Accurate Solutions of Structured Linear Systems

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- Here we will present a method that gets (hra) for any Cauchy or Vandermonde (and many other classes). It is based on accurate Rank Revealing Decompositions, that are known to exist for many classes of structured matrices.

High relative accuracy

We say that the solution of

$$A\,z = b$$

is computed with high relative accuracy (hra) if

$$\frac{\|\widehat{z} - z\|}{\|z\|} = O(\mathbf{u})$$

with $\widehat{z}$ the computed solution and $\mathbf{u}$ the unit roundoff, independently of the condition number of A.

Rank Revealing Decompositions

- Rank Revealing Decompositions have been widely used to compute
  - Singular Values and Vectors [1999, Demmel et al.]
  - Eigenvalues and Eigenvectors [2003, Dopico&M&Moro; 2005, Dopico&Koev; 2009 Dopico&Koev&M]

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- In this work RRDs will be used to solve linear systems.
- The algorithm presented has $O(n^3)$ complexity.

Cauchy and Vandermonde matrices

Given $x, y \in \mathbb{R}^n$, a Cauchy matrix is given by

$$C_{i,j} = \frac{1}{x_i + y_j}$$

$$C(x,y) = \begin{bmatrix} \frac{1}{x_1+y_1} & \frac{1}{x_1+y_2} & \cdots & \frac{1}{x_1+y_n} \\ \frac{1}{x_2+y_1} & \frac{1}{x_2+y_2} & \cdots & \frac{1}{x_2+y_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{x_n+y_1} & \frac{1}{x_n+y_2} & \cdots & \frac{1}{x_n+y_n} \end{bmatrix} \in \mathbb{R}^{n \times n}$$

$C(x,y)$ is Totally Positive if

$$x_1 + y_1 > 0$$
$$x_1 \le x_2 \le \ldots \le x_{n-1} \le x_n$$
$$y_1 \le y_2 \le \ldots \le y_{n-1} \le y_n$$

Cauchy and Vandermonde matrices

Given $x \in \mathbb{R}^n$, a Vandermonde matrix is given by

$$V_{i,j} = x_j^{i-1}$$

$$V(x) = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \\ x_1^2 & x_2^2 & \cdots & x_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{n-1} & x_2^{n-1} & \cdots & x_n^{n-1} \end{bmatrix} \in \mathbb{R}^{n\times n}$$

$V(x)$ is Totally Positive if

$$0 < x_1 < x_2 < \ldots < x_n$$

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- There exist fast $O(n^2)$ algorithms to solve linear systems. [1970, Björk&Pereyra; 1999, Boros&Kailath&Olshevsky]
- For these fast algorithms hra is achieved (guaranteed for certain rhs) when they are totally positive.

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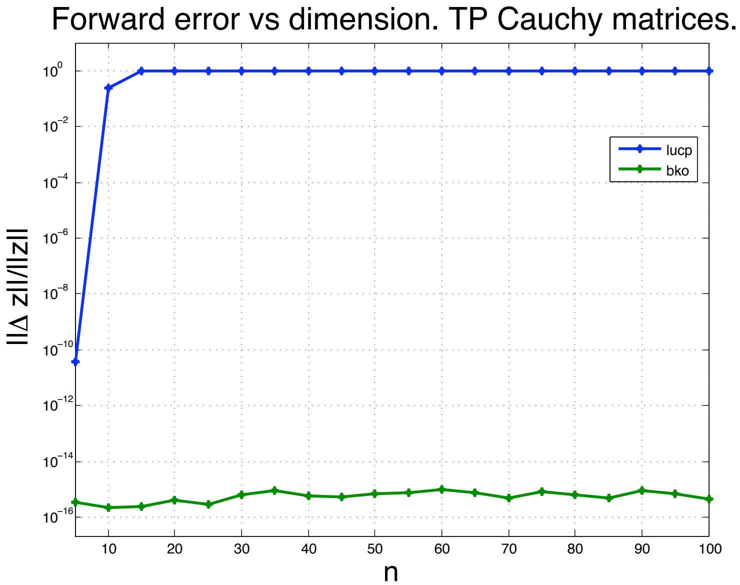
- Backward errors related to the perturbation of the rhs. [1987, Higham; 1999, Boros&Kailath&Olshevsky]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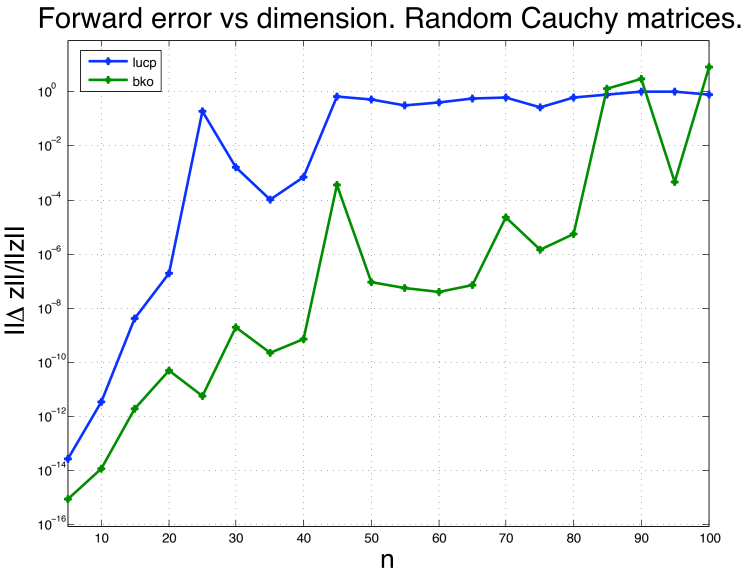
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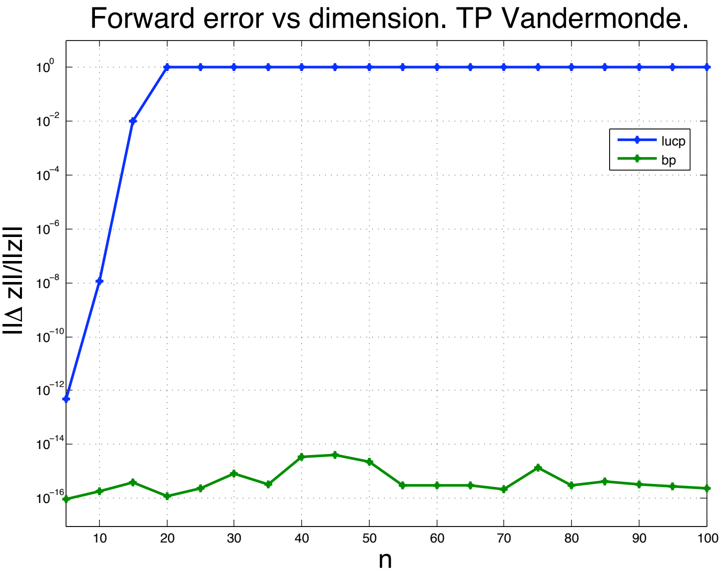
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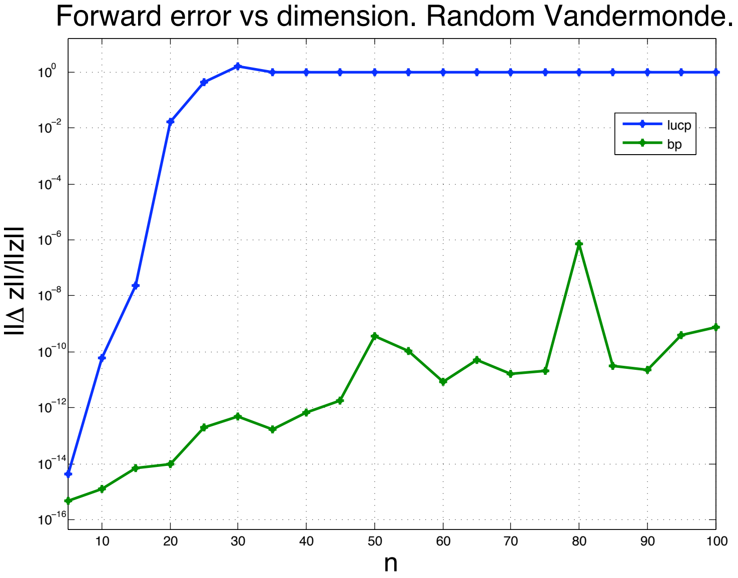
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Perturbing the right-hand side

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

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

then

$$\frac{\|\Delta z\|_2}{\|z\|_2} \leq \frac{\|A^{-1}\|_2 \|\Delta b\|_2}{\|z\|_2} = \kappa_2(A, b)\frac{\|\Delta b\|_2}{\|b\|_2}$$

with

$$\kappa_2(A, b) \equiv \frac{\|A^{-1}\|_2 \|b\|_2}{\|z\|_2} = \frac{\|b\|_2}{\sigma_n \|z\|_2}$$

being σ_n the smallest singular value of A.

Effective conditioning

Theorem (Chan & Foulser, 1988)

If

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

is a (partitioned) SVD of A, and $A\,z = b$, then

$$\kappa_2(A,b) = \frac{\|b\|_2}{\sigma_n \|z\|_2} \leq \frac{\sigma_{n+1-k}}{\sigma_n} \frac{\|b\|_2}{\|P_k b\|_2}, \quad \forall k = 1:n$$

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

Effective conditioning

For the perturbation problem $A\,(z + \Delta z) = b + \Delta b$ this means

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

with

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

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Notice that, except in an unlikely case where $u_n^T b \approx 0$, we will have

$$\|P_1 b\|_2 = u_n^T b \lesssim \|b\|_2$$

with u_n the last left singular vector of A.

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If, for example, $\|P_1 b\|_2 = u_n^T b \geqslant \frac{\|b\|_2}{n}$, then

$$\frac{\|\Delta z\|_2}{\|z\|_2} \le n\,\frac{\|\Delta b\|_2}{\|b\|_2}$$

Algorithm

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

- Step 1: Compute an accurate RRD of $A = XDY^T$
- Step 2: Solve the three systems

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

Rank Revealing Decomposition

1. Given $A \in \mathbb{C}^{m\times n}$, with $rank(A) = r$,

$$A = XDY^T,$$

with $X \in \mathbb{C}^{m\times r}$, $Y \in \mathbb{C}^{n\times r}$ and $D \in \mathbb{C}^{r\times r}$ diagonal, it is called a Rank Revealing Decomposition (RRD) of A if

$$\kappa(X), \kappa(Y) \gtrsim 1 \quad \text{and} \quad \kappa(D) \approx \kappa(A).$$

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$$\kappa(X), \kappa(Y) \gtrsim 1 \quad \text{and} \quad \kappa(D) \approx \kappa(A).$$

2. We say that an RRD, $A = XDY^T$, is accurate if the computed factors $\widehat{X}, \widehat{Y}$ and $\widehat{D}$ obey

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

Structured matrices and RRDs

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

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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]
  - ...

Backward Error

Theorem

If $\widehat{z}$ is the computed solution of $XDY^Tz = b$ using previous Algorithm, with roundoff error $\mathbf{u}$, then

$$(X + \Delta X)(D + \Delta D)(Y + \Delta Y)^T \widehat{z} = b$$

with

$$\|\Delta X\| \leq O(\mathbf{u})\|X\|, \quad \|\Delta Y\| \leq O(\mathbf{u})\|Y\|, \quad |\Delta D| \leq O(\mathbf{u})|D|$$

RRD Perturbation Theory

Theorem

Let $A = XDY^T \in \mathbb{R}^{n\times n}$ *be an RRD of* A *and* z *the solution of* $XDY^Tz = b$*, then the solution of*

$$(X + \Delta X)(D + \Delta D)(Y + \Delta Y)^T(z + \Delta z) = b$$

obeys, if $\|\Delta X\| \leq \epsilon \, \|X\|, \|\Delta Y\| \leq \epsilon \, \|Y\|, |\Delta D| \leq \epsilon \, |D|,$

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$$\frac{\|\Delta z\|_2}{\|z\|_2} \leq \frac{\|b\|_2}{\sigma_n \|z\|_2} \left[2\kappa_2(X) + \kappa_2(Y)\right] O(\epsilon)$$

with $\kappa_2(X) = \|X^{-1}\|_2 \|X\|_2, \kappa_2(Y) = \|Y^{-1}\|_2 \|Y\|_2$.

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being u_n the last left singular vector of A.

Numerical Experiments: Cauchy matrices

We have built Cauchy matrices with

- TP matrices (ordered x and y vectors) and non TP matrices (random x and y vectors)
- Random rhs vector b
- Sizes `5:5:100`
- $10^6 \lesssim \kappa(C(x,y)) \lesssim 10^{200}$

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We have used four algorithms

- GECP
- BKO fast ($O(n^2)$) algorithm (Boros-Kailath-Olshevsky)
- GS-Cauchy [BKO] fast algorithm with pre-pivoting (Rational Leja ordering)
- Rank Revealing ($O(n^3)$) algorithm (Demmel)+ MATLAB (`Y\D\X\b`)

Computable bound

We have checked the bound in the forward error

$$\frac{\|\Delta z\|_2}{\|z\|_2} \leq \frac{\|b\|_2}{\sigma_n \|z\|_2} \left[2\kappa_2(X) + \kappa_2(Y)\right] O(\mathbf{u})$$

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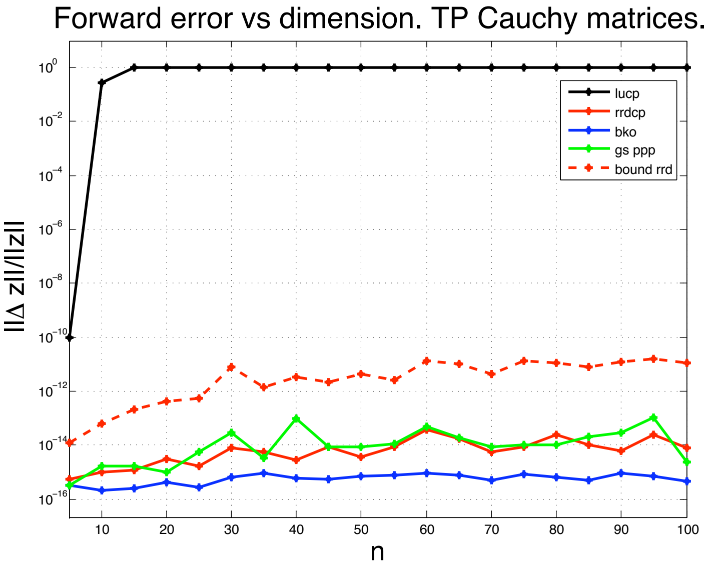
we get the computable approximation

$$\texttt{bound\_rrd} = \frac{\|\widehat{Y}^{-1}\|_2 \|\widehat{X}^{-1}\|_2}{|d_n|} \frac{\|b\|_2}{\|\widehat{z}\|_2} \left[2\kappa_2(\widehat{X}) + \kappa_2(\widehat{Y})\right] \mathbf{u}$$

independent of σ_n or A^{-1}.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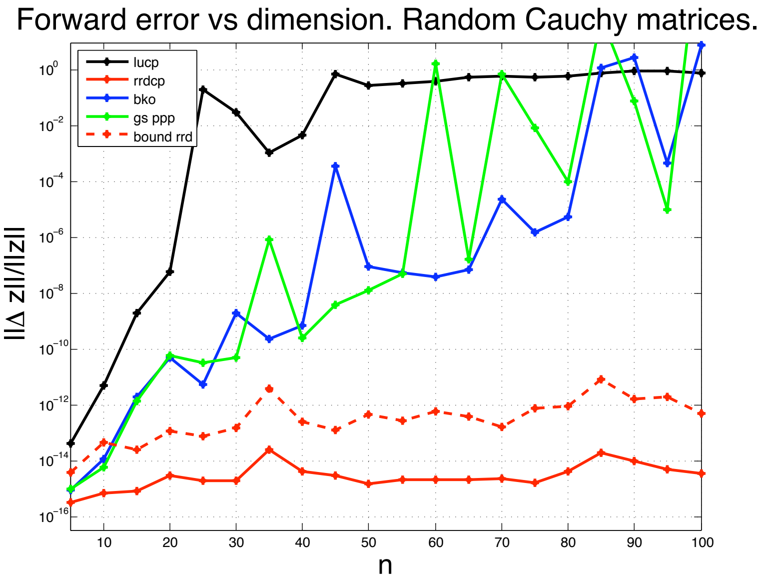
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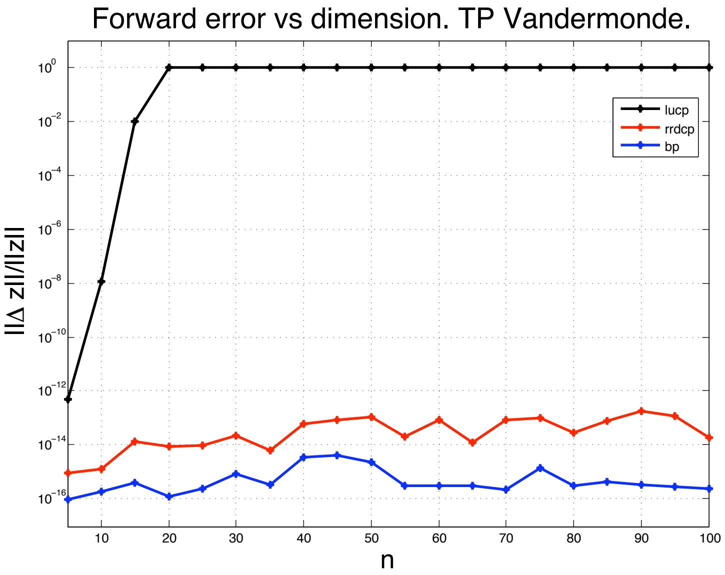

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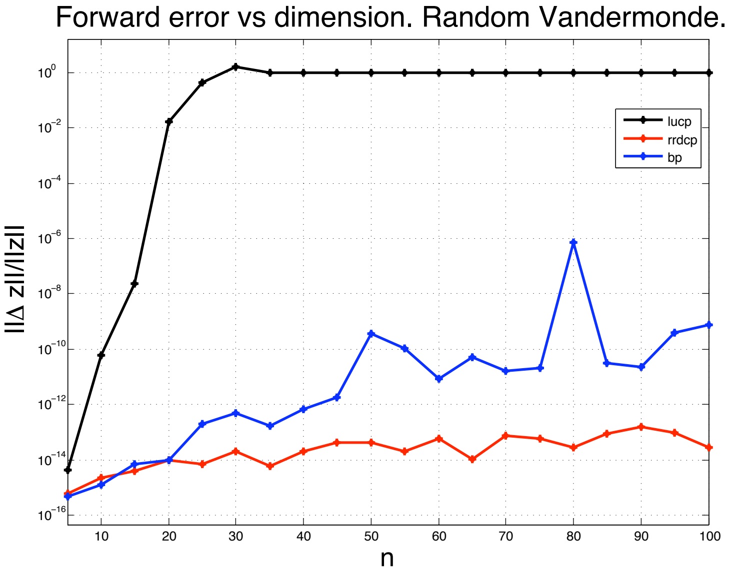
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Conclusions

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- We have used an $O(n^3)$ algorithm that uses an accurate RRD.
- We have shown satisfactory numerical results for Cauchy and Vandermonde matrices.
- It will work for any kind of matrices for which accurate RRDs can be computed, now or in the future, and for, almost, any b.

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Thank you for your attention.