ACCURATE ALGORITHMS FOR STRUCTURED EIGENVALUE PROBLEMS

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THE MEANING OF ACCURACY IN THIS TALK

1- Given an $n \times n$ matrix A, we will say that an algorithm computes **all** its **eigenvalues** to **high relative accuracy (hra)** if the computed eigenvalues satisfy

$$|\widehat{\lambda} - \lambda| = O(\epsilon)\,|\lambda|,$$

where ϵ is the machine precision. In addition,

- the cost is $O(n^3)$ flops,
- and extra precision is not used.

2- For **eigenvectors** of general matrices the meaning is not clear (**OPEN PROBLEM**).

3- For **e-vectors of** symmetric matrices: $\theta(v_i, \widehat{v}_i) = \dfrac{O(\epsilon)}{\min\limits_{j \neq i} \left| \frac{\lambda_i - \lambda_j}{\lambda_i} \right|}$

4- Similar for SVD.

HRA IS NOT OBTAINED FROM STANDARD ALGORITHMS

EXAMPLE: HILBERT MATRIX

$$H_{100} = \left[\frac{1}{i+j-1}\right]_{i,j=1}^{100}$$

Eigenvalues: $\lambda_1 > \lambda_2 > \ldots > \lambda_{100} > 0$. $\epsilon \approx 10^{-16}$.

	λ_{100}
EXACT	$5.77970086283480\,2\,E-151$
Accurate Alg.	$5.77970086283481\,3\,E-151$
MATLAB	$-1.21607266026676\,0\,E-019$

- Accurate algorithm has a good behavior for all eigenvalues.
- Standard algorithms compute the eigenvalues with errors

$$\frac{|\widehat{\lambda}_i - \lambda_i|}{|\lambda_i|} = O(\epsilon)\frac{|\lambda|_{\max}}{|\lambda_i|} \qquad \left(H_{100}\colon\ \frac{|\lambda|_{\max}}{|\lambda|_{\min}} \approx 3.8\,E+150\right)$$

KEYS ON PRESENT HRA ALGORITHMS

- They only exist for some classes of matrices.

- They do not work (in general) on the entries of the matrix.

- They work on an adequate representation of the matrix.

- The parameters defining this representation determine accurately the eigenvalues and/or eigenvectors. This means that there exists an underlying perturbation theory.

- At present, **there are many symmetric eigenproblems** (and SVD problems) for which hra-algorithms exist. All of them are in the **unifying framework Rank Revealing Decomposition plus Jacobi type algorithm**.

- There are **only two types of nonsymmetric matrices** for which hra computations of eigenvalues (not eigenvectors) are possible.

OUTLINE OF THE TALK

A. Accurate algorithms for **symmetric** eigenproblems:

1. Rank Revealing Decompositions (RRD).
2. Accurate algorithms of Jacobi type on RRDs.
3. Accurate computations of RRDs.

B. Accurate algorithms for **nonsymmetric** eigenproblems:

1. Totally nonnegative matrices.
2. Certain sign regular matrices.

- **Our goal is to present**
  - Key ideas on this topic.
  - Open problems.
  - Most recent developments.

Rank Revealing Decompositions (RRD)

Definition (Demmel et al, 1999): Let A be an $m \times n$ matrix. Then

$$A = XDY^T$$

is a RRD of A if D **is diagonal, and** X **and** Y **have full rank and are well conditioned**.

- In practice, RRDs may be computed as an LDU factorization coming from Gaussian Elimination with complete pivoting (GECP).
- If $X = Y$ then $A = A^T$ and the RRD is a **symmetric RRD**.
- In practice, symmetric RRDs may be computed by the diagonal pivoting method with the Bunch-Parlett complete pivoting strategy.
- Nonsymmetric RRDs of symmetric matrices may be also considered.

RRDs and HRA computations for SVD

Theorem (Demmel et al, 1999): If the computed factors $\widehat{X}, \widehat{D}$, and $\widehat{Y}$ of a RRD

$$A = XDY^T$$

of A satisfy the **forward error bounds**

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

then **two different Jacobi type algorithms can be applied on** $\widehat{X}, \widehat{D}$, **and** $\widehat{Y}$ to compute the SVD of A to HRA with relative errors

$$O(\epsilon \max\{\kappa_2(X), \kappa_2(Y)\}).$$

- **Accuracy in a finite computation (RRD-GECP) guarantees accuracy in SVD.**

Symmetric RRDs and HRA computations

Theorem (FMD, Koev, 2006): If the computed factors $\widehat{X}$ and $\widehat{D}$ of a RRD

$$A = XDX^T$$

of **symmetric matrix** A satisfy the **forward error bounds**

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

then **two different Jacobi type algorithms can be applied on $\widehat{X}$ and $\widehat{D}$** to compute the eigenvalues and eigenvectors of A to HRA with relative errors

$$O(\epsilon\,\kappa_2(X)).$$

REMARK: Computing accurate RRDs (symmetric or not) is only possible for particular types of matrices through special structured implementations of GECP and its variants.

HRA algorithms on RRDs of symmetric matrices (I)

There are, at present, essentially three:

1- (Demmel, Veselić, 1992) Given RRD $A = XDX^T$ **positive definite**:

1. Compute SVD of $X\sqrt{D}$ with **one-sided Jacobi** on the left with an stringent stopping criterion.
2. Compute eigenvalues (σ_i^2) of $A = X\sqrt{D}(X\sqrt{D})^T$. Eigenvectors are the left singular vectors.

Remarks: Fully satisfactory algorithm because:

- The symmetry is preserved.
- Only orthogonal transformations are used.

HRA algorithms on RRDs of symmetric matrices (II)

2- (Veselić, Slapničar, 1993; Slapničar, 2003) Given RRD $A = XDX^T$:

1. Write $A = X\sqrt{|D|}\,J\,(X\sqrt{|D|})^T$ with $J = \mathrm{diag}\{\pm 1\}$.
2. Compute **Hyperbolic SVD** of
$$X\sqrt{|D|} = U\Sigma H^T \text{ where } U^TU = I,\ H^TJH = J$$
with **hyperbolic one-sided Jacobi** on the right
3. $A = U\,(\Sigma^2 J)\,U^T$ is the spectral decomposition of A.

Remarks: Not fully satisfactory. Main features:

- The symmetry is preserved.
- Hyperbolic rotations are used.
- So, it does not take advantage of all the properties of symmetric matrices.
- HRA error bounds depend on a proviso.
- It works very well in practice.

HRA algorithms on RRDs of symmetric matrices (III)

3- (FMD, Molera, Moro 2003; FMD, Molera 2007) Given RRD $A = XDX^T$ (or $A = XDY^T$ although $A = A^T$):

1. Compute SVD of $A = U\Sigma V^T$ from RRD using Jacobi type algorithm by Demmel et al. (1999).

2. Compute eigenvalues and eigenvectors from SVD by using $A = A^T$.

Remarks: Not fully satisfactory. Main features

- The symmetry is not preserved. It allows us flexibility by using nonsymmetric RRDs.
- Only orthogonal transformations are used.
- HRA error bounds are perfect for eigenvalues.
- HRA error bounds are perfect for eigenvectors,
- but this requires a delicate process.

HRA algorithms on RRDs of symmetric matrices (IV)

Open problem: Given a symmetric RRD $A = XDX^T$ of a symmetric indefinite matrix **to find an algorithm** that computes

- the eigenvalues and eigenvectors to HRA,
- using only orthogonal transformations,
- and preserving the symmetry.

Hopefully the solution is coming soon: joint work in progress with Koev and Molera based on

- new theoretical properties of symmetric RRDs,
- Jacobi type algorithm,
- very natural and simple algorithm,
- the code exists and works perfectly.

Accurate computations of RRDs (I)

- **For nonsymmetric matrices:**

  1. Cauchy, Scaled-Cauchy, Vandermonde (Demmel).
  2. Diagonally dominant M-matrices, Polynomial Vandermonde (Demmel and Koev), (Peña).
  3. Graded Matrices (Demmel et al.)
  4. Acyclic Matrices (include bidiagonal) (Demmel and Gragg).
  5. DSTU, TSC (Demmel et al.).
  6. Totally nonnegative (FMD and Koev).
  7. Diagonally Dominant Matrices (Q. Ye)....

Different techniques for each class: highly structured implementations of **GECP** in most cases.

Accurate computations of RRDs (II)

- **For symmetric matrices preserving the symmetry:**

  1. Well Scaled Symmetric Positive Definite (Demmel and Veselić).
  2. Symmetric Cauchy and Scaled-Cauchy (FMD and Koev).
  3. Symmetric Vandermonde (FMD and Koev).
  4. Symmetric Totally nonnegative (FMD and Koev).
  5. Symmetric Graded Matrices (FMD and Molera).
  6. Symmetric DSTU and TSC (Peláez and Moro)....

Different techniques for each class: highly structured implementations of **diagonal pivoting method with Bunch-Parlett pivoting strategy** in most cases.

HRA algorithms on NONSYMMETRIC matrices

At present, it is possible to compute to hra the **eigenvalues** of **only two types of nonsymmetric matrices**:

- Nonsingular totally nonnegative (TN) matrices (positive e-values) (Koev, 2005)

- Matrices that are obtained by reversing the order of the columns (or the rows) of nonsingular TN matrices (positive and negative e-values) (Koev, FMD, 2007)

HRA algorithms in both cases transform the eigenvalue problem into a symmetric one that is solved by computing the singular values of a positive bidiagonal matrix.

Open Problem 1: No results on eigenvectors for any class of nonsymmetric matrices.

Open Problem 2: No results on classes of nonsymmetric matrices with complex eigenvalues.

Summary of nonsingular TN matrices (I)

- **Definition:** matrices with all minors nonnegative are called Totally Nonnegative (TN).
- They include notoriously ill-conditioned matrices
  - Hilbert matrix,
  - Vandermonde and Cauchy matrices with increasing nonnegative nodes,
  - Bernstein Vandermonde,
  - Positive Diagonal Scaling of previous ones....
- They appear in a wide area of problems: mechanical vibration problems, CAD,...

Summary of nonsingular TN matrices (II)

- **Most relevant property for HRA:** Any nonsingular TN matrix can be uniquely factorized as product of **nonnegative bidiagonal factors**, i.e.,

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

  D positive diagonal.

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

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

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

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

- **The parameters of the bidiagonal factorization ($\mathcal{BD}(A)$) of A determine very accurately the eigenvalues of A** (Koev, 2005)

Summary of nonsingular TN matrices (III)

Example: If $\delta > 0$ this matrix in nonsing. TN

$$\underbrace{\begin{bmatrix} 1 & 1 \\ 1 & 1+\delta \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 1 & \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & \\ & \delta \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}}_{\mathcal{BD}(A)}$$

δ	λ_1	λ_2
10^{-3}	$\approx 5 \cdot 10^{-4}$	≈ 2
10^{-6}	$\approx 5 \cdot 10^{-7}$	≈ 2

- Relative perturbation of order 10^{-3} in the $(2,2)$ entry of the matrix produces a relative variation of the smallest eigenvalue of order 1.

- Theorem (Koev, 2005): Relative perturbations of order α in the entries of $\mathcal{BD}(A)$ produce relative variations in the eigenvalues of order $2n^2\alpha$.

HRA algorithm for certain sign regular (SR) matrices (I)

- **Definition:** An $n \times n$ matrix all of whose nonzero kth order minors, $k = 1, \ldots, n$, have the same sign ρ_k is called *sign regular* (SR).

- We only consider one type of sign regular matrices: **nonsingular TN matrices with the columns (or the rows) in reverse order**. We denote these matrices as TN^J.

- These matrices have $\rho_k = (-1)^{k(k-1)/2}$ and are the only SR matrices (except TN and their negatives) that can be, at present, parameterized and easily generated.

- They are the **only type** of nonsymmetric matrices having nonpositive eigenvalues for which hra computations of its eigenvalues may be performed.

HRA algorithm for certain sign regular (SR) matrices (II)

- The eigenvalues of a TN^J matrix are real and if

$$|\lambda_1| \geq \ldots \geq |\lambda_n| > 0$$

then $\mathrm{sign}(\lambda_i) = (-1)^{i-1}$.

- TN^J matrices include Vandermonde and Cauchy matrices

$$V = \left[x_i^{j-1}\right]_{i,j=1}^n \quad \text{and} \quad C = \left[\frac{1}{x_i + y_j}\right]_{i,j=1}^n,$$

with $x_1 > x_2 > \ldots > x_n > 0$ and $x_1 > x_2 > \ldots > x_n > 0$, $0 < y_1 < y_2 < \ldots < y_n$.

- SVDs of TN and TN^J trivially related, **but this is no longer true for eigenvalues.**

HRA algorithm for certain sign regular (SR) matrices (III)

EXAMPLE 1:

$$A = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \text{ nondiagonalizable and e-values } \quad \{1, 1\}$$

$$A^C = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}, \text{ diagonalizable and e-values } \quad \frac{1 \pm \sqrt{5}}{2}$$

EXAMPLE 2:

$$V(x_1, x_2, x_3) = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix} \qquad V^R(x_1, x_2, x_3) = \begin{bmatrix} 1 & x_3 & x_3^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_1 & x_1^2 \end{bmatrix}$$

e-val $V(10^{-6}, 1, 10^{6}) = \{10^{12}, 1.0\ldots, 1.0\ldots\}$ (this is TN)

e-val of $V^R(10^{-6}, 1, 10^{6}) = \{1.0\ldots \cdot 10^{6}, -1.0.. \cdot 10^{5}\ldots, 1.0..\}$ (TN^J)

HRA algorithm for certain sign regular (SR) matrices (IV)

- **KEY POINT 1:** Every TN^J (by columns) matrix can be uniquely represented with nonnegative bidiagonals as

$$A = \overbrace{L^{(1)} \cdots L^{(n-1)} \cdot D \cdot U^{(n-1)} \cdots U^{(1)} \cdot J}^{\mathcal{BD}^J(A)},$$

where, $J = \begin{bmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{bmatrix}, \quad L^{(k)} = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & l_1^{(k)} & 1 & & \\ & & \ddots & \ddots & \\ & & & l_k^{(k)} & 1 \end{bmatrix},$

D is diagonal nonsingular, and $U^{(k)}$ is upper bidiagonal.

- **KEY POINT 2:** The nontrivial entries of $\mathcal{BD}^J(A)$ determine accurately the eigenvalues of A (Koev, FMD, 2007).

- **KEY POINT 3:** All steps in the next algorithm are performed on $\mathcal{BD}^J(A)$.

HRA algorithm for certain sign regular (SR) matrices (V)

Algorithm (Koev,FMD, 2007) Given $\mathcal{BD}^J(A)$ of a nonsingular TN^J matrix A computes the eigenvalues of A to hra.

1. Similarity transformations are used to reduce A to a nonnegative anti-bidiagonal

$$C = \begin{bmatrix} & & & b_1 & a_1 \\ & & \cdot & a_2 & \\ & \cdot & \cdot & & \\ b_{n-1} & a_{n-1} & & & \\ a_n & & & & \end{bmatrix} \in \mathrm{TN}^J$$

without cancellations.

2. A positive diagonal similarity transforms C into a symmetric anti-bidiagonal matrix

$$G = \begin{bmatrix} & & & b'_1 & a'_1 \\ & & \cdot & a'_2 & \\ & \cdot & \cdot & & \\ b'_1 & a'_2 & & & \\ a'_1 & & & & \end{bmatrix} \in \mathrm{TN}^J.$$

HRA algorithm for certain sign regular (SR) matrices (VI)

3. The absolute values, $|\lambda_1| \geq \ldots \geq |\lambda_n|$, of the eigenvalues of

$$G = \begin{bmatrix} & & & b'_1 & a'_1 \\ & & \cdot & a'_2 & \\ & \cdot & \cdot & & \\ b'_1 & a'_2 & & & \\ a'_1 & & & & \end{bmatrix} \in \mathsf{TN}^J.$$

are the singular values of

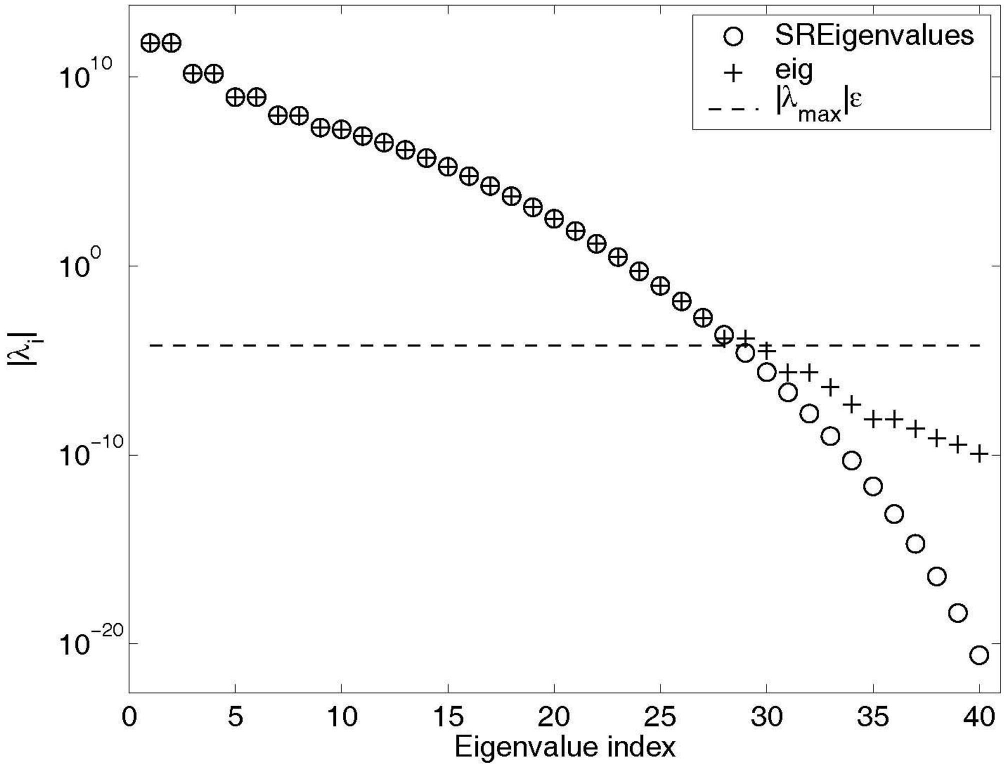
$$G \cdot J = \begin{bmatrix} a'_1 & b'_1 & & & \\ & a'_2 & \cdot & & \\ & & \cdot & \cdot & \\ & & & a'_2 & b'_2 \\ & & & & a'_1 \end{bmatrix} \in \mathsf{TN}^J,$$

and the signs are $(-1)^{(i-1)}$.

Singular values of $G \cdot J$ are computed to hra by Demmel/Kahan's zero shift QR, or Fernando and Parlett's dqds.

Note: Step 2 more complicated if some $b_i = 0$.

EXAMPLE: V is a 40×40 Vandermonde matrix with nodes $4, 3.9, 3.8, \ldots, 0.1$. $\mathcal{BD}^J(V)$ can be accurately computed.



$$\kappa_2(V) = 2.4 \cdot 10^{44}$$

CONCLUSIONS

- Accurate eigenvalue/vectors computations of symmetric matrices are rather well understood.
- Jacobi type algorithms are fundamental in accurate symmetric eigenproblems.
- In symmetric eigenproblems rank revealing decompositions play a key role both as numerical tool and a unifying concept.
- RRDs allow us to compute accurately eigenvalues for many classes of symmetric matrices.
- Only two types of nonsymmetric accurate eigenvalue (not vector) algorithms have been found so far.
- The final (iterative) step of these nonsymmetric accurate eigenvalue algorithms is the accurate computation of singular values of bidiagonal matrices.