## On Incremental 2-norm Condition Estimators

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## Outline

(1) Introduction: The Problem
(2) The two strategies
(3) ICE and INE with inverse factors

4 INE maximization versus ICE maximization
(5) Numerical experiments
(6) Conclusions

## Introduction: The Problem

Matrix condition number: an important quantity used in numerical linear algebra. We consider square nonsingular matrices:

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- Estimating sensitivity to perturbations
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- Assessing quality of computed solutions
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- Monitor and control adaptive computational processes.
- Here: $A$ upper triangular (no loss of generality - computations typically based on triangular decomposition)
- Euclidean norm


## Introduction: Earlier work

- Turing (1948); Wilkinson (1961)
- Gragg, Stewart (1976); Cline, Moler, Stewart, Wilkinson (1979); Cline, Conn, van Loan (1982); van Loan (1987)


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- 1-norm: Hager (1984), Higham (1987, 1988, 1989, 1990) [175], Higham, Tisseur (2000).


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- 1-norm: Hager (1984), Higham (1987, 1988, 1989, 1990) [175], Higham, Tisseur (2000).
- Incremental: Bischof (1990, 1991), Bischof, Pierce, Lewis (1990), Bischof, Tang (1992); Ferng, Golub, Plemmons (1991); Pierce, Plemmons (1992); 2-norm estimator based on pivoted QLP: Stewart (1998); Duff, Vömel (2002)


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- See also other techniques in various applications: adaptive filters, recursive least-squares, ACE for multilevel PDE solvers.


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- An immediate application is dropping and pivoting in preconditioner computation (see Bollhöfer, Saad (2001-2006)).


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- An immediate application is dropping and pivoting in preconditioner computation (see Bollhöfer, Saad (2001-2006)).
- Starting point: the methods by Bischof (1990) (incremental condition number estimation - ICE) and Duff, Vömel (2002) (incremental norm estimation - INE).


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ICE - Bischof (1990)

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\hat{R}=\left[\begin{array}{cc}
R & v \\
0 & \gamma
\end{array}\right]
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- Using a left extremal (minimum or maximum) singular vector $u_{e x t}$, if $R=U \Sigma V^{T} \Rightarrow\left\|u_{e x t}^{T} R\right\|=\left\|u_{e x t}^{T} U \Sigma V^{T}\right\|=\sigma_{e x t}(R)$.


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- Bischof (1990): estimates to extremal singular values and left singular vectors:

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\begin{gathered}
\sigma_{\text {ext }}^{C}(R)=\left\|y_{e x t}^{T} R\right\| \approx \sigma_{\text {ext }}(R) \\
\left\|\hat{y}_{e x t}^{T} \hat{R}\right\|=\operatorname{ext}_{\|[s, c]\|=1}\left\|\left[\begin{array}{ll}
s y_{e x t}^{T}, & c
\end{array}\right]\left[\begin{array}{cc}
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- $s_{\text {ext }}$ and $c_{e x t}$ : components of the eigenvector corresponding to the extremal (minimum or maximum) eigenvalue of $B_{\text {ext }}^{C}$

$$
B_{e x t}^{C} \equiv\left[\begin{array}{cc}
\sigma_{e x t}^{C}(R)^{2}+\left(y_{e x t}^{T} v\right)^{2} & \gamma\left(y_{e x t}^{T} v\right) \\
\gamma\left(y_{e x t}^{T} v\right) & \gamma^{2}
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- Again, $s_{\text {ext }}$ and $c_{\text {ext }}$ : components of the eigenvector corresponding to the extremal (minimum or maximum) eigenvalue of $B_{e x t}^{N}$

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## ICE and INE when both direct and inverse factors available: ICE

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- Estimation of $\sigma_{-}(R)$ is often harder than estimation of $\sigma_{+}(R)$. With $R^{-1}$ this can be circumvented using $1 / \sigma_{+}\left(R^{-1}\right)$. However:


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## Theorem

Computing the inverse factor $R^{-1}$ in addition to $R$ does not give any improvement for ICE:

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## Theorem

Computing the inverse factor $R^{-1}$ in addition to $R$ does not give any improvement for ICE: Let $R$ be a nonsingular upper triangular matrix. Then the ICE estimates of the singular values of $R$ and $R^{-1}$ satisfy

$$
\sigma_{-}^{C}(R)=1 / \sigma_{+}^{C}\left(R^{-1}\right)
$$

The approximate left singular vectors $y_{-}$and $x_{+}$corresponding to the ICE estimates for $R$ and $R^{-1}$, respectively, satisfy

$$
\sigma_{-}^{C}(R) x_{+}^{T}=y_{-}^{T} R
$$

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INE maximization applied to $R^{-1}$ may provide a better estimate than INE minimization applied to $R$ :

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1 / \sigma_{+}^{N}\left(\hat{R}^{-1}\right) \leq \sigma_{-}^{N}(\hat{R})
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with equality if and only if $v$ is collinear with the left singular vector corresponding to the smallest singular value of $R$.

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Rather technical in case the assumption is relaxed to $1 / \sigma_{+}^{N}\left(R^{-1}\right) \leq \sigma_{-}^{N}(R)$. Superiority of maximization does not apply always, but might explain the name incremental norm estimation.

Small example: ICE and INE with maximization and minimization

$$
R=\left[\begin{array}{ccc}
2 & 0 & 1 \\
& 1 & 0 \\
& & 1
\end{array}\right], \quad \sigma_{-}(R)=0.874
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\hat{R}=\left[\begin{array}{llll}
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0.5381 \approx 1 / \sigma_{+}^{N}\left(\hat{R}^{-1}\right)<\sigma_{-}^{N}(\hat{R}) \approx 0.835
\end{gathered}
$$

## An example showing the possible gap between the ICE and INE estimates



Figure: INE estimation of the smallest singular value of the 1D Laplacians of size one until hundred: INE with minimization (solid line), INE with maximization (circles) and exact minimum singular values (crosses).

## Example: INE with maximization and exact smallest singular value



Figure : INE estimation of the smallest singular value of the 1D Laplacians of size fifty until hundred (zoom of previous figure for INE with maximization and exact minimum singular values).

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## INE versus ICE

## Theorem

Consider norm estimation of the extended matrix

$$
\hat{R}=\left[\begin{array}{cc}
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\end{array}\right]
$$

let ICE and INE start with $\sigma_{+} \equiv \sigma_{+}^{C}(R)=\sigma_{+}^{N}(R)$; let $y$ be the ICE approximate LSV, $z$ be the INE approximate RSV and $w=R z / \sigma^{+}$. We have $\sigma_{+}^{N}(\hat{R}) \geq \sigma_{+}^{C}(\hat{R})$ if

$$
\left(v^{T} w\right)^{2} \geq \rho_{1}
$$

where $\rho_{1}$ is the smaller root of the quadratic equation in $\left(v^{T} w\right)^{2}$,

$$
\begin{aligned}
\left(v^{T} w\right)^{4} & +\left(\frac{\gamma^{2}+\left(v^{T} y\right)^{2}}{\sigma_{+}^{2}}\left(v^{T} v-\left(v^{T} y\right)^{2}\right)-v^{T} v-\left(v^{T} y\right)^{2}\right)\left(v^{T} w\right)^{2} \\
& +\left(v^{T} y\right)^{2}\left(\frac{\gamma^{2}+v^{T} v}{\sigma_{+}^{2}}\left(\left(v^{T} y\right)^{2}-v^{T} v\right)+v^{T} v\right)=0
\end{aligned}
$$

## Example: ICE versus INE



Figure: Value of $\rho_{1}$ in dependence of $\left(v^{T} y\right)^{2}\left(\mathrm{x}\right.$-axis) and $\gamma^{2}(\mathrm{y}$-axis) with $\sigma_{+}=1,\|v\|^{2}=0.1$.

## Example: ICE versus INE



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Figure: Value of $\rho_{1}$ in dependence of $\left(v^{T} y\right)^{2}\left(\mathrm{x}\right.$-axis) and $\gamma^{2}(\mathrm{y}$-axis) with $\sigma_{+}=1,\|v\|^{2}=10$.

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Figure: Value of $\rho_{1}$ in dependence of $\left(v^{T} y\right)^{2}\left(\mathrm{x}\right.$-axis) and $\gamma^{2}(\mathrm{y}$-axis) with $\sigma_{+}=1, \Delta=0.6,\|v\|^{2}=0.1$.

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## Comparison 1

Example 1: 50 matrices $A=\operatorname{rand}(100,100)-\operatorname{rand}(100,100)$, dimension 100 , colamd, $R$ from the QR decomposition of $A$. (Bischof, 1990, Section 4).


Figure : Ratio of estimate to real condition number for the 50 matrices in example 1. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

## Comparison 2

Example 2: 50 matrices $A=U \Sigma V^{T}$ of size 100, prescribed condition number $\kappa$ choosing

$$
\Sigma=\operatorname{diag}\left(\sigma_{1}, \ldots, \sigma_{100}\right), \text { with } \quad \sigma_{k}=\alpha^{k}, \quad 1 \leq k \leq 100, \quad \alpha=\kappa^{-\frac{1}{99}}
$$

$U$ and $V$ are random unitary factors, $R$ from the QR decomposition of $A$ with colamd, ( Bischof, 1990, Section 4, Test 2; Duff, Vömel, 2002, Section 5, Table 5.4). With $\kappa(A)=10$ we obtain:


## Comparison 3



Figure : Ratio of estimate to real condition number for the 50 matrices in example 2 with $\kappa(A)=100$. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

## Comparison 4



Figure : Ratio of estimate to real condition number for the 50 matrices in example 2 with $\kappa(A)=1000$. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

## Matrices from MatrixMarket



Figure : Ratio of estimate to actual condition number for the 20 matrices from the Matrix Market collection without column pivoting. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

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Figure : Ratio of estimate to actual condition number for the 20 matrices from the Matrix Market collection with column pivoting. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

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- Future work: block algorithm, using the estimator inside a incomplete decomposition.


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- INE strategy using both the direct and inverse factor and maximization only is a method of choice yielding a highly accurate 2-norm estimator.
- Future work: block algorithm, using the estimator inside a incomplete decomposition.

For more details see:
J. Duintjer Tebbens, M. Tůma: On Incremental Condition Estimators in the 2-Norm , Preprint NCCM/2013/15, submitted, May 2013.

## Last but not least

## Thank you for your attention!

