Do we understand Gaussian elimination?

Miroslav Tůma

Institute of Computer Science

Academy of Sciences of the Czech Republic

tuma@cs.cas.cz

based on joint work with **Michele Benzi, Rafael Bru, Jurjen Duintjer Tebbens, José Marín, José Mas, Miroslav Rozložník, Jennifer Scott** et al.

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Motivation: I.

Solving large, sparse systems of linear algebraic equations

$$Ax = b$$

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Contemporary decompositional interpretation of the Gaussian elimination (GE): Householder at the end of the latest 50's.

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Contemporary decompositional interpretation of the Gaussian elimination (GE): Householder at the end of the latest 50's.

Both different and similar role of GE in the two basic solving approaches:

- Direct methods and iterative methods

Case of our interest: Relaxed GE (incomplete decompositions of various kinds).

Motivation: II.

Incomplete decompositions and their implementation.

- GE: We need sparsity (in the input matrix, elimination graphs' estimates, intermediate data) and the speed of the whole computation.

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- The sparsity does not seem to be particularly critical when considering plain incomplete decompositions (ID). But, fast implementations of contemporary ID may cause problems.
- Fortunately, some data structures originally developed for direct methods (and not used there anymore) can be successfully used.

Fast implementations of sophisticated GE modifications are possible

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Incomplete decompositions and robustness

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- Partial robustness: in its evaluation (breakdown-free property).
  - May be based on relaxing accuracy of decomposition (decomposing a different matrix)
  - Or, may promote density of the decomposition (restricting the incompleteness (numerically or structurally))
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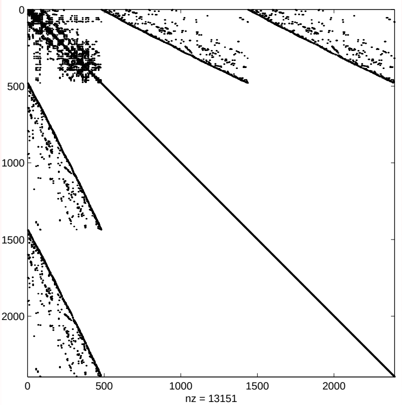
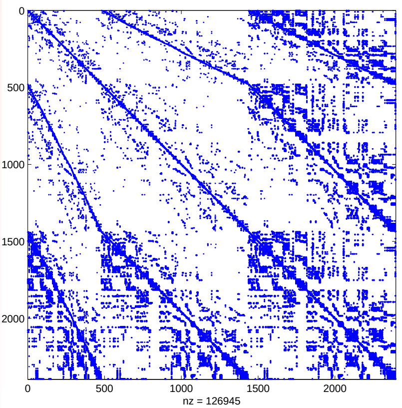
In the other words, how far are we from GE-aware decompositions?

Motivation: IV.

ID affects the iterative method via its inverse.



matrix ADD20



rather precise inverse
(2 its BiCGStab)

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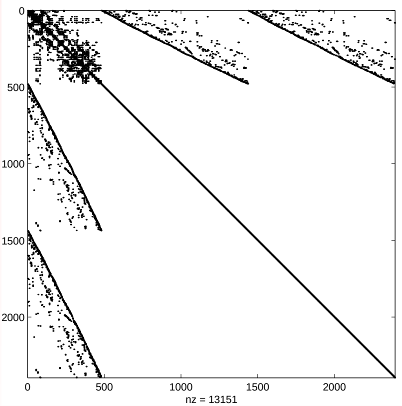

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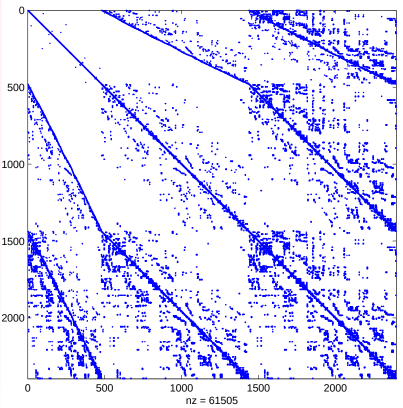

less precise inverse

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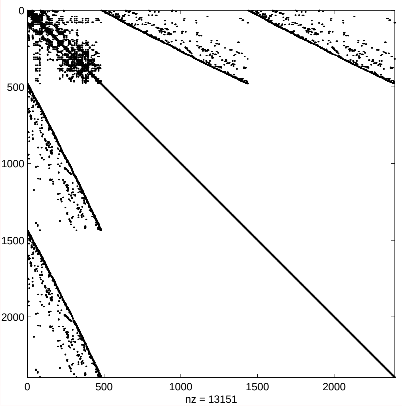

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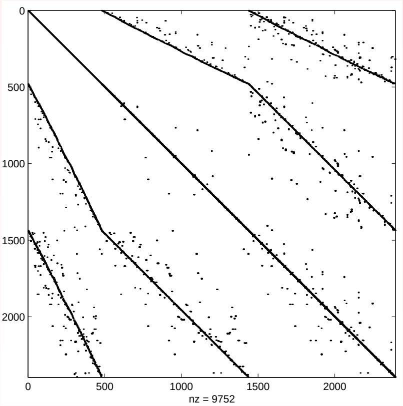

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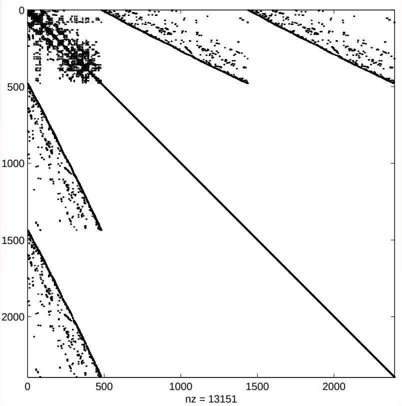

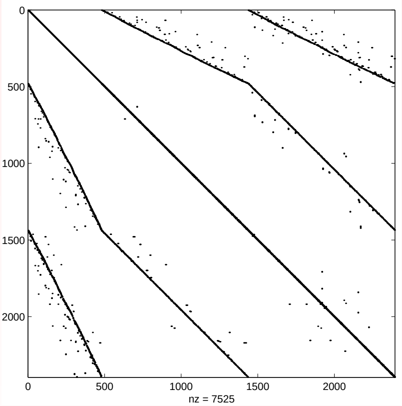

matrix ADD20 rough inverse

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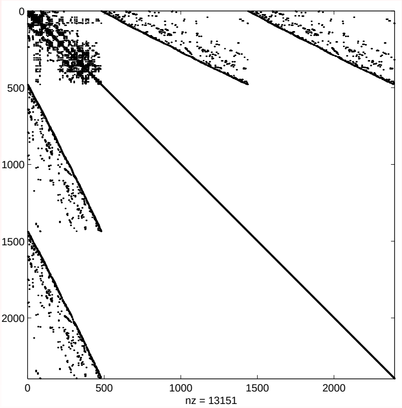

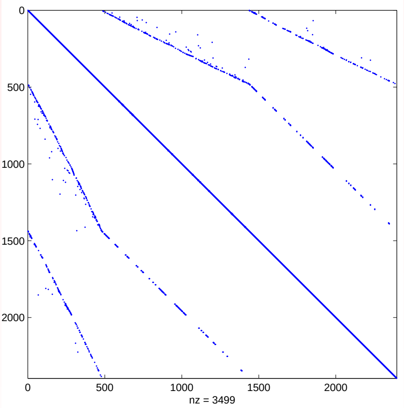

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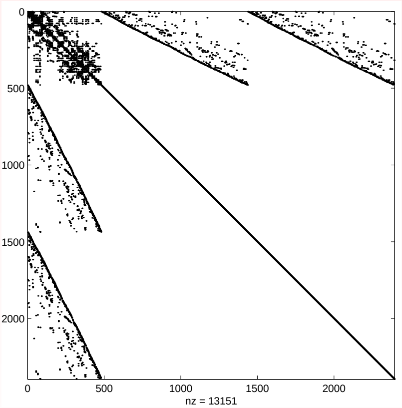

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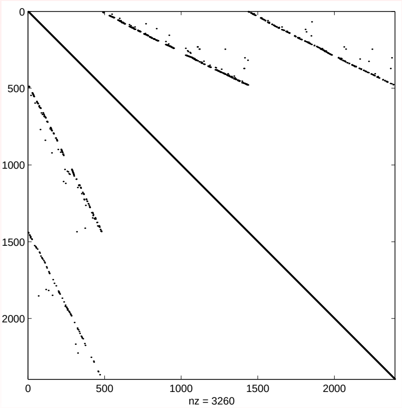

ILU decomposition
(similar size as the "very rough inverse")

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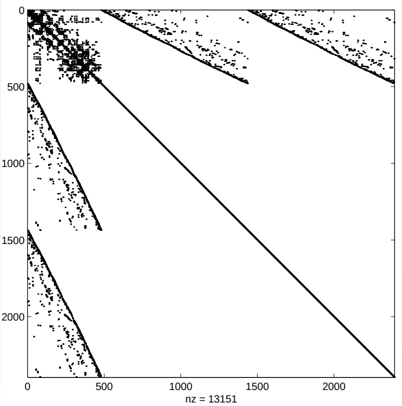

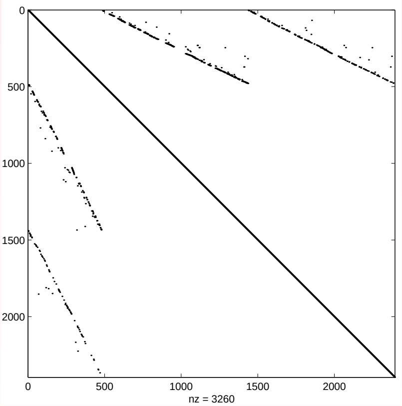

matrix ADD20

inverted ILU decomposition

Concluded motivation

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What we do not discuss here?

- Modifications of the basic algorithm (basic diagonal modifications, general diagonal compensations with respect to some matvecs etc.)
- a priori diagonal changes
- matrix pre/post processings
- embedding into a more general (e.g. multilevel) scheme.
- Analysis of the described schemes

Summarizing our starting points and goals

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Here we try to get inside GE, not to study/defend a synthetic approach.

Outline

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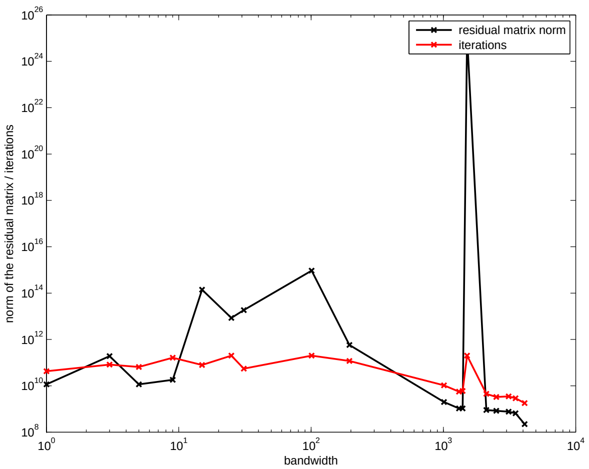
Limits of ID: BCSSTK38, $n = 8032$, $nz = 181,746$

ID: Limitations in predictability and efficiency



- Generally no clear dependence on the error size, pattern etc.
- This is a very common kind of behavior

Outline

Generalized Gram-Schmidt (GGS)

Generalized Gram-Schmidt: basics of SPD case

- Orthogonalize columns of I using the inner product $\langle\ ,\ \rangle_A$
- We get (instead of $A = QDR$ with R unit upper triangular):

$$I = ZU$$

  - U is unit upper triangular, as usual ($U = L^T$ for $A = LL^T$).
  - Z is orthogonal in $\langle\ ,\ \rangle_A$

$$Z^T AZ = D \quad (\text{Biconjugate decomposition})$$

  - But: Z is unit upper triangular as well ($Z = L^{-T}$ for $A = LL^T$)
- Easy to reveal decomposed matrix inverse:

$$A^{-1} = ZD^{-1}Z^T,$$

Generalized Gram-Schmidt: II.

Resulting direct and inverse ID may be practical in the incomplete case

$$I = ZDU$$

$$A \approx LL^T, \; U \approx L^T, \; Z \approx L^{-1}$$

- Origins: more papers in 40's and early 50's (Escalator method by Morris (1946), Vector method by Purcell (1952), Fox, Huskey, Wilkinson (1948)).
- The sparse incomplete method can be implemented: AINV (Benzi, Meyer, T., 1996; Benzi, T., 1998)
- Computational procedures to compute sparse incomplete U in this way: RIF (Benzi, T., 2003)
- As we will see, both Z and U can be computed breakdown-free, but this is not all that we may want.

Generalized Gram-Schmidt: III.

Generalized Gram-Schmidt: the (SPD) algorithm

$$I = ZU \equiv [z_1, \ldots, z_n]\ (u_{ij})_{i,j}$$

```
for i=1, n
    for j=1, i-1 with nonzero
```
$u_{ij} = e_j^T A {z_i}^{(j)}$

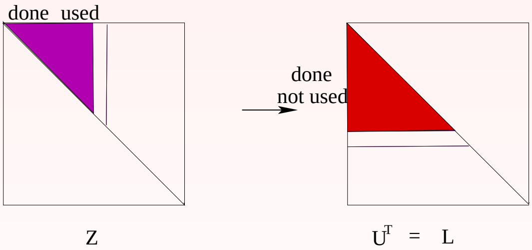
$${z_i}^{(j)} = {z_i}^{(j-1)} - {z_j}^{(j-1)} \frac{e_j^T A {z_i}^{(j-1)}}{e_j^T A {z_j}^{(j-1)}}$$

```
    end j
end i
```

- Forcing partial robustness: different formulas which are the same in exact arithmetic: the breakdown-free variant SAINV
- But: in order to get U we must get Z: direct factor is obtained via the inverse factor

Generalized Gram-Schmidt: IV.

Generalized Gram-Schmidt $I = ZU$: the data dependence graphically



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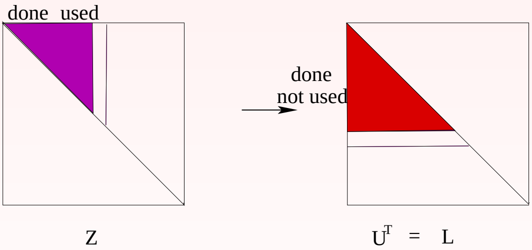

One way transfer of information

Summarization the two general problems

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- We have (some) answers for both of these problems
- 1. Arbitrary direct-inverse decompositions
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Of course, it remains a lot to do to improve GE-based decompositions from inside.

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New shifted biconjugation

- Note: general nonsymmetric formulation is used here

$$A^{-1} = ZZ^T \longleftarrow A^{-1} = ZD^{-1}W^T$$

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Nonsymmetric recursions:

$$z_i^{(j)} = z_i^{(j-1)} - z_j^{(j-1)} \frac{a^j z_i^{(j-1)}}{a^j z_j^{(j-1)}}, \quad w_i^{(j)} = w_i^{(j-1)} - w_j^{(j-1)} \frac{a_j^T w_i^{(j-1)}}{a_j^T w_j^{(j-1)}}$$

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$$\Downarrow$$

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Analogical recursions:

$$z_i = se_i - \sum_{j=1}^{i-1} \frac{v_j^T e_i}{d_j} z_j \quad , \; v_i = (a^i - se^i)^T - \sum_{j=1}^{i-1} \frac{z_j^T (a^i - se^i)}{d_j} v_j,$$

Z and D are the same in both recursions

More on the new biconjugation

- The $(s^{-1}I - A^{-1})^{-1})$ biconjugation introduced by Bru, Cerdán, Marín, Mas, 2003. The incomplete algorithm was proposed as an approximate inverse preconditioner. (factor Z)

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- The $(s^{-1}I - A^{-1})^{-1})$ biconjugation introduced by Bru, Cerdán, Marín, Mas, 2003. The incomplete algorithm was proposed as an approximate inverse preconditioner. (factor Z)
- It was shown that this new biconjugation can be used to get a direct decomposition (factor U) as well, Bru, Marín, Mas, T., 2008.

$$s^{-1}I - A^{-1} = ZD^{-1}V^T \text{ and } A = LDU \text{ and } Z = U^{-1}$$

$$s^{-1}I - U^{-1}D^{-1}L^{-1} = U^{-1}D^{-1}V^T$$

$$s^{-1}I = U^{-1}D^{-1}(L^{-1} + V^T)$$

upper triangular ↗ ↖ lower triangular

More on the new biconjugation: II.

Pictorially

$$V = \begin{bmatrix} \ddots & & -sL^{-T} \\ & & \\ & \ddots & \\ & & \\ U^T D & & \ddots \end{bmatrix}, \qquad \mathrm{diag}(V) = D - sI. \tag{1}$$

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- V obtained by a simple recursion for its columns
- The new recursions provide scaled U and L^{-1} at the same time!
- Dropping can interconnect their computation.

Balanced incomplete factorization (BIF) experiments

SPD experiments: I.

Example: matrix PWTK, n=217,918, nnz=5,926,171

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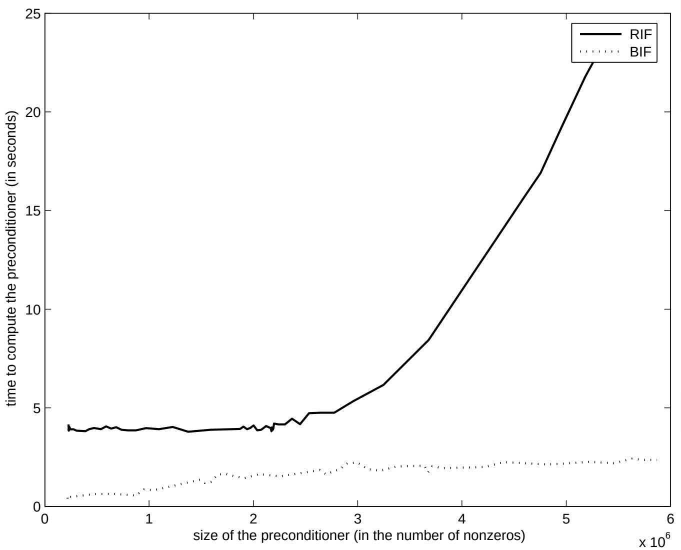

Balanced incomplete factorization (BIF) experiments: II.

Of course: not only pros; cons as well

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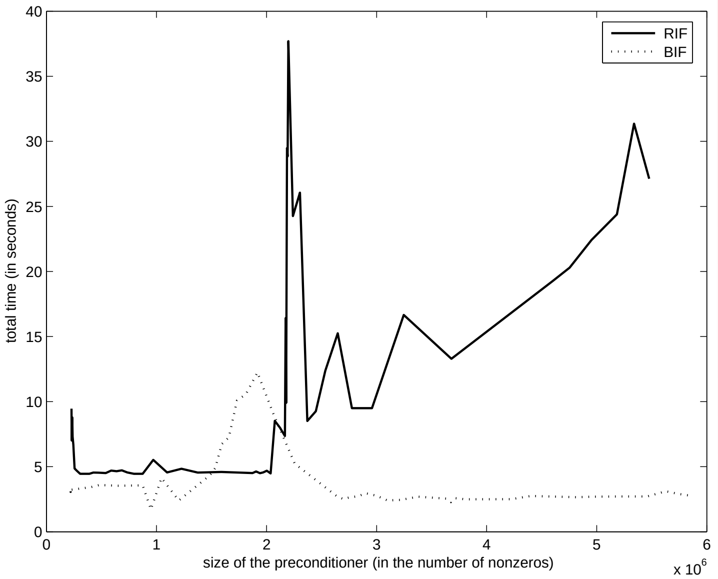
- The convergence curve is often rather flat if we run many iterations. Is the accuracy sufficient for solving sequences from nonlinear solvers?

Balanced incomplete factorization (BIF) experiments: III.

SPD experiments: II.



Direct-inverse decomposition

- Vector formulation of the shifted biconjugation can hide important details Bru, Mas, Marín, T. 2009

$$v_i = (a^i - se^i)^T - \sum_{j=1}^{i-1} \frac{z_j^T (a^i - se^i)}{d_j} v_j,$$

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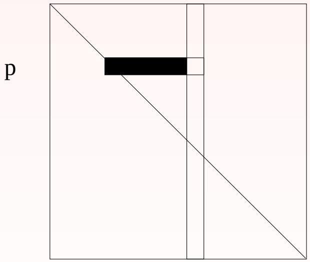

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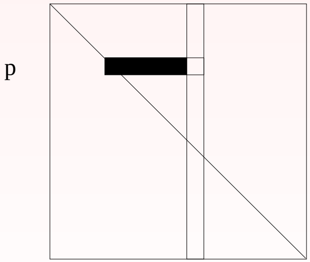

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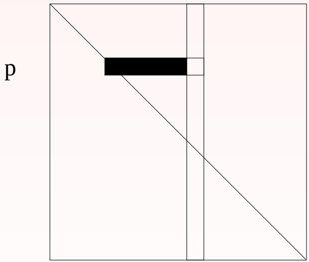

- v_{pi}: just the entries of V with indices $p+1, \ldots, i-1$ are involved
- good, but not enough: the inverse factor still updated only by entries of the inverse factor

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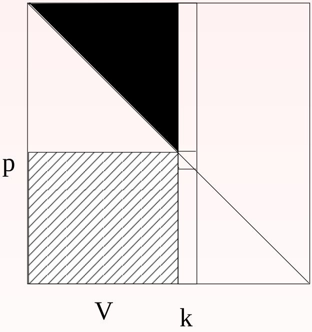

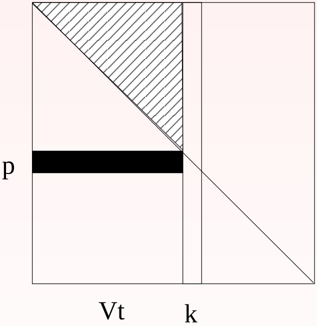

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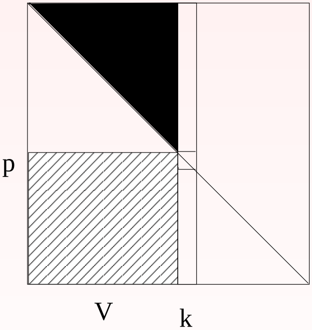

- $v_{1:p-1}$ computed using fully filled areas

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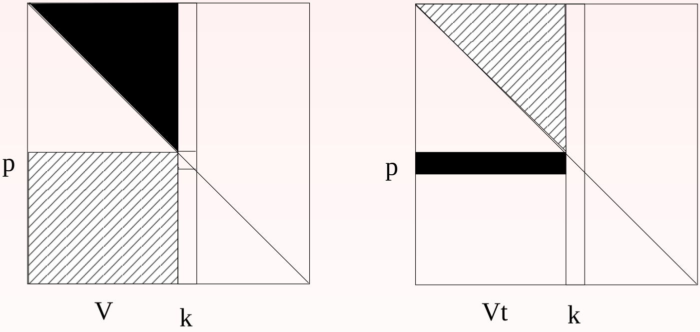

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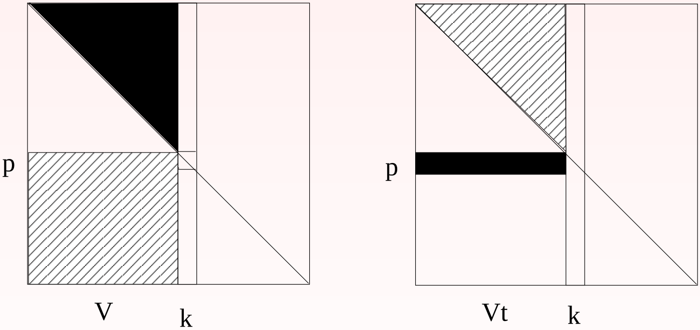

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- $v_{p+1:n}$ computed using dashed areas
- direct and inverse factors influence each other

Direct-inverse (NBIF) decomposition: experiments: II.

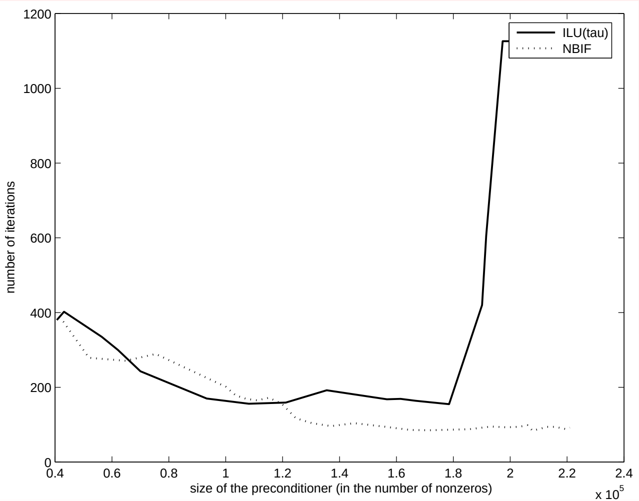

Figure: Sizes of NBIF and ILU(τ) preconditioners versus iteration counts of the preconditioned BiCGStab method for the matrix CHEM_MASTER1.

Outline

Condition number estimation

Condition number estimation in the 2-norm
(Duintjer Tebbens et al., 2009)

- Two basic approaches: Incremental condition estimation using left singular vectors (ICE, Bischof, 1990) and Incremental norm estimation using right singular vectors (INE, Duff, Vömel, 2002)

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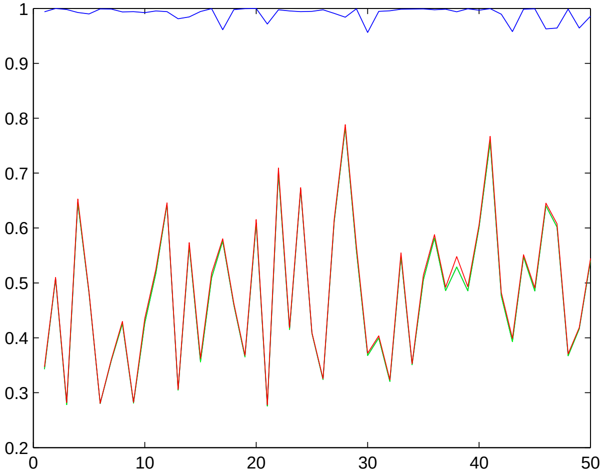
$$\kappa(R) \approx \frac{\sigma_{maxL}(R)}{\sigma_{minL}(R)} \; (ICE) \longrightarrow \ldots \longrightarrow \kappa(R) \approx \sigma_{maxR}(R)\sigma_{minRI}(R)$$

yellow (green) curve **blue curve**

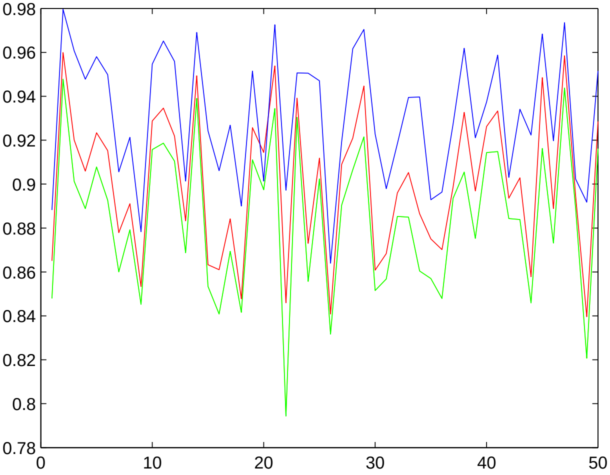
Condition number estimation: II.

50 Random matrices A forming AA^T



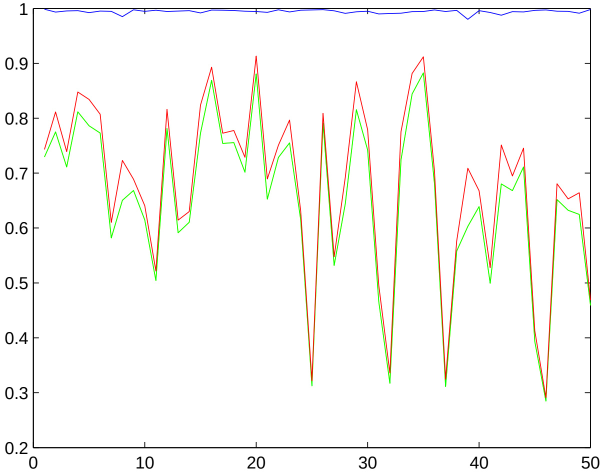
Condition number estimation: III.

50 Random matrices A forming $A + A^T$ with an additional shift



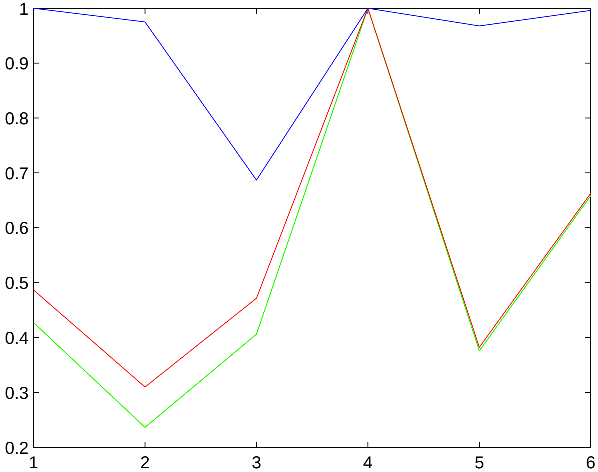
Condition number estimation: IV.

50 Random matrices A forming $A + A^T$, different shift



Condition number estimation: V.

6 Harwell-Boeing matrices, not via BIF



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Biconjugation described via projections

Stabilization: $e_j^T A {z_i}^{(j-1)} \longrightarrow z_j^{(j-1)} A {z_i}^{(j-1)}$

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Algorithm

Non-stabilized Generalized GS via projections; the main loop

(1) for $i = 1, \ldots, n$:
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Generalization of GS neither classical nor modified!

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- Generalization of GS is fully modified. Projector properties may be the reason we were looking for.
- Are we able to describe a direct decomposition via orthogonal projections?. Yes, we can.

Inverse biconjugation

Let $\bar{P}_i$ be the projector $\bar{P}_i = I - z_i z_i^T A^{-1}/d_i$.

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- The algorithm computes a direct $(L^T DL)$ decomposition.
- Is it a practical way to get a direct incomplete decomposition?

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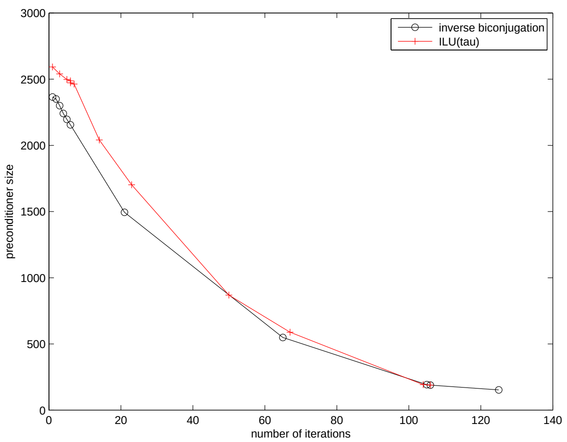

- still very preliminary experiments for BCSSTK05
- more possible ways which are more or less “stable”
- unclear practical implications.

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The way from efficient rules of decomposition to fully GE-aware algorithms may be very long

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