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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Outline

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

Outline

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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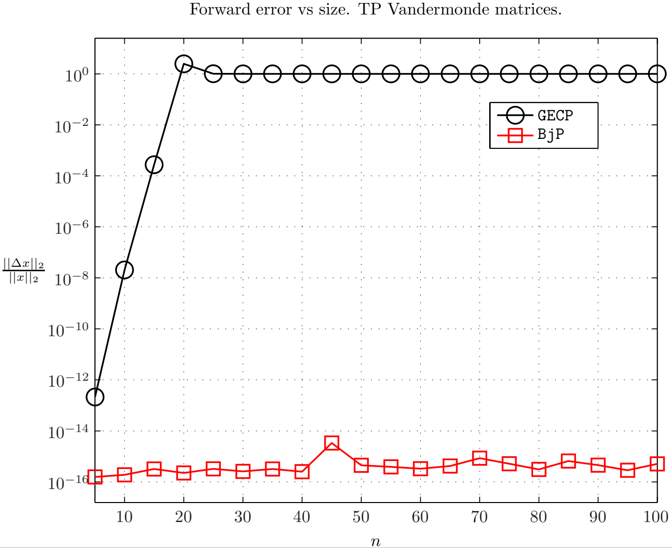

TP Cauchy matrices

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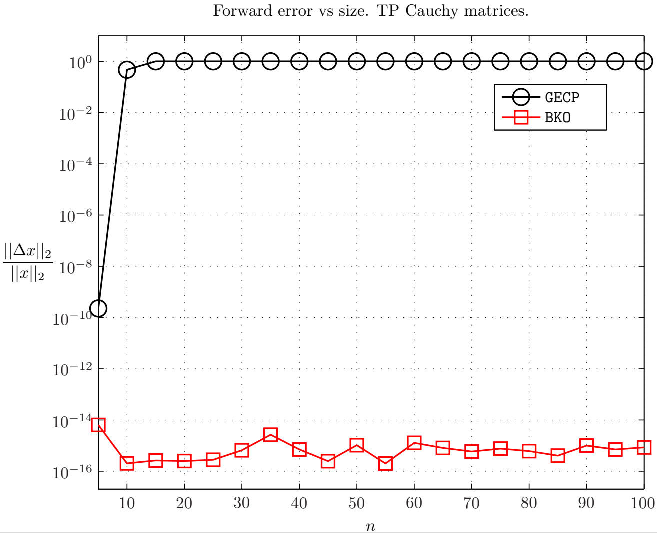

New methods

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 $A\,x \approx b$,
- for "almost any" rhs b,
- 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

- RRDs can be computed in practice from Gaussian Elimination with Complete Pivoting (GECP) (i.e., direct methods).

Structured matrices and accurate RRDs

- 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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- Eigenvalues and eigenvectors of symmetric matrices
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  [2009, Dopico&Koev&M]

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- Linear systems of equations
  [2011, IMA Journal of Numerical Analysis, Dopico&M]

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- Linear systems of equations
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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

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

$O(n^3)$ 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

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

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RRD Perturbation Theory

We are interested in computing the minimal 2-norm solution of

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$$\begin{aligned}\widetilde{A} &= (X + \Delta X)(D + \Delta D)(Y + \Delta Y) \\ &= (I + \Delta X X^{\dagger}) X (I + \Delta D D^{-1}) D Y (I + Y^{\dagger} \Delta Y)\end{aligned}$$

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&=: (I + E) X D Y (I + F),
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$$\begin{aligned}
\widetilde{A} &= (X + \Delta X)(D + \Delta D)(Y + \Delta Y) \\
&= (I + \Delta X X^{\dagger})X(I + \Delta D D^{-1})DY(I + Y^{\dagger}\Delta Y) \\
&= (I + \Delta X X^{\dagger})(I + X \Delta D D^{-1} X^{\dagger})XDY(I + Y^{\dagger}\Delta Y) \\
&=: (I + E)XDY(I + F),
\end{aligned}$$

where $E = \Delta X X^{\dagger} + X \Delta D D^{-1} X^{\dagger} + \Delta X \Delta D D^{-1} X^{\dagger}$ and $F = Y^{\dagger}\Delta Y$.

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\end{aligned}$$

where $\|E\| \leq O(\mathtt{u})\kappa(X)$ and $\|F\| \leq O(\mathtt{u})\kappa(Y)$, if $\Delta X, \Delta Y$ come from previous error analysis.

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.*

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

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

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

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

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

where $\widehat{E} = (I+E)^{-1}E$ *and* $\widehat{F} = (I+F)^{-1}F$.

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* $\|h\|_2 \leq \epsilon \|b\|_2$.
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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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RRD Perturbation Theory

$$\kappa_f(X, D, Y, b) :=$$

$$:= \lim_{\epsilon \to 0} \sup \left\{ \frac{\|\widetilde{x} - x\|}{\epsilon \|x\|} \; : \; (X + \Delta X)\,(D + \Delta D\,)\,(Y + \Delta Y)\,\widetilde{x} = b + h, \right.$$

$$\left. \|h\| \leqslant \epsilon \|b\|, \;\; \|\Delta X\| \leqslant \epsilon\, \|X\|, \;\; |\Delta D\,| \leqslant \epsilon\, |D|, \;\; \|\Delta Y\| \leqslant \epsilon\, \|Y\| \right\}$$

Theorem

$$\kappa_f(X, D, Y, b) \leq \left(\kappa(Y) + [1 + 2\,\kappa(X)]\;\; \frac{\|A^{-1}\|\,\|b\|}{\|x\|} \right) \leq 3\,\kappa_f(X, D, Y, b)$$

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

$$\frac{\|\Delta x_0\|}{\|x_0\|} \leqslant \frac{\|A^\dagger\|\|\Delta b\|}{\|x_0\|} = \kappa(A, b)\frac{\|\Delta b\|}{\|b\|}$$

with

$$\kappa(A, b) \equiv \frac{\|A^\dagger\|\|b\|}{\|x_0\|} \leqslant \|A^\dagger\|\|A\|\frac{\|b\|}{\|P_A(b)\|} = \frac{\kappa(A)}{\cos\theta}.$$

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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
```

Perturbing the right-hand side

If $A \in \mathbb{C}^{n\times n}$ is invertible and

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

then

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Example in MATLAB:

```
>> v= vander(randn(20,1)); b=randn(20,1);
>> cond(v)= 7.1021e+11
>> norm(inv(v)) = 1.4857e+11
>> norm(x) = 5.4507e+10
>> norm(b) = 3.0934
>> norm(inv(v))*norm(b)/norm(x) = 8.4317
```

Effective conditioning

Theorem (Chan & Foulser, 1988)

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

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

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

$$\frac{\|\Delta x_0\|_2}{\|x_0\|_2} \leqslant \kappa_2(A,b)\frac{\|\Delta b\|_2}{\|b\|_2} \leqslant \kappa_{eff}(A,b)\frac{\|\Delta b\|_2}{\|b\|_2}$$

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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

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$$\frac{\|\widehat{x}_0 - x_0\|}{\|x_0\|} \leqslant \mathtt{u} \left(P_1\ \kappa_2(\widehat{Y}) + P_2\ \kappa_2(\widehat{X})\ \frac{\|A^\dagger\|\ \|b\|}{\|x_0\|} \right) + O(\mathtt{u}^2)$$

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$$\frac{\|\widehat{x}_0 - x_0\|}{\|x_0\|} \leqslant \mathtt{u} \left(P_1 \; \kappa_2(\widehat{Y}) + P_2 \; \kappa_2(\widehat{X}) \; \frac{\sigma_{r+1-k}}{\sigma_r} \frac{\|b\|}{\|P_k b\|} \right) + O(\mathtt{u}^2)$$

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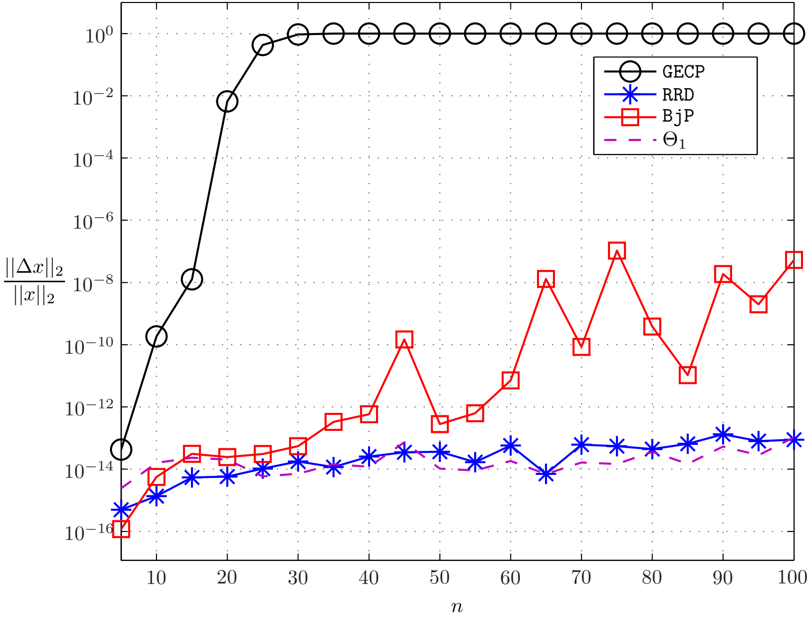
Theorem

If $\widehat{x}_0$ is the computed solution of $A\,x \approx b$ using previous algorithm, with roundoff error $\mathtt{u}$, then,

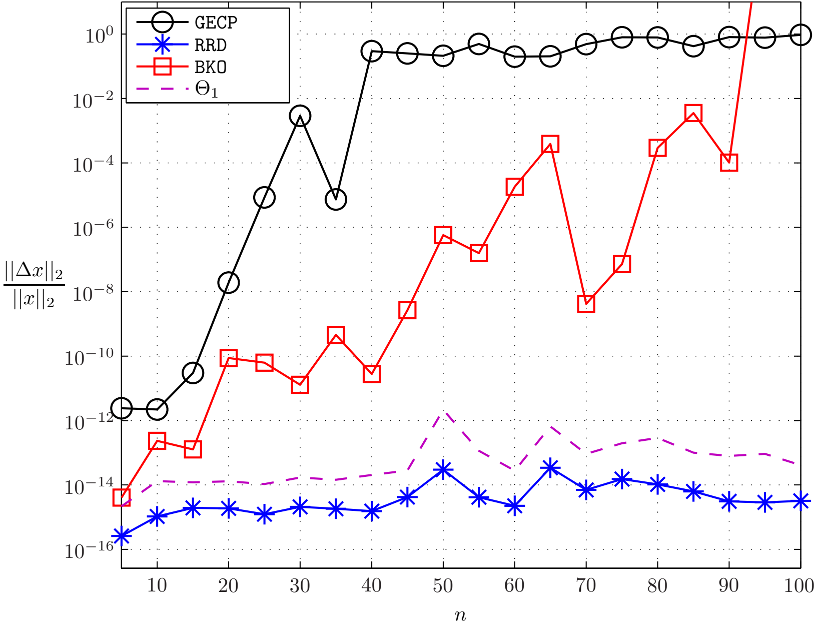
$$\frac{\|\widehat{x}_0 - x_0\|}{\|x_0\|} \leqslant \mathtt{u} \left(P_1\ \kappa_2(\widehat{Y}) + P_2\ \kappa_2(\widehat{X})\ \frac{\|b\|}{\|P_1 b\|} \right) + O(\mathtt{u}^2)$$

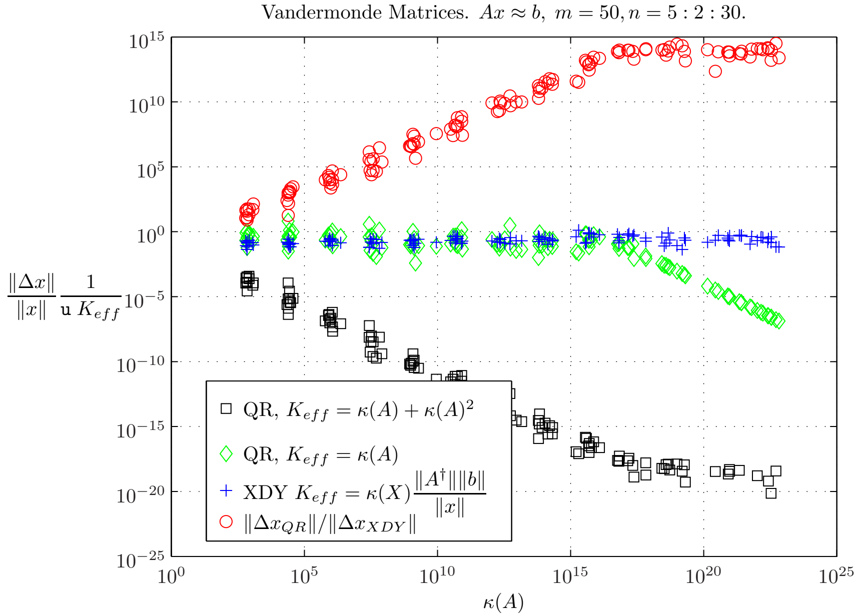
Outline

Forward error vs size. Random Vandermonde matrices.



Forward error vs size. Random Cauchy matrices.





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