Accurate Solution of Structured Linear Systems and Least squares Problems through Rank Revealing Decompositions

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Joint work with
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Householder Symposium XVIII
June 12-17, 2011
Granlibakken Conference Center, Tahoe City, California,

Outline

1. High relative accuracy and structured matrices
2. RRD and accurate computations
3. Algorithms and error analysis
4. Perturbation theory
5. Numerical Experiments

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Problem

Given a structured and potentially bad conditioned (Band, Toeplitz, Hankel, Vandermonde, Cauchy, Quasiseparable, Graded, etc ...) matrix A, is it possible to solve

- a linear system

$$A\,x = b, \quad A \in \mathbb{C}^{n\times n}, \exists A^{-1}$$

- or, to compute the minimal length solution of a least squares problem

$$A\,x \approx b, \quad A \in \mathbb{C}^{m\times n}, \quad rank(A) = r \leq n \leq m$$

with high relative accuracy (hra)?

High relative accuracy

We say that the solution x of a problem is computed with high relative accuracy (hra) if

$$\frac{\|\widehat{x} - x\|}{\|x\|} = O(\mathtt{u})$$

with $\widehat{x}$ the computed solution and $\mathtt{u}$ the unit roundof ($\mathtt{u} = 1.11\ 10^{-16}$), independently of the condition number of A.

TP Vandermonde matrices

$O(n^2)$ algorithm: [1970, Björk&Pereyra; 1987, Higham]

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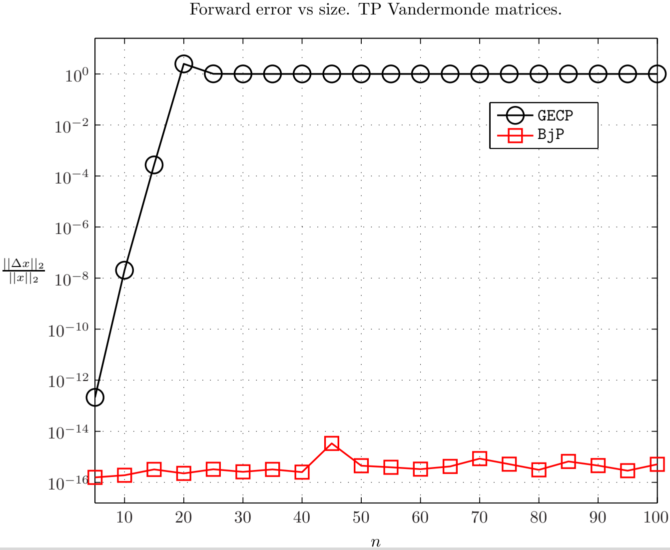

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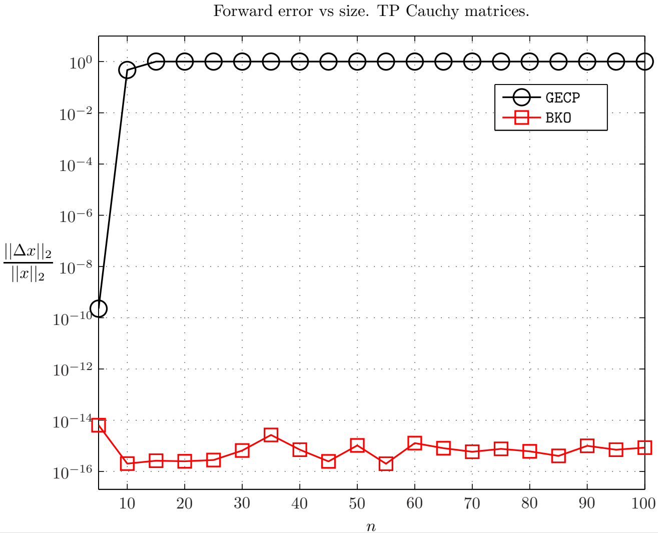

New methods

The methods we are going to present here

- Solve with high relative accuracy linear systems $A\,x = b$ and least squares problems $A\,x \approx b$,
- for "almost any" rhs b,
- it applies to matrices for which there is a Accurate Rank Revealing Decomposition.

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- Solve with high relative accuracy linear systems $A\,x = b$ and least squares problems $A\,x \approx b$,
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- it applies to matrices for which there is a Accurate Rank Revealing Decomposition.

Accurate Rank Revealing Decompositions are known to exist for many classes of structured matrices (in particular, Cauchy, Vandermonde, Graded).

Outline

Rank Revealing Decomposition (RRD)

- RRD

$$A = XDY = \begin{bmatrix} \times & \times \\ \times & \times \\ \times & \times \\ \times & \times \\ \times & \times \end{bmatrix} \begin{bmatrix} \times & \\ & \times \end{bmatrix} \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \end{bmatrix}$$

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- $A \in \mathbb{C}^{m \times n}$, $rank(A) = r$,

$$X \in \mathbb{C}^{m\times r}, \quad Y \in \mathbb{C}^{r\times n}, \quad D \in \mathbb{C}^{r\times r} \text{ diagonal}$$

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- $$\kappa(X), \kappa(Y) \gtrsim 1, \quad \kappa(D) \approx \kappa(A)$$

Structured matrices and accurate RRDs

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- RRDs can be computed in practice from Gaussian Elimination with Complete Pivoting (GECP) (i.e., direct methods).
- But accurate RRDs can only be computed for matrices with special structures:
  - Scaled-Cauchy, Vandermonde (DFT + GECP). [Demmel]
  - Diagonally Dominant M-Matrices. [Demmel and Koev]
  - Polynomial Vandermonde. [Demmel and Koev]
  - Well Scaled Positive Definite. [Demmel and Veselić]
  - Acyclic Matrices (include bidiagonal). [Demmel and Gragg]
  - Diagonally Dominant. [Qiang Ye, Dopico and Koev]
  - DSTU. [Demmel]
  - Graded Matrices. [Dopico, M, Ceballos]

Rank Revealing Decomposition

Theorem (Demmel et al. 1999)

An SVD with high relative accuracy can be computed for a matrix A if and only if an accurate RRD can be computed.

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We say that the computed factors $\widehat{X}, \widehat{Y}$ and $\widehat{D}$, produce an accurate RRD of $A = XDY$ if they obey

$$\frac{\|\widehat{X} - X\|}{\|X\|} = O(\mathtt{u}), \frac{\|\widehat{Y} - Y\|}{\|Y\|} = O(\mathtt{u}) \quad \text{and} \quad \frac{|\widehat{D} - D|}{|D|} = O(\mathtt{u})$$

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- Least squares problems
  [2011, Castro&Ceballos&Dopico&M]

Outline

Algorithm: Linear Systems

- Input: $A \in \mathbb{R}^{n\times n},\ b \in \mathbb{R}^n$
- Output: x solution of $A\,x = b$

1. Compute an accurate RRD of $A = XDY$
2. Solve the three systems

$$\begin{array}{ccc} X\,s = b & \longrightarrow & s \\ D\,w = s & \longrightarrow & w \\ Y\,x = w & \longrightarrow & x \end{array}$$

$O(n^3)$ complexity

Algorithm: Least squares Problems

- Input: $A \in \mathbb{C}^{m \times n}$, $b \in \mathbb{C}^{m}$
- Output: $x_0 = A^{\dagger} b$

1. Compute an accurate RRD of $A = XDY$
2. Compute the solution x_1 of $\min_{x \in \mathbb{C}^n} \|b - X\,x\|_2$ using QR Householder.
3. Solve, for x_2, the diagonal linear system, $D\,x_2 = x_1$.
4. Compute the minimal 2-norm solution x_0 of $Yx = x_2$ using QR Householder on Y^*.

$O(n^3)$ complexity

Backward Error

Theorem

The computed minimal 2-norm solution of $XDYx \approx b$, with roundoff error $\mathtt{u}$, is the exact minimal 2-norm solution of

$$(X + \Delta X)(D + \Delta D)(Y + \Delta Y)\widehat{x} \approx b$$

with

$$\|\Delta X\| \leqslant O(\mathtt{u})\|X\|, \quad \|\Delta Y\| \leqslant O(\mathtt{u})\|Y\|, \quad |\Delta D| \leqslant O(\mathtt{u})|D|$$

Outline

Moore-Penrose Pseudoinverse Multiplicative Perturbation Theory

Theorem

Let $A \in \mathbb{C}^{m\times n}$ *and* $\widetilde{A} = (I+E)A(I+F)$ *where* $I+E$ *and* $I+F$ *are nonsingular. Then*

$$\widetilde{A}^{\dagger} = P_{\widetilde{A}^*}(I+F)^{-1}A^{\dagger}(I+E)^{-1}P_{\widetilde{A}}$$

where $P_{\widetilde{A}} = \widetilde{A}\widetilde{A}^{\dagger}$ *and* $P_{\widetilde{A}^*} = \widetilde{A}^{\dagger}\widetilde{A}$

RRD Perturbation Theory

Theorem

Let

- x_0 *be the minimum* 2*-norm solution of*

$$\min_{x\in\mathbb{C}^n} \|b - XDY\,x\|_2,$$

- $\widetilde{x}_0$ *be the minimum* 2*-norm solution of*

$$\min_{x\in\mathbb{C}^n} \|b + h - (X + \Delta X)(D + \Delta D)(Y + \Delta Y)\,x\|_2$$

$\|\Delta X\|_2 \leq \epsilon\|X\|_2$, $\|\Delta Y\|_2 \leq \epsilon\|Y\|_2$, $|\Delta D| \leq \epsilon|D|$, *and* $\|h\|_2 \leq \epsilon\|b\|_2$.
Then:

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Then:

$$\frac{\|\widetilde{x}_0 - x_0\|_2}{\|x_0\|_2} \leq \epsilon \left(P_1\, \kappa_2(Y) + P_2\, \kappa_2(X)\, \frac{\|A^\dagger\|_2 \|b\|_2}{\|x_0\|_2} \right) + O(\epsilon^2).$$

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Perturbing the right-hand side

The minimal length solutions of the least squares problems

$$A\,x \approx b \quad \text{and} \quad A\,(x + \Delta x) \approx b + \Delta b$$

are related as

$$\frac{\|\Delta x\|}{\|x\|} \leqslant \frac{\|A^\dagger\|\|\Delta b\|}{\|x\|} = \kappa(A, b)\frac{\|\Delta b\|}{\|b\|}$$

with

$$\kappa(A, b) \equiv \frac{\|A^\dagger\|\|b\|}{\|x\|} \leqslant \|A^\dagger\|\|A\|\frac{\|b\|}{\|P_r(b)\|} = \frac{\kappa(A)}{\cos\theta}.$$

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Example in MATLAB:

```
>> m=30;n=15;v= vander(randn(m,1)); v=fliplr(v);
>> v=v(:,1:n);b=randn(m,1);
>> cond(v)= 1.6234e+07
>> cond(v)*norm(b)/norm(v*x) = 2.3898e+07
>> norm(x) = 230.23
>> norm(b) = 5.1154
>> norm(pinv(v))*norm(b)/norm(x) = 4.181
```

Effective conditioning

Theorem (Chan & Foulser, 1988)

If $A \in \mathbb{C}^{m\times n}, \quad rank(A) = r \le n \le m$

$$A = U\Sigma V^H = [\widetilde{U}\ U_k] \begin{bmatrix} \widetilde{\Sigma} & 0 \\ 0 & \Sigma_k \end{bmatrix} \begin{bmatrix} \widetilde{V} \\ V_k \end{bmatrix}$$

is a (partitioned) reduced SVD of A*, and* $x = A^{\dagger} b$*, then*

$$\kappa_2(A, b) = \frac{\|b\|_2}{\sigma_r \|x\|_2} \leqslant \frac{\sigma_{r+1-k}}{\sigma_r} \frac{\|b\|_2}{\|P_k b\|_2}, \quad \forall k = 1 : r$$

where $P_k = U_k U_k^*$ *is the orthogonal projector onto the subspace spanned by the last* k *left singular vectors of* A*.*

Effective conditioning

For the perturbation problem $A\,(x+\Delta x) \approx b+\Delta b$ this means

$$\frac{\|\Delta x\|_2}{\|x\|_2} \leqslant \kappa_2(A,b)\frac{\|\Delta b\|_2}{\|b\|_2} \leqslant \kappa_{eff}(A,b)\frac{\|\Delta b\|_2}{\|b\|_2}$$

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with

$$\kappa_{eff}(A,b) = \min_{k=1:r}\left\{\frac{\sigma_{r+1-k}}{\sigma_r}\frac{\|b\|_2}{\|P_k b\|_2}\right\} \leqslant \frac{\|b\|_2}{\|P_1 b\|_2}$$

Forward Error

Theorem

If $\widehat{x}$ *is the computed solution of* $A\,x \approx b$ *using previous algorithm, with roundoff error* `u`, *then*

Forward Error

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If $\widehat{x}$ is the computed solution of $A\,x \approx b$ using previous algorithm, with roundoff error $\mathtt{u}$, *then*

$$\frac{\|\widehat{x} - x\|}{\|x\|} \leqslant \mathtt{u} \left(P_1\ \kappa_2(\widehat{Y}) + P_2\ \kappa_2(\widehat{X})\ \frac{\|A^\dagger\|\ \|b\|}{\|x\|} \right) + O(\mathtt{u}^2)$$

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$k = 1 : r$.

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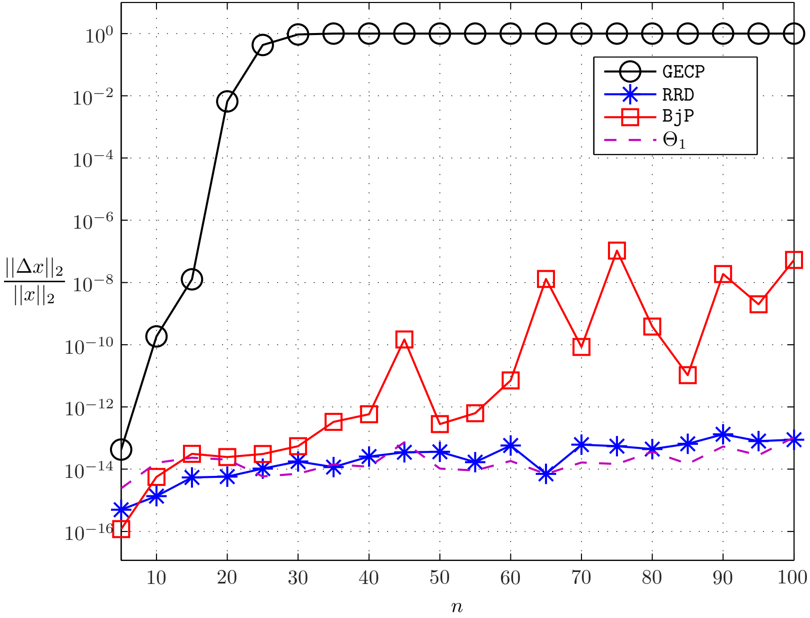
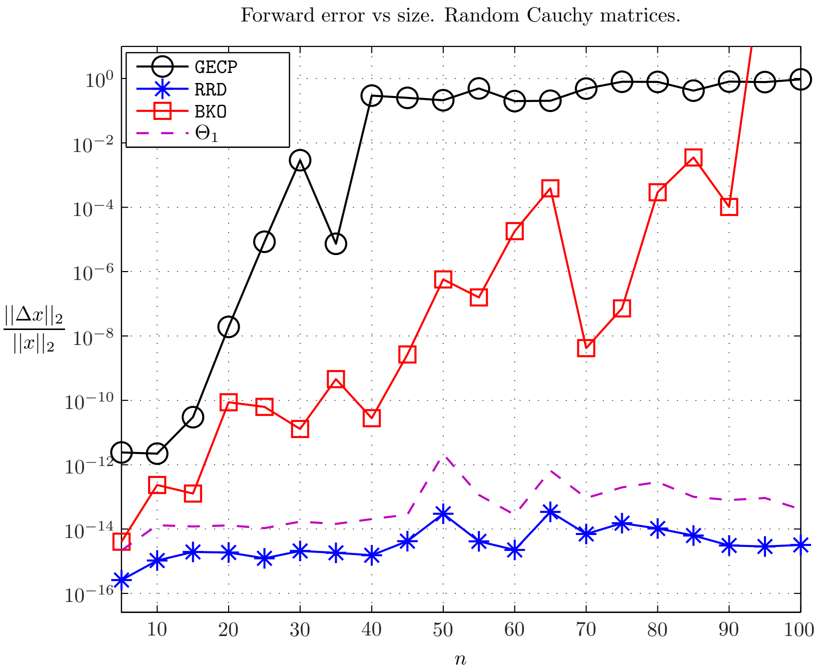
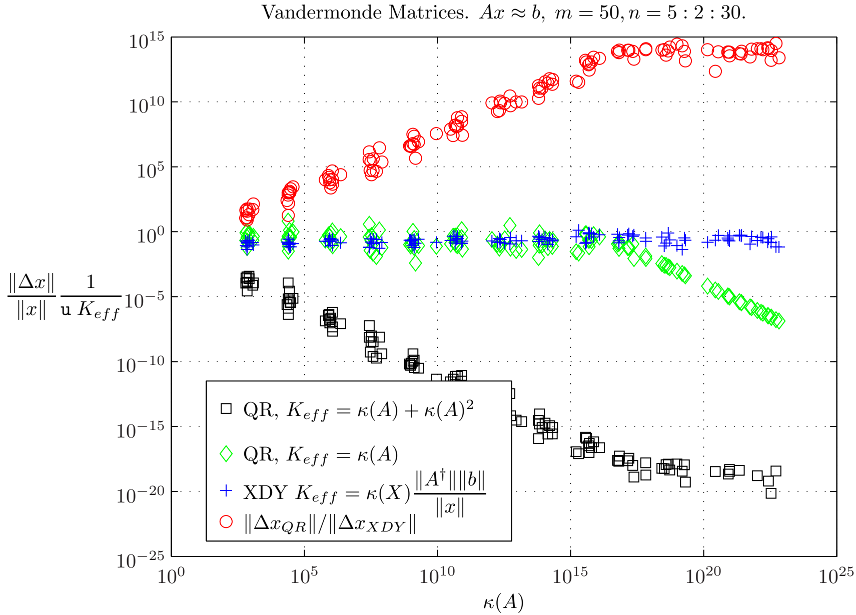
Outline

Forward error vs size. Random Vandermonde matrices.




Forward error vs size. Random Cauchy matrices.
GECP
RRD
BKO
Θ1
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−14
10^−16
||Δx||2 / ||x||2
10
20
30
40
50
60
70
80
90
100
n



Vandermonde Matrices. $Ax \approx b,\ m = 50, n = 5:2:30$.
10^{15}
10^{10}
10^{5}
10^{0}
10^{-5}
10^{-10}
10^{-15}
10^{-20}
10^{-25}
$\frac{\|\Delta x\|}{\|x\|}\frac{1}{\mathrm{u}\,K_{eff}}$
10^{0} 10^{5} 10^{10} 10^{15} 10^{20} 10^{25}
$\kappa(A)$
QR, $K_{eff} = \kappa(A) + \kappa(A)^2$
QR, $K_{eff} = \kappa(A)$
XDY $K_{eff} = \kappa(X)\frac{\|A^\dagger\|\|b\|}{\|x\|}$
$\|\Delta x_{QR}\|/\|\Delta x_{XDY}\|$

Conclusions

- It is possible now to compute accurately solutions of structured systems with huge condition numbers.
- It is necessary to take advantage of the structure of the matrix.
- New multiplicative perturbation results are necessary.
- RRD play a central and important role.

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Thanks for your attention