r$ and WELL-CONDITIONED.

$D$ $r \times r$ and DIAGONAL.

$Y$ $n \times r$ and WELL-CONDITIONED.

# RRDs Computed with high relative accuracy

$$A = XDY^T$$

Computed factors satisfy:

$$|D_{ii} - \widehat{D}_{ii}| = O(\epsilon)|D_{ii}|,$$
$$\|X - \widehat{X}\|_2 = O(\epsilon)\|X\|_2,$$
$$\|Y - \hat{Y}\|_2 = O(\epsilon)\|Y\|_2.$$

$\epsilon$ is the machine precision.

# Applications of Accurate RRDs

- Given an accurate RRD there are O(n$^3$) algorithms to compute SVDs to high relative accuracy (Demmel et al. (1999)).

$$|\hat{\sigma}_i - \sigma_i| \leq O(\kappa\epsilon)|\sigma_i|$$

$$\max\{\theta(v_i, \hat{v}_i), \theta(u_i, \hat{u}_i)\} \leq \frac{O(\kappa\epsilon)}{\min_{j \neq i} \left|\frac{\sigma_i - \sigma_j}{\sigma_i}\right|}$$

where $\kappa = \max\{\kappa_2(X), \kappa_2(Y)\}$.

- Reliable determination of numerical rank.

- Approximation by matrices of smaller rank.

# How to compute accurate RRDs

- Rank Revealing property: In practice

$$LDU$$

from Gaussian Elimination with Complete Pivoting (GECP).

Guaranteed RRDs by Pan (2000), Miranian and Gu (2003).

- Accuracy: Only for matrices with special structures.
  - Demmel: Scaled-Cauchy, Vandermonde (DFT + GECP).
  - Demmel and Koev: M-Matrices, Polynomial Vandermonde.
  - Demmel and Veselic: Well Scaled Positive Definite Matrices.
  - Demmel and Gragg: Acyclic Matrices (include bidiagonal…)

ACCURACY IN A FINITE COMPUTATION (GECP) GUARANTEES ACCURACY IN SVD

# Our goal: Compute Accurate Symmetric RRDs

For symmetric matrices $A = A^T$ compute:

$$A = XDX^T$$

$X$ WELL-CONDITIONED and $D$ DIAGONAL.

$$|D_{ii} - \widehat{D}_{ii}| = O(\epsilon)|D_{ii}|,$$
$$\|X - \widehat{X}\|_2 = O(\epsilon)\|X\|_2.$$

We consider four classes of symmetric matrices:

- Symmetric Scaled Cauchy Matrices
- Symmetric Vandermonde Matrices
- Symmetric Totally Nonnegative Matrices
- Symmetric Graded Matrices

# Remarks on computing symmetric RRDs

- For symmetric indefinite matrices GECP does not preserve, in general, the symmetry.

- Given an accurate symmetric RRD, eigenvalues and vectors can be computed with high relative accuracy using the O($n^3$) symmetric J orthogonal algorithm (Veselic-Slapnicar) :

$$\frac{|\widehat{\lambda}_i - \lambda_i|}{|\lambda_i|} \leq O(\kappa_2(X)\epsilon) \quad \text{and} \quad \theta(v_i, \widehat{v}_i) \leq \frac{O(\kappa_2(X)\epsilon)}{\min\limits_{j \neq i} \left| \frac{\lambda_i - \lambda_j}{\lambda_i} \right|} \quad i = 1 : n$$

- The same accuracy can be obtained given an accurate nonsymmetric RRD of a symmetric matrix using the O($n^3$) SSVD algorithm (FMD, Molera and Moro).

# Symmetric RRDs of Scaled Cauchy Matrices (I)

$$\left[\frac{s_i s_j}{x_i + x_j}\right]_{i,j=1}^{n} = XDX^T$$

Algorithm

1. Compute accurate Schur Complements (Gohberg, Kailath, Olshevsky) and (Demmel)

$$S_{rs}^{(m)} = S_{rs}^{(m-1)} \frac{(x_r - x_m)(x_s - x_m)}{(x_m + x_s)(x_r + x_m)}$$

2. Use Diagonal Pivoting Method with the Bunch-Parlett complete pivoting strategy.
3. Orthogonal diagonalization of the 2 x 2 pivots.

CAREFUL ERROR ANALYSIS IS NEEDED, BUT IT IS GENERAL IF ACCURATE SCHUR COMPLEMENTS ARE AVAILABLE.

This approach has been used by M. J. Peláez and J. Moro to compute accurate SYMMETRIC RRDs of DSTU and TSC matrices

# Symmetric RRDs of Scaled Cauchy Matrices (II)

- Diagonal Pivoting Method

$$PAP^T = L\, D_b\, L^T$$

  - P is a permutation matrix
  - L is unit lower triangular
  - $D_b$ is block diagonal with blocks 1 x 1 and 2 x 2

P PERMUTATION FOR THE REST OF THE TALK!!!!!

- Bunch-Parlett Complete Pivoting Strategy

The 2 x 2 pivots are chosen if the elements of the corresponding Schur Complement, S, satisfy:

$$0.64 \cdot \max_{i,j} |s_{ij}| > \max_{i} |s_{ii}|$$

- Cost: $\frac{2}{3}n^3 + O(n^2)$

# RRDs of Symmetric Vandermonde Matrices (I)

Let $a$ be a real number

$$A = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & a & a^2 & \dots & a^{n-1} \\ 1 & a^2 & a^4 & \dots & a^{2(n-1)} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & a^{n-1} & a^{2(n-1)} & \dots & a^{(n-1)^2} \end{bmatrix}$$

## Remarks

1. The NONSYMMETRIC approach does NOT respect the symmetry:

SCALED CAUCHY = VANDERMONDE x DFT

2. Schur complements of Vandermonde matrices are NOT Vandermonde.
3. Pivoting strategies DESTROY the symmetric Vandermonde structure.
4. We avoid pivoting and use EXACT formulas for A = $LDL^T$ and its converse.

# RRDs of Symmetric Vandermonde Matrices (II)

$$\begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & a & a^2 & \dots & a^{n-1} \\ 1 & a^2 & a^4 & \dots & a^{2(n-1)} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & a^{n-1} & a^{2(n-1)} & \dots & a^{(n-1)^2} \end{bmatrix} = LDL^T = A$$

$$d_i = a^{\frac{1}{2}(i-2)(i-1)} \cdot \prod_{t=1}^{i-1} (a^t - 1),$$

$$l_{ij} = \prod_{t=1}^{j-1} \frac{1 - a^{i-j+t}}{1 - a^t}.$$

The LDL$^T$ can be accurately computed in 2 n$^2$ flops

CONDITION NUMBER OF L?

# RRDs of Symmetric Vandermonde Matrices (III)

Lemma: If $|a| \le \frac{2}{3}$ then $\kappa_1(L) = O(n^2)$.

$$\begin{array}{c} \text{Large} \\ \Bigg\downarrow \\ \text{Small} \end{array} \quad \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & a & a^2 & \dots & a^{n-1} \\ 1 & a^2 & a^4 & \dots & a^{2(n-1)} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 1 & a^{n-1} & a^{2(n-1)} & \dots & a^{(n-1)^2} \end{bmatrix} = LDL^T = A$$

Large $\longrightarrow$ Small

# RRDs of Symmetric Vandermonde Matrices (IV)

If $|a| \geq \frac{3}{2}$, the converse of $A$ is used:

$$A = \begin{bmatrix} 0 & \dots & 0 & 1 \\ 0 & \dots & 1 & 0 \\ 0 & \vdots & 0 & 0 \\ 1 & \dots & 0 & 0 \end{bmatrix} \underbrace{\begin{bmatrix} a^{(n-1)^2} & a^{(n-1)(n-2)} & \dots & 1 \\ a^{(n-1)(n-2)} & a^{(n-2)^2} & \dots & 1 \\ \vdots & \vdots & \dots & \vdots \\ 1 & 1 & \dots & 1 \end{bmatrix}}_{\bar{L}\bar{D}\bar{L}^T} \begin{bmatrix} 0 & \dots & 0 & 1 \\ 0 & \dots & 1 & 0 \\ 0 & \vdots & 0 & 0 \\ 1 & \dots & 0 & 0 \end{bmatrix}$$

$\bar{L}\bar{D}\bar{L}^T$ is accurately computed with EXACT formulas, with $2n^2$ cost, and, if $|a| \geq \frac{3}{2}$ then $\kappa_1(\bar{L}) = O(n^2)$.

$\frac{2}{3} < |a| < \frac{3}{2}$? At present only NONSYMMETRIC approach

# RRDs of Totally Nonnegative Matrices (I)

- Matrices with all minors nonnegative are called totally nonnegative (TN). We consider only nonsingular matrices.
- TN can be parametrized as products of nonnegative bidiagonal matrices.

$$A = L^{(1)} \cdot L^{(2)} \dots L^{(n-1)} \cdot D \cdot U^{(n-1)} \dots U^{(2)} \cdot U^{(1)}$$

$A$ TN $n \times n$ matrix and $D$ diagonal.

$L^{(k)}$ lower unit bidiagonal.

$L^{(k)}$ has its first $n-1-k$ subdiag. entries zero.

$U^{(k)}$ upper unit bidiagonal.

$U^{(k)}$ has its first $n-1-k$ super. entries zero.

BIDIAGONAL FACTORIZATION NEED NOT BE AN RRD OF A

# Very Good Numerical Virtues of BD(A)

P. Koev has shown that given the bidiagonal factorization of a TN matrix, BD(A), it is possible to compute accurately and efficiently O($n^3$):

1. Eigenvalues of nonsymmetric TN.
2. Singular values and vectors of TNs.
3. Inverse.
4. BDs of products of TNs.
5. LDU decompositions.
6. BDs of Schur complements.
7. BDs of submatrices and Minors.
8. Apply Givens rotations: BD(A) $\longrightarrow$ BD(GA).
9. QR factorization……………

# RRDs of Totally Nonnegative Matrices (II)

Our Goal: Compute accurate RRDs given BD(A)

1. In $O(n^3)$ time
2. Using a finite process,
3. and, respecting the symmetry.

This is nontrivial because

PIVOTING STRATEGIES DESTROY TN STRUCTURE.

TWO ALGORITHMS:

SYMMETRIC AND NONSYMMETRIC

# Accurate RRDs of nonsymmetric TNs

1. BD(A) $\longrightarrow$ BD(B) by applying Given rotations, and B bidiagonal:

$$A = Q\, B\, H^T$$

2. $B = P_1$ LDU $P_2$ using accurate GECP for acyclic matrices (Demmel et al.)

$$A = (Q\, P_1\, L)\;\; D\;\; (U\, P_2\, H^T)$$

COST: 14 $n^3$

# Accurate RRDs of Symmetric TNs (I)

$$A = L^{(1)} \cdot L^{(2)} \cdots L^{(n-1)} \cdot D \cdot (L^{(n-1)})^T \cdots (L^{(2)})^T \cdot (L^{(1)})^T$$

A is POSITIVE DEFINITE

COMPLETE PIVOTING IS DIAGONAL PIVOTING, AND IT PRESERVES THE SYMMETRY

# Accurate RRDs of Symmetric TNs (II)

1. BD(A) $\longrightarrow$ BD(T), by applying Givens rotations, and T tridiagonal

$$A = Q\,T\,Q^T$$

2. Compute a symmetric RRD of T

$$T = P\,L\,D\,L^T\,P^T$$

   a) GECP (DIAGONAL SYMMETRIC PIVOTING) .
   b) ELEMENTS OF D AND L COMPUTED AS SIGNED QUOTIENTS OF MINORS OF T.
   c) MINORS OF T COST O(n) FLOPS.
   d) SUBTRACTION FREE APPROACH

3. Multiply to get: $A = Q\,TQ^T = (Q\,P\,L)\,D\,(Q\,P\,L)^T$

COST: $21n^3 + O(n^2)$

# RRDs of graded matrices

$A$ $n \times n$ is GRADED if $A = S_1 B S_2$ with

1. $S_1 = \text{diag}[(S_1)_1, \ldots, (S_1)_n]$ with $(S_1)_i > 0$
2. $S_2 = \text{diag}[(S_2)_1, \ldots, (S_2)_n]$ with $(S_2)_i > 0$
3. $B$ is well conditioned

The GRADING FACTOR is $\tau_L = \max \left\{ \max_{1 \leq j < i \leq n} \frac{(S_1)_i}{(S_1)_j}, \max_{1 \leq j < i \leq n} \frac{(S_2)_i}{(S_2)_j} \right\}$.

If $\tau_L << 1$ we say that $A$ is strongly graded.

# What is known for RRDs of NONSYMMETRIC graded matrices?

Under which conditions does GECP applied on A

$$P_1 A P_2^T = LDU$$

compute an accurate RRD of A?

Notice that $A = S_1 B S_2$ implies

$$P_1 A P_2^T = S_1' P_1 B P_2^T S_2' = S_1' L_B D_B U_B S_2'$$

with $S_1' = P_1 S_1 P_1^T$ and $S_2' = P_2 S_2 P_2^T$.

$P_1 B P_2^T = L_B D_B U_B$ NOT FROM GECP ON B!!!$^{1}$)

# What is known for RRDs of NONSYMMETRIC graded matrices?

$$P_1 A P_2^T = LDU$$ ← COMPUTED WITH GECP

$$P_1 A P_2^T = S_1' P_1 B P_2^T S_2' = S_1' L_B D_B U_B S_2'$$

← JUST FOR THEORY

$A = (P_1^T L) D (U P_2)$ is an ACCURATE RRD if

$$\max\left\{ \max_{1 \leq j < i \leq n} \frac{(S_1')_i}{(S_1')_j}, \max_{1 \leq j < i \leq n} \frac{(S_2')_i}{(S_2')_j} \right\} \kappa(L_B)\kappa(D_B)\kappa(U_B)$$

IS SMALL. Demmel et al. (1999)

# Accurate RRDs of SYMMETRIC graded matrices (I)

Under which conditions the DIAGONAL PIVOTING METHOD with the BUNCH PARLETT COMPLETE PIVOTING STRATEGY

$$PAP^T = LDL^T$$

compute an accurate SYMMETRIC RRD of A?

$$A = A^T = SBS$$

$D$ has $1 \times 1$ and $2 \times 2$ pivots

# Accurate RRDs of SYMMETRIC GRADED MATRICES (II)

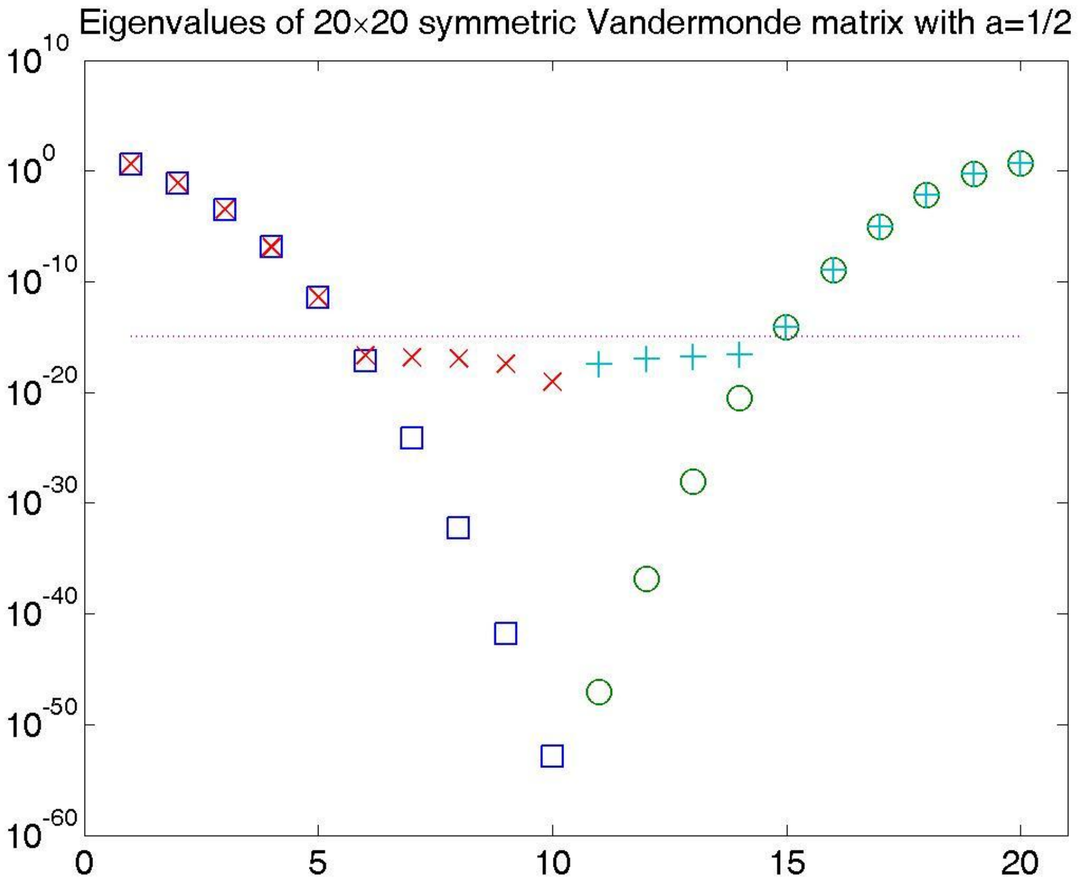
$A = A^T = (P^T L) D (P^T L)^T$ is an ACCURATE SYMMETRIC RRD if

$$\max_{\text{all } \{i,i+1\} 2\times 2 \text{ pivot positions}} \max \left\{ \frac{S'_{i+1}}{S'_i}, \frac{S'_i}{S'_{i+1}} \right\}$$

$$\times \max_{1 \leq j < i \leq n} \frac{(S')_i}{(S')_j} \kappa(L_B)^2 \kappa(D_B)$$

IS SMALL.

# Numerical Example: Symmetric Vandermonde for a=1/2



# CONCLUSIONS

- If accurate RRDs for a nonsymmetric class of matrices can be computed, accurate symmetric RRDs can (almost always) be computed for the symmetric counterparts.

- Different classes of matrices require very different approaches: there is not an UNIVERSAL approach.

- If accurate Schur complements are available DIAGONAL PIVOTING METHOD WITH BUNCH AND PARLETT STRATEGY will do the job.

- Nonsymmetric RRDs plus SSVD algorithm computes accurate eigenvalues and eigenventors.