A way to improve incremental 2-norm condition estimation

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The condition number

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The condition number is used, among others, to

- assess the quality of computed solutions
- estimate the sensitivity to perturbations
- monitor and control adaptive computational processes.

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- We are particularly interested in the adaptive process of incomplete LU factorization using dropping and pivoting.
- It is important to monitor the condition number of the submatrices that are computed progressively in the incomplete factorization process:
- If A is incompletely factorized as

  $$A \approx LU,$$

  then the preconditioned matrix is, e.g.

  $$L^{-1}AU^{-1}$$

  (or $AU^{-1}L^{-1}$ or other variants) and the norms of L^{-1} and U^{-1} directly influence the stability of the preconditioned system.

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- More precisely, dropping of new entries for the kth leading submatrix constructed in the ILU process is done according to the rule

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- The information the size of $\|e_k^T L^{-1}\|_\infty$ is obtained by using a cheap condition estimator for the ∞-norm.
- In recently introduced mixed direct/inverse decomposition methods called Balanced Incomplete Factorization (BIF) for Cholesky (or LDU) decomposition [Bru & Marín & Mas & Tůma 2008, 2010] similar dropping rules are used, but in this type of incomplete decomposition the inverse triangular factors are available as a by-product of the factorization process.

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- In this talk we present a relatively accurate 2-norm condition estimator which is very suited for use during incomplete factorization and which assumes that inverses of triangular factors are available (or can be computed cheaply).

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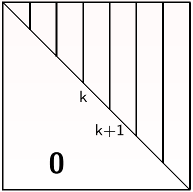
$\kappa(R)$ can be cheaply estimated with a technique called *incremental* condition number estimation, which is suited for incomplete factorization. Main idea: Subsequent estimation for all principal leading submatrices:

$R =$



$\Rightarrow$ every column is accessed only once.

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- Other papers on incremental condition estimation include [Bischof 1991], [Bischof & Pierce & Lewis 1990], [Bischof & Tang 1992], [Ferng & Golub & Plemmons 1991], [Pierce & Plemmons 1992], [Stewart 1998], [Duff & Vömel 2002].

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- The starting point for our method: the methods by Bischof (1990) (incremental condition number estimation - ICE, denoted with a superscript C) and Duff, Vömel (2002) (incremental norm estimation - INE, denoted with a superscript N).

ICE - Bischof (1990)

Consider two leading principal submatrices R and $\hat{R}$ such that

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then with a left minimum singular vector u_-, clearly

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and we get an incremented approximate left minimum singular vector $\hat{y}_-$ for $\hat{R}$ from y_- putting

$$\|\hat{y}_-^T \hat{R}\| = \mathrm{min}_{s^2+c^2=1} \left\| \begin{bmatrix} s\, y_-^T, & c \end{bmatrix} \begin{bmatrix} R & v \\ 0 & \gamma \end{bmatrix} \right\|.$$

ICE - Bischof (1990)

This minimization problem is easily solved by taking s and c as the entries of the eigenvector corresponding to the minimum eigenvalue of

$$\begin{bmatrix} \sigma_{-}^{C}(R)^2 + (y_{-}^{T}v)^2 & \gamma(y_{-}^{T}v) \\ \gamma(y_{-}^{T}v) & \gamma^2 \end{bmatrix}.$$

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Then the incremented estimate for $\hat{R}$ is defined as

$$\|\hat{y}_-^T \hat{R}\| = \|[\ s\, y_-^T, \quad c\ ]\hat{R}\| \equiv \sigma_-^C(\hat{R}) \approx \sigma_-(\hat{R}).$$

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To find an estimate for $\sigma_+(\hat{R})$ one applies the same technique but starting with an approximate left maximum singular vector y_+ and incrementing it using the maximum eigenvector of

$$\begin{bmatrix} \sigma_+^C(R)^2 + (y_+^T v)^2 & \gamma(y_+^T v) \\ \gamma(y_+^T v) & \gamma^2 \end{bmatrix}.$$

INE - Duff, Vömel (2002)

Considering again

$$\hat{R} = \begin{bmatrix} R & v \\ 0 & \gamma \end{bmatrix},$$

Duff and Vömel (2002) compute estimates to extremal (minimum or maximum) singular values and right singular vectors: Starting from

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Again, s and c are the components of the eigenvector corresponding to the extremal (minimum or maximum) eigenvalue of

$$\begin{bmatrix} \sigma_{ext}^N(R)^2 & z_{ext}^T R^T v \\ z_{ext}^T R^T v & v^T v + \gamma^2 \end{bmatrix}.$$

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- Based on their definitions, it is very hard to guess which technique will perform better.
- For dense matrices ICE seems to be superior in general, but INE has been advocated for sparse matrices.
- But if we need only estimates of the maximum singular value $\sigma_+(R)$, INE usually does better. This is why INE is called incremental *norm* estimation.

Experiment

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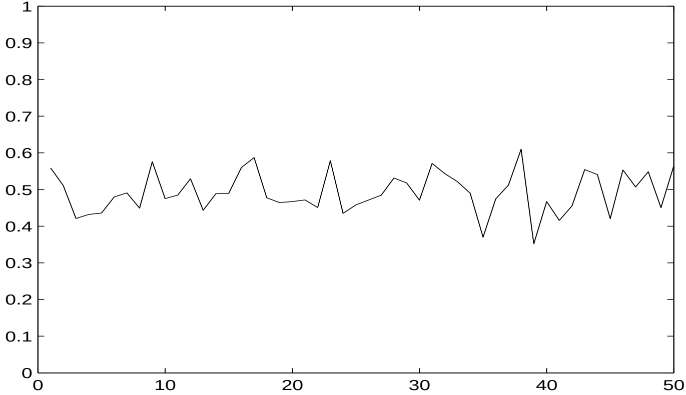
- We compute the estimations $\sigma_+^C(R)$ and $\sigma_-^C(R)$
- In the following graph we display the quality of the estimations through the number

$$\frac{\left(\frac{\sigma_+^C(R)}{\sigma_-^C(R)}\right)^2}{\kappa(A)},$$

where $\kappa(A)$ is the true condition number. Note that we always have

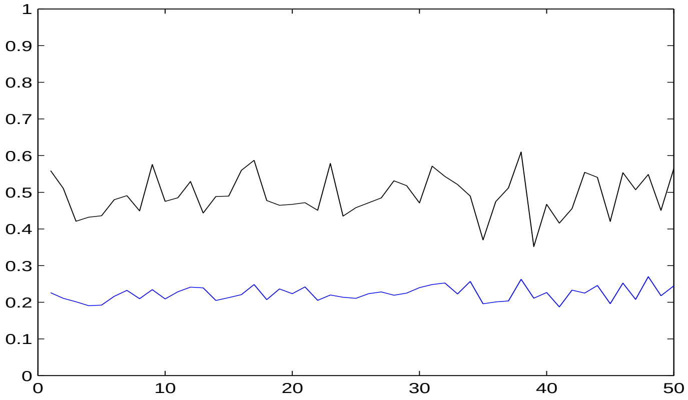
$$\left(\frac{\sigma_+^C(R)}{\sigma_-^C(R)}\right)^2 \leq \kappa(A).$$

Experiment with ICE



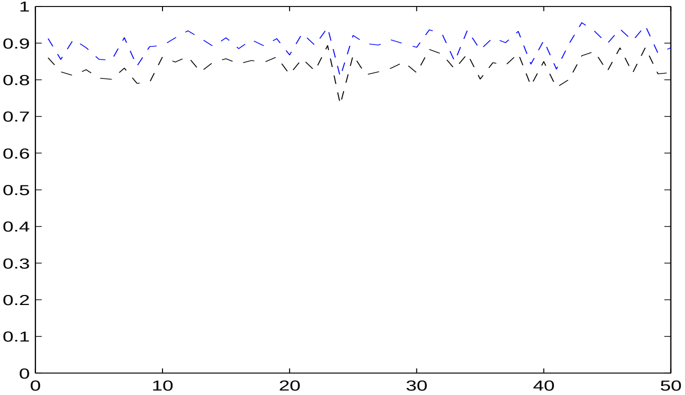
Quality of the estimator ICE for 50 random upper triangular matrices of dimension 100.

Experiment with ICE and INE



Quality of the estimator ICE (black) and of the estimator INE (blue) for 50 random upper triangular matrices of dimension 100.

Experiment with ICE and INE: Only norm estimates



Quality of the ICE technique used to estimate the largest singular value (black) and of the INE technique used to estimate the largest singular value (blue) for 50 random upper triangular matrices of dimension 100.

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

We now assume we have both R and R^{-1}

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Then we can for instance run ICE on R^{-1} and use the additional estimations

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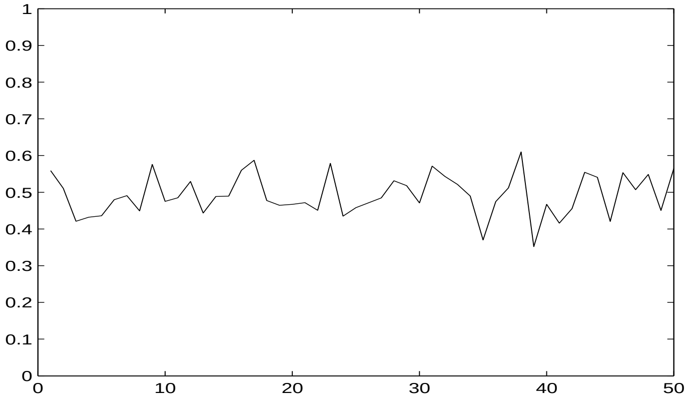
In the following graph we use the same data as before and take the best of both estimations, we display

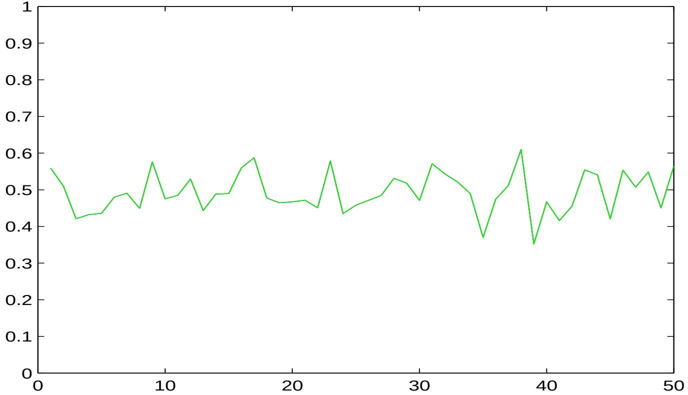
$$\frac{\left(\frac{\max(\sigma_+^C(R),\sigma_-^C(R^{-1})^{-1})}{\min(\sigma_-^C(R),\sigma_+^C(R^{-1})^{-1})}\right)^2}{\kappa(A)}.$$

Experiment with ICE



Quality of the estimator ICE for 50 random upper triangular matrices of dimension 100.

Experiment with ICE when both direct and inverse factors



Quality of the estimator ICE without (black) and with exploiting the inverse (green).

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Theorem

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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*

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

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

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Similarly, one can prove $\sigma_+^C(R) = 1/\sigma_-^C(R^{-1})$.

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Theorem

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INE maximization applied to R^{-1} **may provide a better estimate** *than INE minimization applied to* R: *Let R be a nonsingular upper triangular matrix. Assume that the INE estimates of the singular values of R and R^{-1} are exact:*

$$1/\sigma_+^N(R^{-1}) = \sigma_-^N(R) = \sigma_-(R).$$

Then the INE estimates of the singular values related to the incremented matrix satisfy

$$1/\sigma_+^N(\hat{R}^{-1}) \leq \sigma_-^N(\hat{R})$$

with equality if and only if v is collinear with the left singular vector corresponding to the smallest singular value of R.

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

An analogue of the previous theorem for estimates of the maximum singular value shows that

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In this sense, for INE maximization performs better than minimization.

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In case the assumption is relaxed to $1/\sigma_+^N(R^{-1}) \leq \sigma_-^N(R)$ we obtain a rather technical theorem, saying essentially that maximization with R^{-1} is in most cases superior to minimization with R.

Small example: ICE and INE with and without inverse

$$R = \begin{bmatrix} 2 & 0 & 1 \\ & 1 & 0 \\ & & 1 \end{bmatrix}, \qquad \sigma_-(R) = 0.874$$

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$$\hat{R} = \begin{bmatrix} 2 & 0 & 1 & 1 \\ & 1 & 0 & 1 \\ & & 1 & 1 \\ & & & 1 \end{bmatrix}, \qquad \sigma_-(\hat{R}) = 0.5155$$

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$\sigma_-^N(\hat{R}) = 0.835$, but $1/\sigma_+^N(\widehat{R^{-1}}) = 0.5381$.

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However, a counterexample is given by

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We now give a striking example.

An example showing the possible gap between INE with and without using the inverse

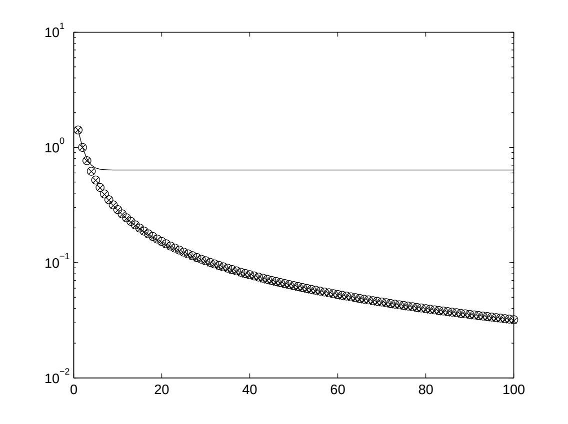

Figure : INE estimation of the smallest singular value of the 1D Laplacians of size one until hundred: INE with minimization (solid line), INE with maximization (circles) and exact minimum singular values (crosses).

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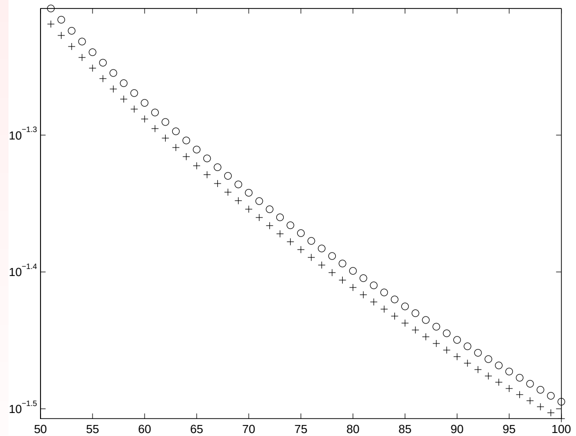
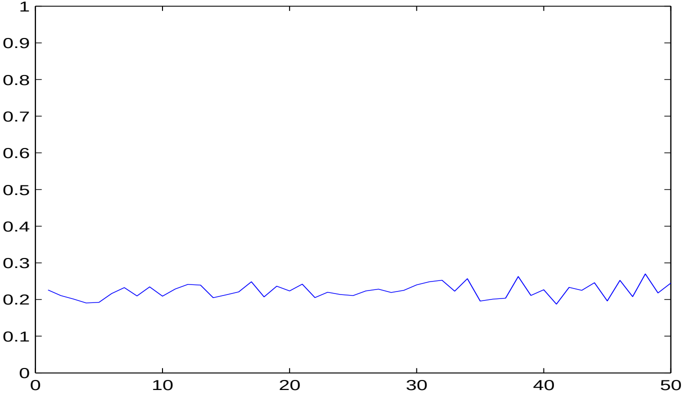


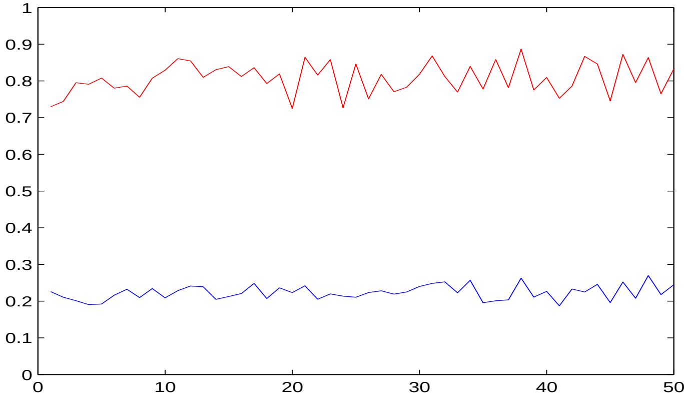
Figure : INE estimation of the smallest singular value of the 1D Laplacians of size fifty until hundred (zoom of previous figure for INE with maximization and exact minimum singular values).

Experiment with INE



Quality of the estimator INE for 50 random upper triangular matrices of dimension 100.

Experiment with INE when both direct and inverse factors available



Quality of the standard INE estimator (blue) and of INE using maximization and R^{-1} to estimate the smallest singular value (red).

Why such an improvement?

- This significant improvement is partly explained by the fact that a moderate improvement of the estimate for $\sigma_{min}(R)$ (from using the inverse) has an important impact because $\sigma_{min}(R)$ is typically small and appears in the denominator in

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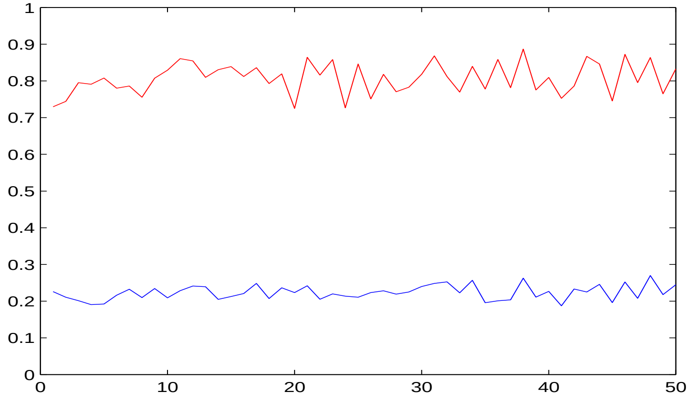
- Similarly, if $\sigma_{min}(R)$ is slightly better estimated with INE than with ICE (expoiting the inverse factor), the improvement for the condition number estimate will be more important.

- This can be expected because we have observed that INE gives better estimates of maximum singular values than ICE, in particular

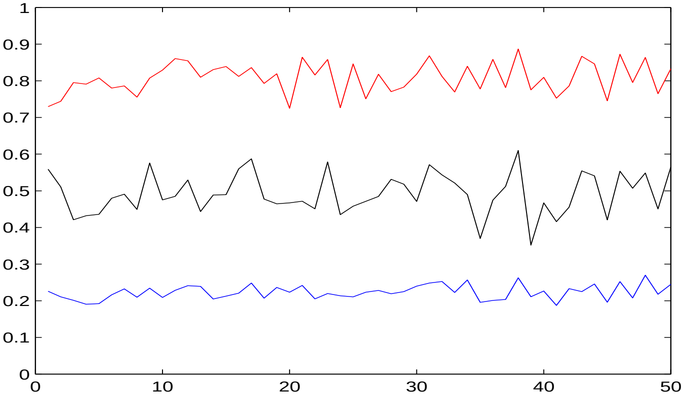
$$1/\sigma_+^N(\hat{R}^{-1}) < 1/\sigma_+^C(\hat{R}^{-1}).$$

Experiment with INE when both direct and inverse factors available



Quality of the standard INE estimator (blue) and of INE using maximization and R^{-1} to estimate the smallest singular value (red).

Experiment with INE and ICE when both direct and inverse factors available



Quality of INE (blue), of INE using maximization and R^{-1} to estimate the smallest singular value (red) and of standard ICE (black).

Short summary

Summarizing, we showed that

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- ICE cannot profit from the presence of the inverse factor.
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- This does not yet explain why INE using maximization (for the inverse factor) is more powerful than ICE using maximization (for either the direct or the inverse factor). This was observed in the experiments.
- We now give theoretical results which make it plausible that INE maximization will tend to perform better than ICE maximization.

A superiority condition for INE

Theorem

Consider norm estimation of the incremented matrix

$$\hat{R} = \left[\begin{array}{cc} R & v \\ 0 & \gamma \end{array} \right],$$

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* $w = Rz/\sigma^+$*. Then*

$$\sigma_+^N(\hat{R}) \geq \sigma_+^C(\hat{R}) \qquad \text{if} \qquad (v^T w)^2 \geq \rho,$$

where the critical value ρ *is the smaller root of the quadratic equation*

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

Graphical demonstration of potential INE superiority

In the next figures,

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- Without loss of generality we can assume $\sigma_+^C(R) = \sigma_+^N(R) = 1$.
- Then the coefficients of the quadratic equation depend on the sizes of v, γ and $(v^T y)^2$ only. We fix $v^T v$.

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- The y-axes represent values of γ^2, i.e. the square of the new diagonal entry.

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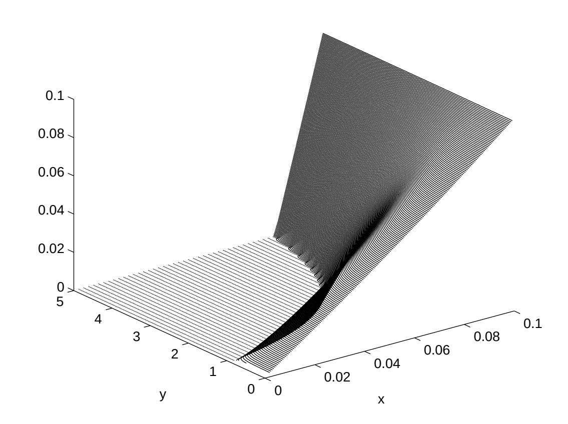

Figure : Critical value ρ in dependence of $(v^T y)^2$ (x-axis) and γ^2 (y-axis) with $\sigma_+ = 1$, $\|v\|^2 = 0.1$.

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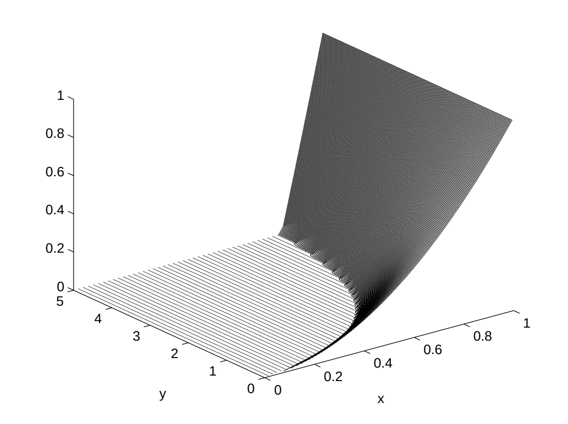

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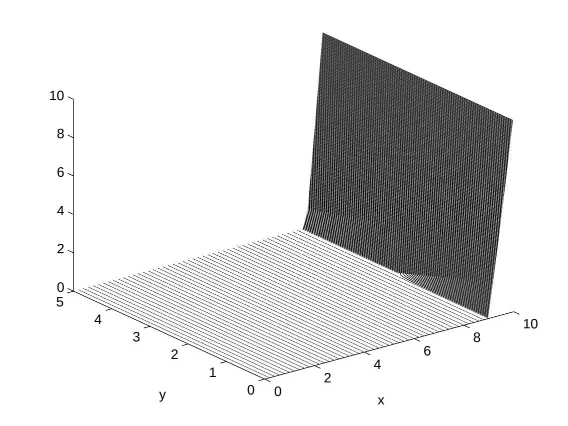

Figure : Critical value ρ in dependence of $(v^T y)^2$ (x-axis) and γ^2 (y-axis) with $\sigma_+ = 1$, $\|v\|^2 = 10$.

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- Let

$$\Delta \equiv \sqrt{(\sigma_+^N)^2 - (\sigma_+^C)^2}, \qquad \sigma_+^N \geq \sigma_+^C.$$

- Intuitively we expect $\Delta > 0$ to even increase the potential superiority of INE over ICE.

Graphical demonstration of potential INE superiority

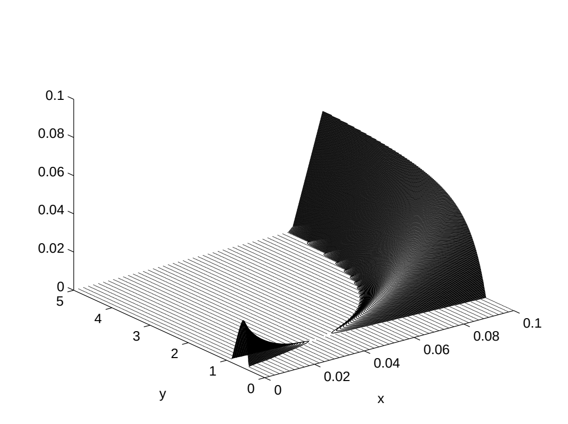

Figure : Critical value ρ in dependence of $(v^T y)^2$ (x-axis) and γ^2 (y-axis) with $\sigma_+ = 1$, $\Delta = 0.6$, $\|v\|^2 = 0.1$.

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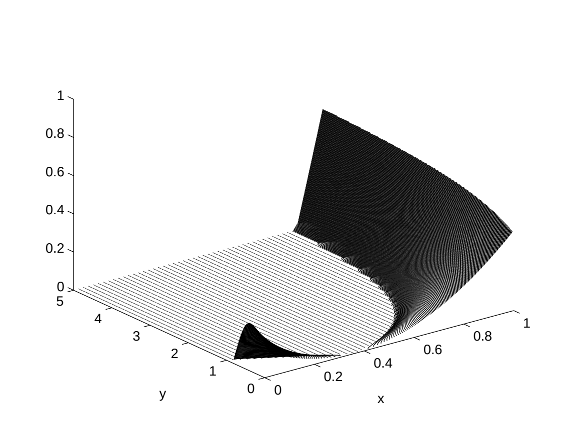

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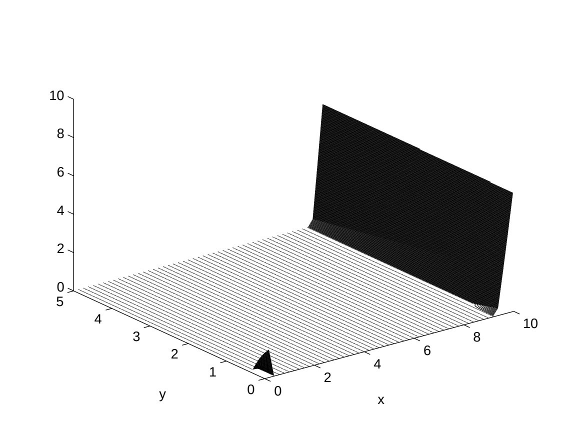

Figure : Critical value ρ in dependence of $(v^T y)^2$ (x-axis) and γ^2 (y-axis) with $\Delta = 0.6$, $\|v\|^2 = 10$.

The compared estimators

We will compare the following estimators:

- The original ICE technique with the estimates defined as

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$$\sigma_+^N(R)/\left(\sigma_+^N(R^{-1})\right)^{-1}.$$
- The INE technique based on minimization only which uses the matrix inverse as well, that is
$$\left(\sigma_-^N(R^{-1})\right)^{-1}/\sigma_-^N(R).$$

Comparison 1

Example 1: 50 matrices A=rand(100,100) - rand(100,100), dimension 100, colamd, R from the QR decomposition of A. [Bischof 1990, Section 4].

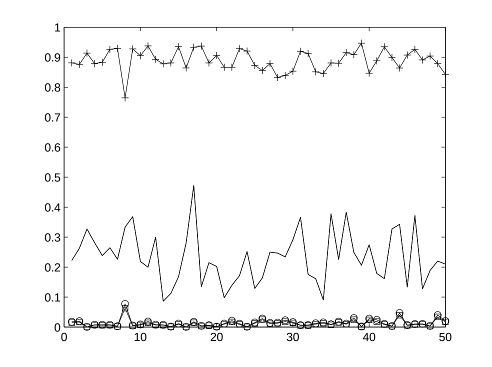

Figure : Ratio of estimate to real condition number for the 50 matrices in example 1. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

Comparison 2

Example 2: 50 matrices $A = U\Sigma V^T$ of size 100 with prescribed condition number κ choosing

$$\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_{100}),$$

with

$$\sigma_k = \alpha^k, \quad 1 \leq k \leq 100, \quad \alpha = \kappa^{-\frac{1}{99}}.$$

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

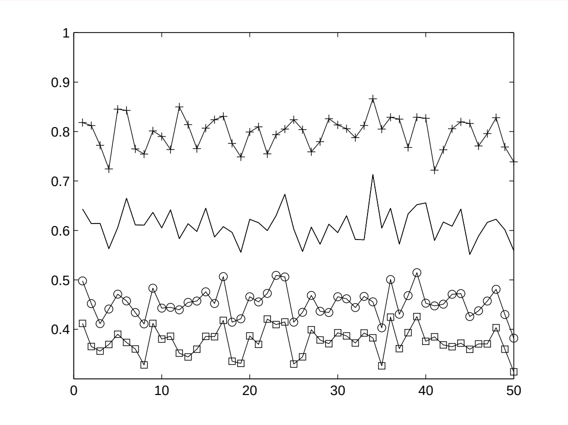

Figure : Ratio of estimate to real condition number for the 50 matrices in example 2 with $\kappa(A) = 10$. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

Comparison 4

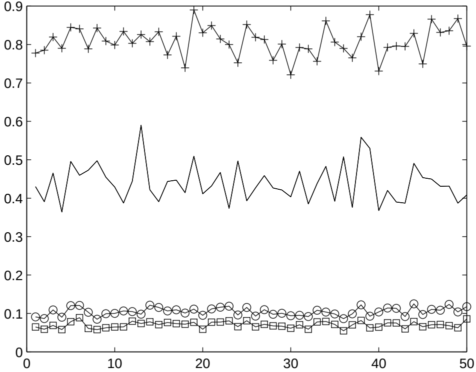

Figure : Ratio of estimate to real condition number for the 50 matrices in example 2 with $\kappa(A) = 100$. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

Comparison 5

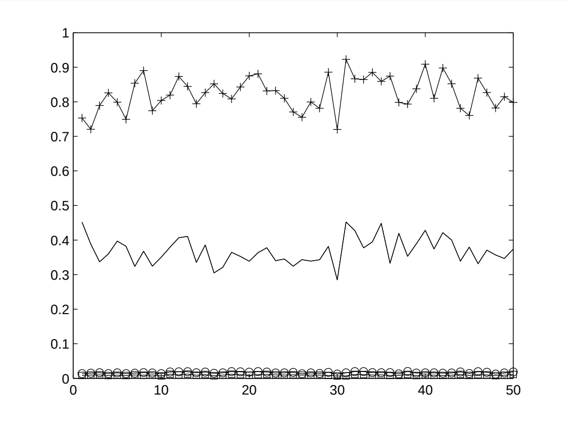

Figure : Ratio of estimate to real condition number for the 50 matrices in example 2 with $\kappa(A) = 1000$. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

Matrices from MatrixMarket

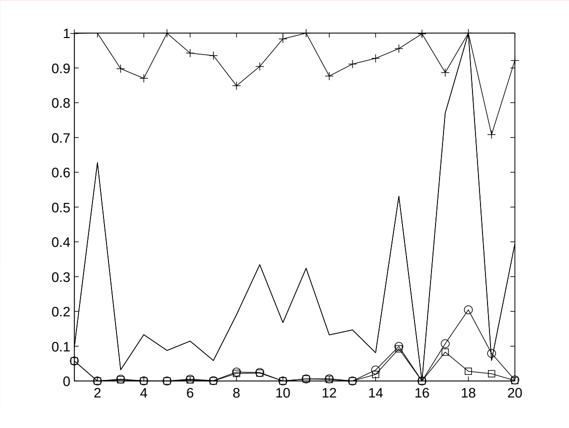

Figure : Ratio of estimate to actual condition number for the 20 matrices from the Matrix Market collection with column pivoting. Solid line: ICE (original), pluses: INE with inverse and using only maximization, circles: INE (original), squares: INE with inverse and using only minimization.

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- 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.

Main references

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Last but not least

Thank you for your attention!