On solving mixed sparse-dense linear least-squares problems Part II: A preconditioned conjugate gradient method

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An aside ...

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- I am aware that for all of this I am greatly indebted to Iain!
- Having spent half a year at CERFACS in 1998, je suis tambien en peu Toulousain, and always like to return to the South of France.
- Iain, Happy Birthday and many more healthy and productive years!

Introduction

Recall the Linear least squares problem (LS):

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad \|Ax - b\|_2,$$

where $A \in \mathbb{R}^{m \times n}$ with $m \geq n$ is large and sparse and $b \in \mathbb{R}^m$.

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Introduction

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Focus again on A having small number of "dense" rows.

Assume the same notation as in the previous talk:

$$A = \begin{pmatrix} A_s \\ A_d \end{pmatrix}$$

where $A_s \in \mathbb{R}^{m_s \times n}$ is sparse but rows of $A_d \in \mathbb{R}^{m_d \times n}$ are dense $(m_s \gg m_d)$. Then

$$C = \begin{pmatrix} A_s^T & A_d^T \end{pmatrix} \begin{pmatrix} A_s \\ A_d \end{pmatrix} = A_s^T A_s + A_d^T A_d$$

Here we consider preconditioned iterative methods

- Preconditioner based on implicitly approximating $C^T C = A^T A$
- Both the sparse part A_s and the dense part A_d should be considered in such approximations (but see the results for unpreconditioned LSQR in Avron, Ng, Toledo, 2009)
- The construction then uses both sparse and dense techniques.
- All of this heavily depends on foundations within the framework of direct methods based on the work of Björck, George, Heath, Ng, Duff and many others.

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- All of this heavily depends on foundations within the framework of direct methods based on the work of Björck, George, Heath, Ng, Duff and many others.
- Crucial practical step: applying factorization $C_s = L_s L_s^T$ to the problem (see, Bjorck, 1986):
- Giving the following equivalent problem

$$\min_z \left\| \begin{pmatrix} B_s \\ B_d \end{pmatrix} z - \begin{pmatrix} b_s \\ b_d \end{pmatrix} \right\|_2, \tag{1}$$

$$B_s = A_s L_s^{-T}, \quad B_d = A_d L_s^{-T}, \quad z = L_s^T x$$

We consider also $C_s \approx L_s L_s^T$.

Preconditioner construction: background 1

- Solving the partial sparse problem $\min_{x_s} \|A_s x_s - b_s\|_2$ approximately
- Completing the result to the exact solution of the original LS problem
- The construction uses residuals that are available in Krylov space accelerators.

Theorem

If $C_s = L_s L_s^T$ and ξ_1 is an approximate solution to the problem $\min_z \|B_s z - b_s\|_2$, the exact least squares solution of the equivalent problem above can be written as $z = \xi_1 + \Gamma_1$, where $\rho_s = b_s - B_s \xi_1$ and $\rho_d = b_d - B_d \xi_1$ and

$$\Gamma_1 = B_s^T \rho_s + B_d^T (I_{m_d} + B_d B_d^T)^{-1} (\rho_d - B_d B_s^T \rho_s). \qquad (2)$$

Preconditioner construction: background 2

- Solving the partial sparse problem $\min_{x_s} \|A_s x_s - b_s\|_2$ exactly
- Completing the result to the exact solution of the original LS problem
- Note that the construction uses residuals that are available in Krylov space accelerators.

Theorem

If $C_s = L_s L_s^T$ and ξ_1 minimizes $\|B_s z - b_s\|_2$ exactly, the exact least squares solution of problem (1) can be written as $z = \xi_1 + \Gamma_1$, , $\rho_s = b_s - B_s \xi_1$ and $\rho_d = b_d - B_d \xi_1$ and

$$\Gamma_1 = B_d^T (I_{m_d} + B_d B_d^T)^{-1} \rho_d. \tag{3}$$

- More possibilities: also the dense part could be approximated
- In fact, ξ_1 can be chosen to solve approximately $\min_\xi \|B_d \xi - b_d\|_2$ instead of $\min_\xi \|B_s \xi - b_s\|_2$

Preconditioned iterations: CGLS1

- Preconditioning reuses some computations of CGLS1.

Algorithm

Preconditioned CGLS1 algorithm $(A_s,\ A_d,\ A_s^T A_s \approx \tilde{L}_s \tilde{L}_s^T;\ z = M^{-1}s))$

0. $r_s^{(0)} = b_s - A_s x^{(0)},\ r_d^{(0)} = b_d - A_d x^{(0)},\ w_s^{(0)} = A_s^T r_s^{(0)},\ w_d^{(0)} = A_d^T r_d^{(0)},$

   $z^{(0)} = M^{-1}(w_s^{(0)} + w_d^{(0)}),\ p^{(0)} = z^{(0)}$

1. **for** $i = 1 : nmax$ **do**

2. $q_s^{(i-1)} = A_s p^{(i-1)},\ q_d^{(i-1)} = A_d p^{(i-1)}, \alpha = \frac{(w_s^{(i-1)} + w_d^{(i-1)}, z^{(i-1)})}{(q_s^{(i-1)}, q_s^{(i-1)}) + (q_d^{(i-1)}, q_d^{(i-1)})}$

3. $x^{(i)} = x^{(i-1)} + \alpha p^{(i-1)},\ r_s^{(i)} = r_s^{(i-1)} - \alpha q_s^{(i-1)},\ r_d^{(i)} = r_d^{(i-1)} - \alpha q_d^{(i-1)}$

4. $z^{(i)} = M^{-1}(A_s^T r_s^{(i)} + A_d^T r_d^{(i)}),\ \beta = \dfrac{(w_s^{(i)} + w_d^{(i)}, z^{(i)})}{(w_s^{(i-1)} + w_d^{(i-1)}, z^{(i-1)})}$

5. $p^{(i)} = z^{(i)} + \beta p^{(i-1)}$

6. **end do**

Experimental evaluation

- Stopping criterion

  C: Stop if $\|r\|_2 < \delta_1$ or $\frac{\|A^T r\|_2}{\|r\|_2} < \frac{\|A^T r_0\|_2}{\|r_0\|_2} * \delta_2$,
  r residual, r_0 initial residual, $\delta_1 = 10^{-8}$ and $\delta_2 = 10^{-6}$.

- Intel(R) Core(TM) i5-4590 CPU at 3.30 GHz, 12 GB of internal memory. Visual Fortran Intel(R) 64 XE compiler

- Most of the matrices from the University of Florida Sparse Matrix Collection
- A prescaled by normalizing its columns
- A row of A considered as dense if the number of entries in the row either exceeds 100 times the average number of entries in a row or is more than 4 times greater than the number of entries in any row in the sparse part A_s.

Experimental evaluation

Table: Statistics: (density= $nnz(C)/n^2$)

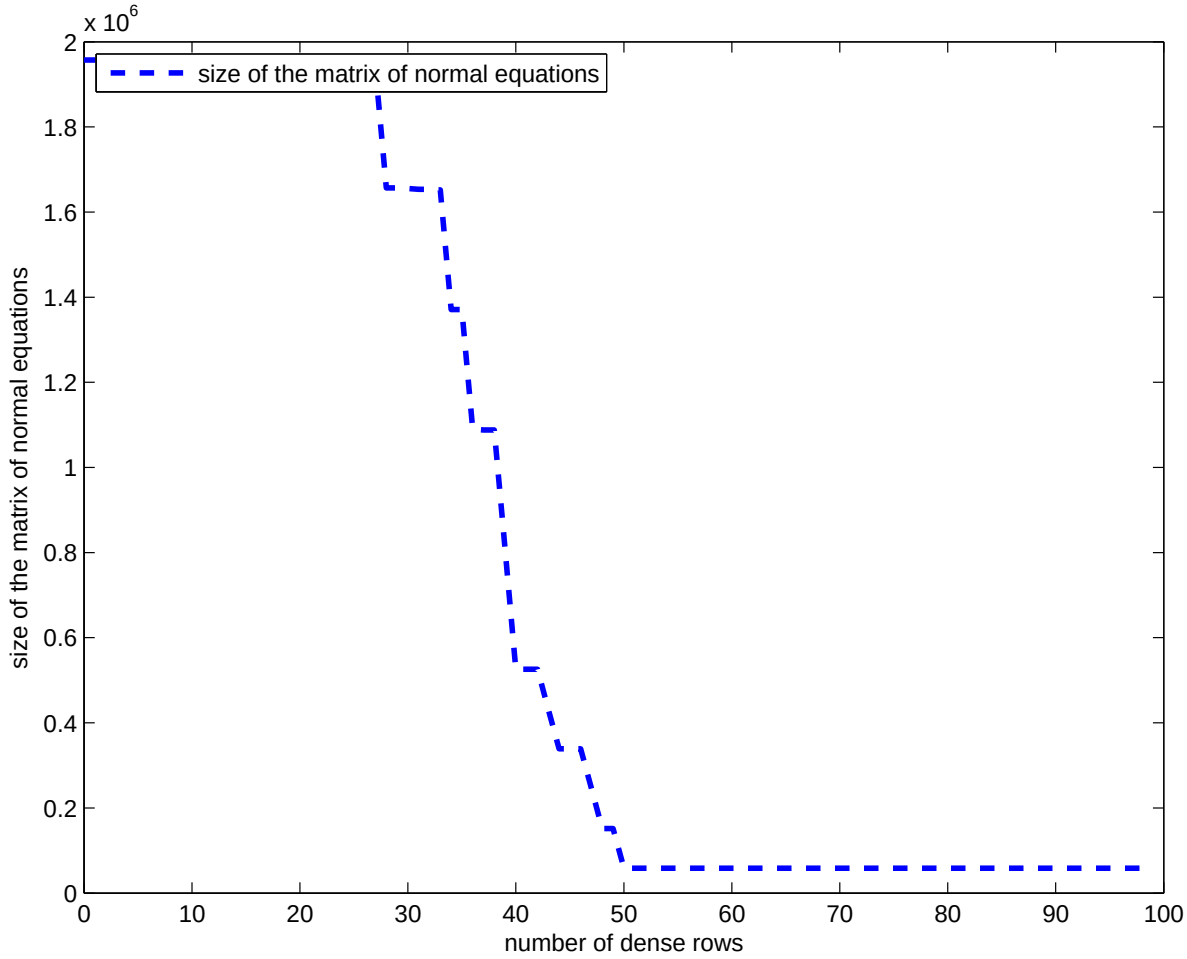
Identifier	m	n	$nnz(A)$	$nnz(C)$	*density*
aircraft	7,517	3,754	20,267	1.4×10^6	0.200
lp_fit2p	13,525	3,000	50,284	4.5×10^6	1.000
scrs8-2r	27,691	14,364	58,439	6.2×10^6	0.143
sctap1-2b	33,858	15,390	99,454	2.6×10^6	0.050
scsd8-2r	60,550	8,650	190,210	2.0×10^6	0.100
scagr7-2r	62,423	35,213	123,239	2.2×10^7	0.036
sc205-2r	62,423	35,213	123,239	6.5×10^6	0.010
sctap1-2r	63,426	28,830	186,366	9.1×10^6	0.050
scfxm1-2r	65,943	37,980	221,388	8.3×10^5	0.014
world	67,147	34,506	198,883	3.1×10^5	0.001
neos1	133,743	131,581	599,590	1.7×10^8	0.027
neos2	134,128	132,568	685,087	2.3×10^8	0.033
stormg2-125	172,431	66,185	433,256	1.0×10^6	0.002
PDE1	270,595	271,792	990,587	1.6×10^{10}	0.670
neos	515,905	479,119	1,526,794	5.3×10^8	0.034
stormg2_1000	1,377,306	528,185	3,459,881	4.2×10^7	0.002
cont1_l	1,921,596	1,918,399	7,031,999	8.2×10^{11}	0.667

Experimental evaluation

	Dense rows not exploited				Dense rows exploited				
Identifier	*size_p*	*T_p*	*Its*	*T_i*	m_d	*size_ps*	*T_p*	*Its*	*T_i*
aircraft	22,509	0.09	44	0.02	17	3,750	0.01	1	0.01
lp_fit2p	17,985	0.26	‡	‡	25	4,940	0.09	1	0.01
scrs8-2r	86,169	0.94	380	0.50	22	36,385	0.01	1	0.02
sctap1-2b	92,325	0.39	639	0.69	34	68,644	0.01	1	0.01
scsd8-2r	51,885	0.25	90	0.11	50	51,855	0.05	7	0.02
scagr7-2r	197,067	3,34	244	0.53	7	152,977	0.06	1	0.01
sc205-2r	211,257	1.56	72	0.19	8	104,022	0.08	1	0.01
sctap1-2r	172,965	1.47	673	1.90	34	127,712	0.03	1	0.01
scfxm1-2r	227,835	0.59	187	0.51	58	227,823	0.14	33	0.23
neos1	789,471	†	†	†	74	789,471	5.27	132	3.71
neos2	†	†	†	†	90	795,323	5.46	157	4.84
stormg2-125	395,595	0.27	‡	‡	121	7,978,135	0.22	16	0.29
PDE1	†	†	†	†	1	1,623,531	12.7	696	1.28
neos	†	†	†	†	20	2,874,699	4.93	232	15.0
stormg2_1000	3,157,095	19.1	‡	‡	121	3,125,987	19.1	18	2.92
cont1_l	†	†	†	†	1	11,510,370	4.82	1	0.33

Moving rows one by one from A_s to A_d

SCSD8-2r_a: size of C_s



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SCSD8-2r_a: iteration counts + $size\_p/size(A^T A)$

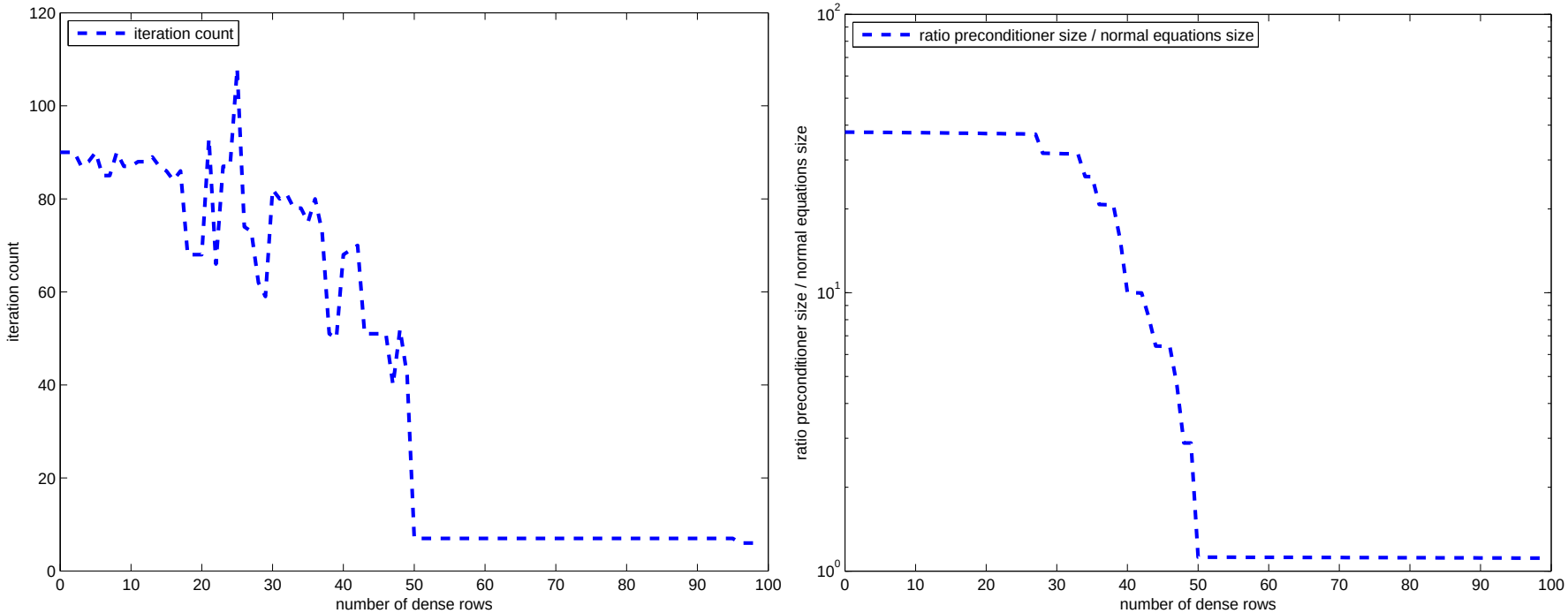

Figure: Problem $Meszaros/scsd8-2r$. Iteration counts (left), and ratio of the preconditioner size to the size of $A^T A$ (right) as the number of dense rows that are removed from A is increased.

Moving rows one by one from A_s to A_d

SCSD8-2r_a: timings

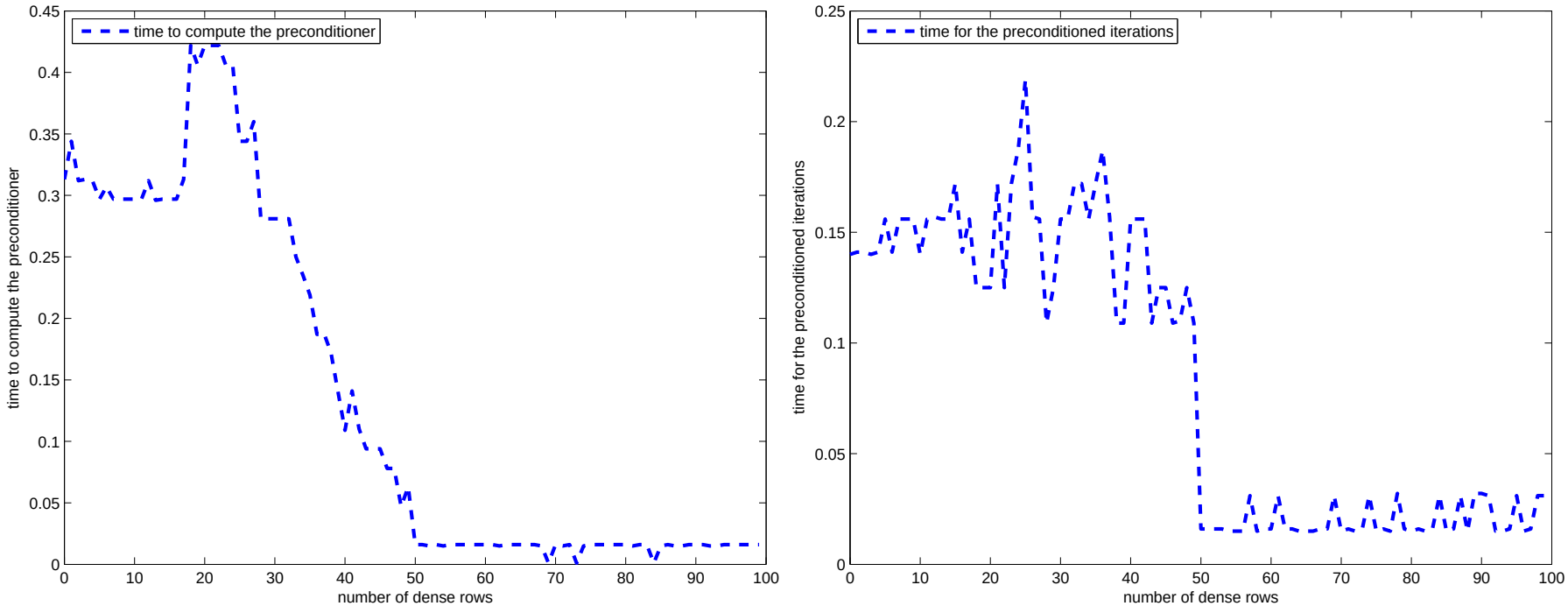

Figure: Problem *Meszaros*/*scsd*8 – 2*r*. Time to compute the preconditioner (left) and time for CGLS (right) as the number of dense rows that are removed from A is increased.

Problem of null columns in A_s after removing A_d

$$A = \begin{pmatrix} A_1 & A_2 \end{pmatrix} \equiv \begin{pmatrix} A_{s_1} & \\ A_{d_1} & A_{d_2} \end{pmatrix}, \tag{4}$$

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- As mentioned in the previous talk: solution can be expressed as a combination of partial solutions of $\min_z \|A_1 z - b\|_2$ and $\min_W \|A_1 W - A_2\|_F$.

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- As mentioned in the previous talk: solution can be expressed as a combination of partial solutions of $\min_z \|A_1 z - b\|_2$ and $\min_W \|A_1 W - A_2\|_F$.
- What about some other preprocessing?
  - E.g., sparsifying the dense rows
  - Such strategy called stretching discussed by Grcar (1990), Vanderbei (1991), Alvarado (1997), Adler (2000), Adler, Björck (2000).

Matrix stretching for the LS problems: generic example

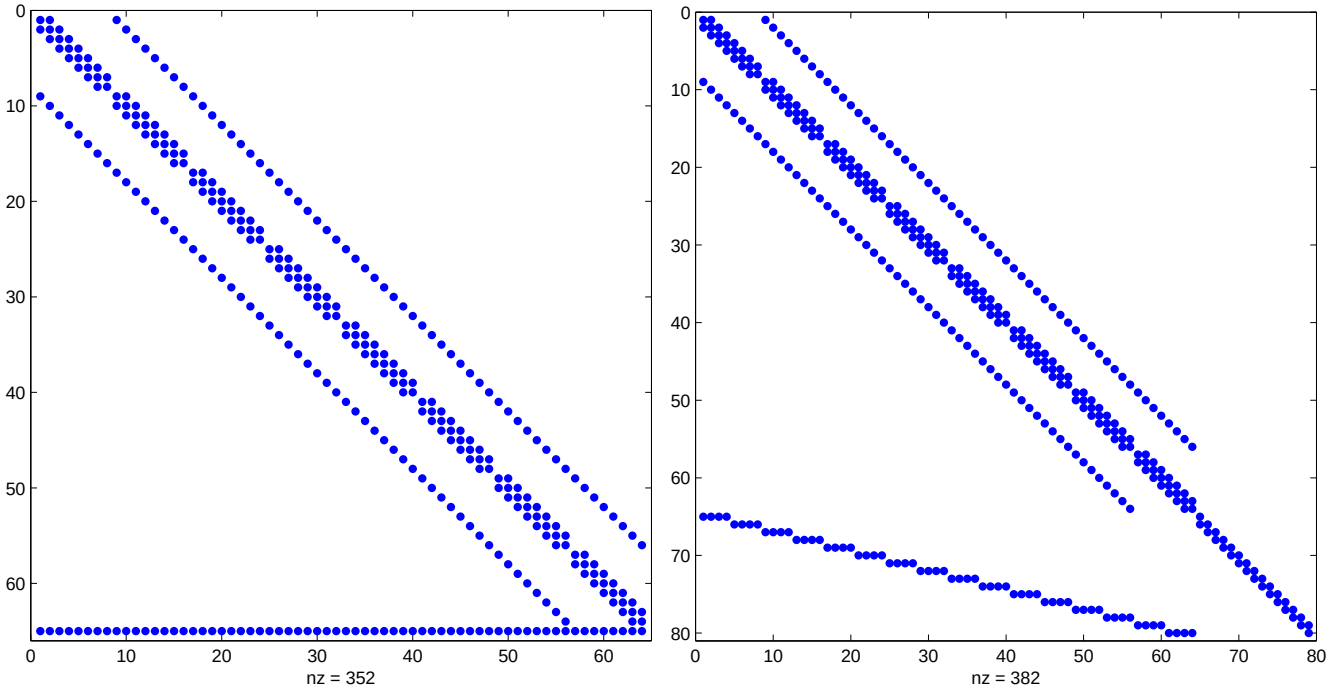

Figure: Matrices based on discrete 2D Laplacian: unstretched (left), stretched (right).

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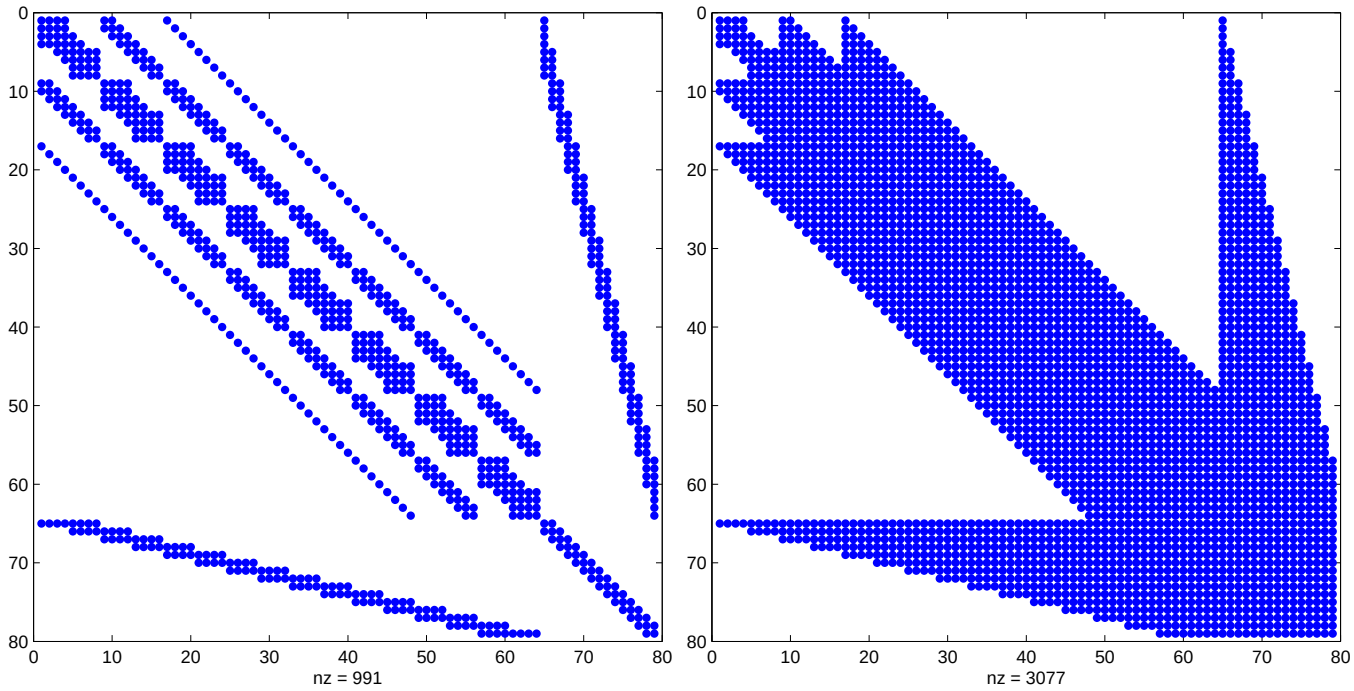

Figure: $A^T A$ (left) and its Cholesky factor (right).

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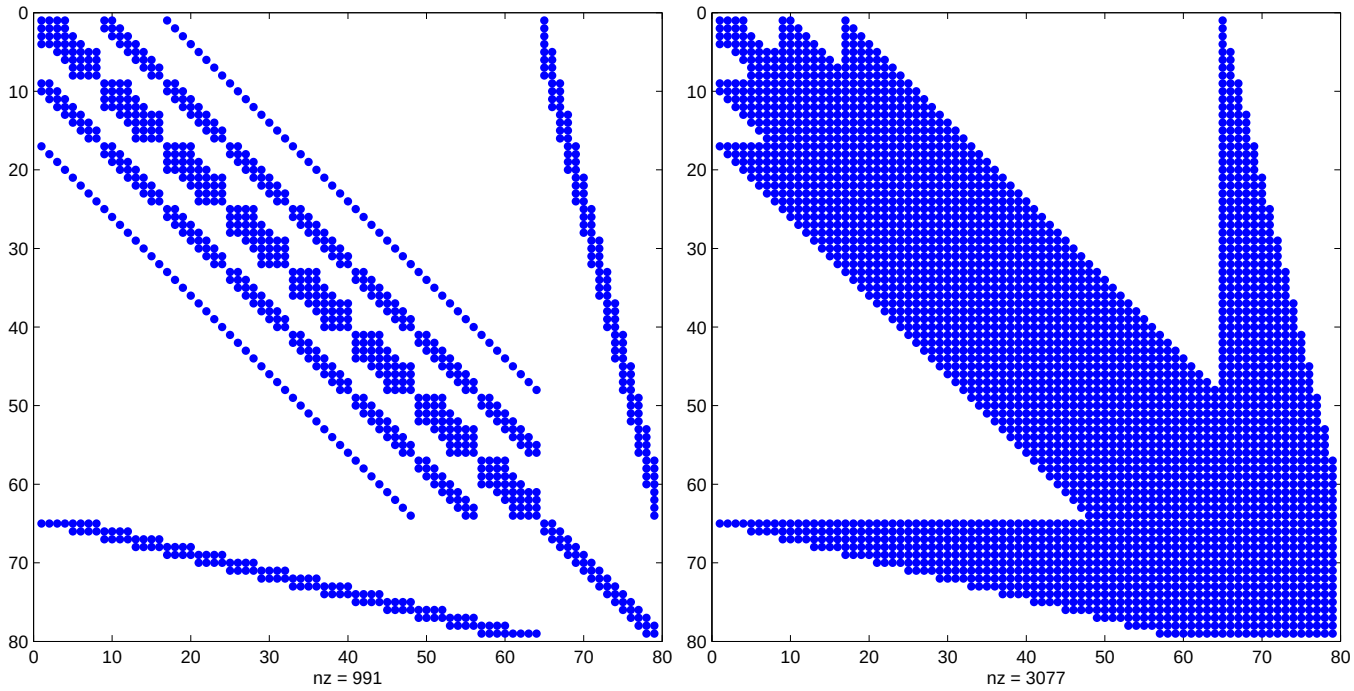

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Matrix stretching for the LS problems: fill-in

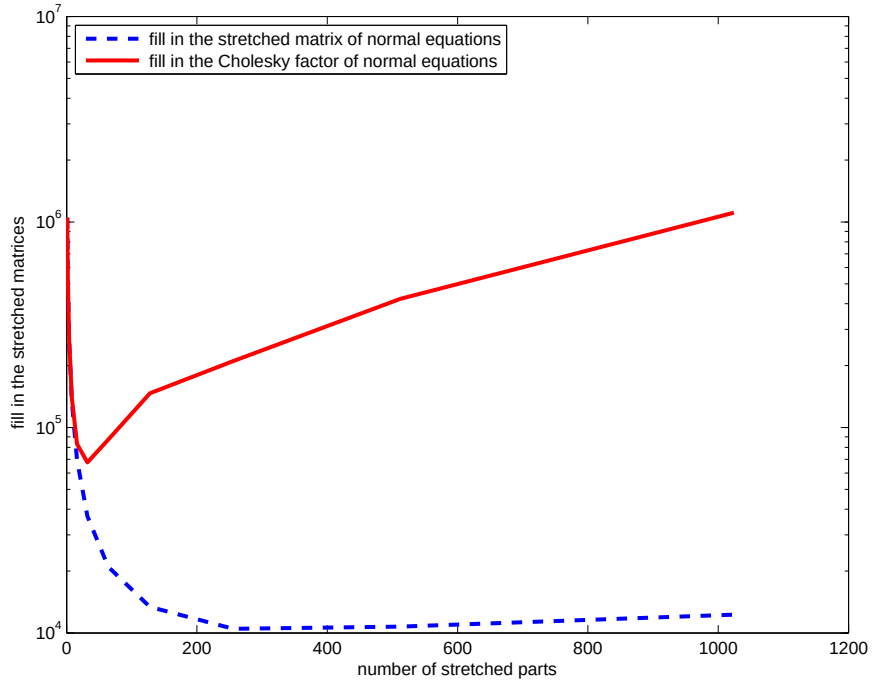

Figure: Fill-in in $A^T A$ and its Cholesky factor (triangular parts).

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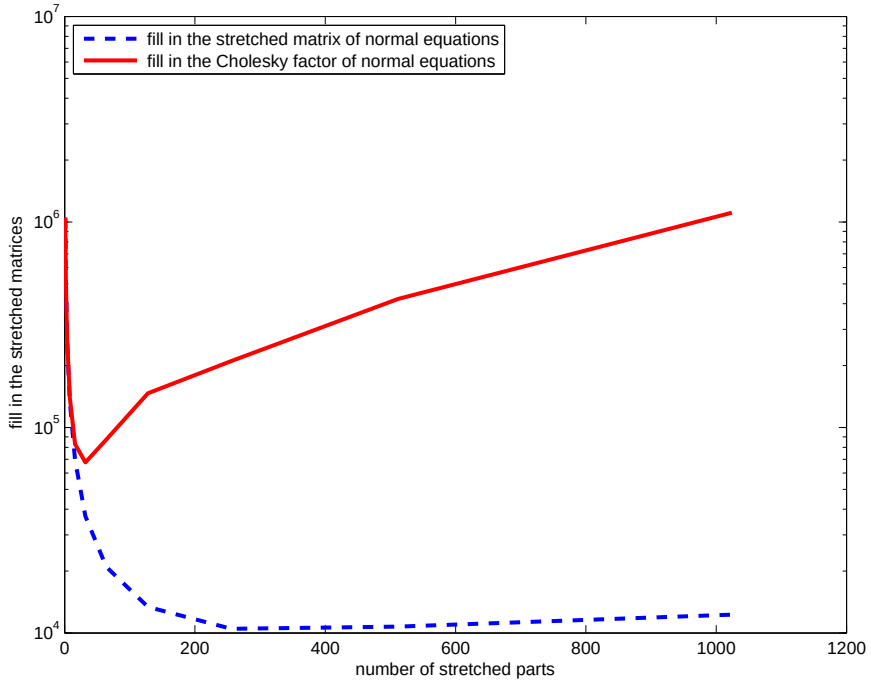

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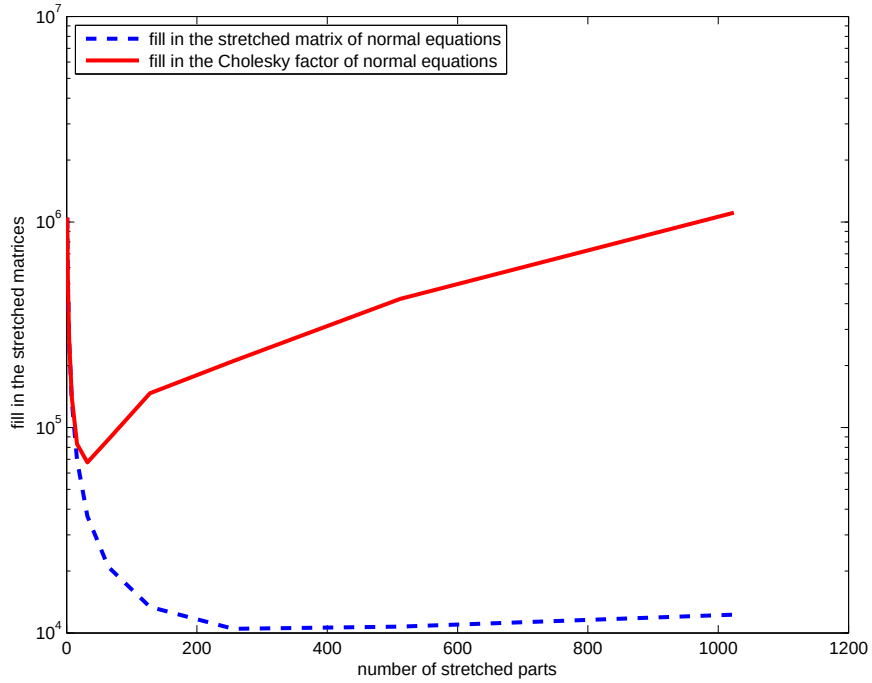

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- More general cases: problems with both fill-in and conditioning (despite the nice result by Adlers and Björck).

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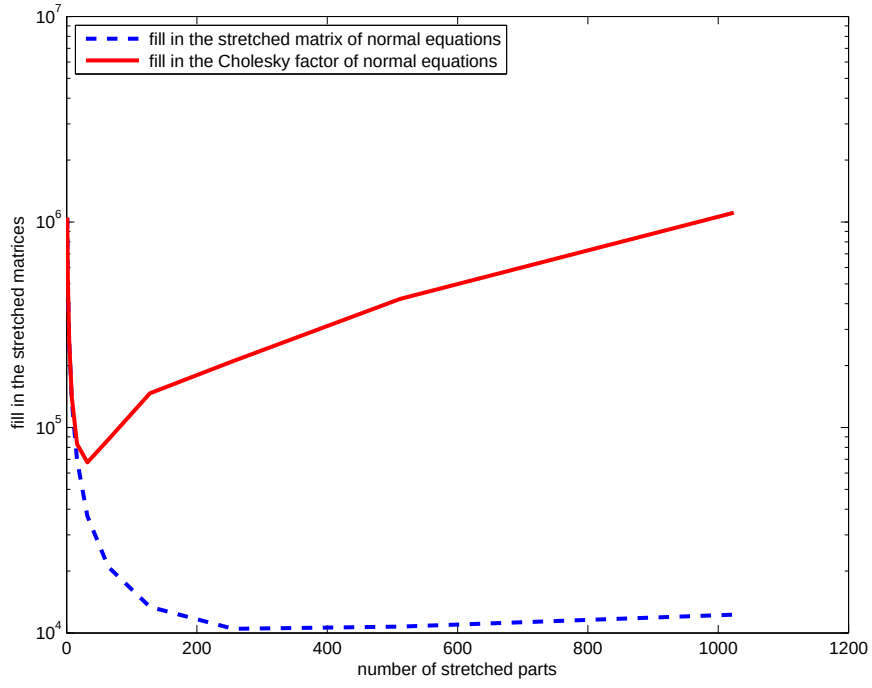

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- Worse, but still not tragic ... Again, reorderings can help.
- More general cases: problems with both fill-in and conditioning (despite the nice result by Adlers and Björck).
- The problem with fill-in is primarily not in additional memory, but in contributing to loss of information in preconditioners!

Our solution (sketched here): make a bridge between A_s and A_d

- Also positive results: stretching just to make a bridge between A_s and A_d
- Matrix AIRCRAFT, stretching used to replace the combination of the partial solutions.
- The decrease in the left automatic due to the IC.

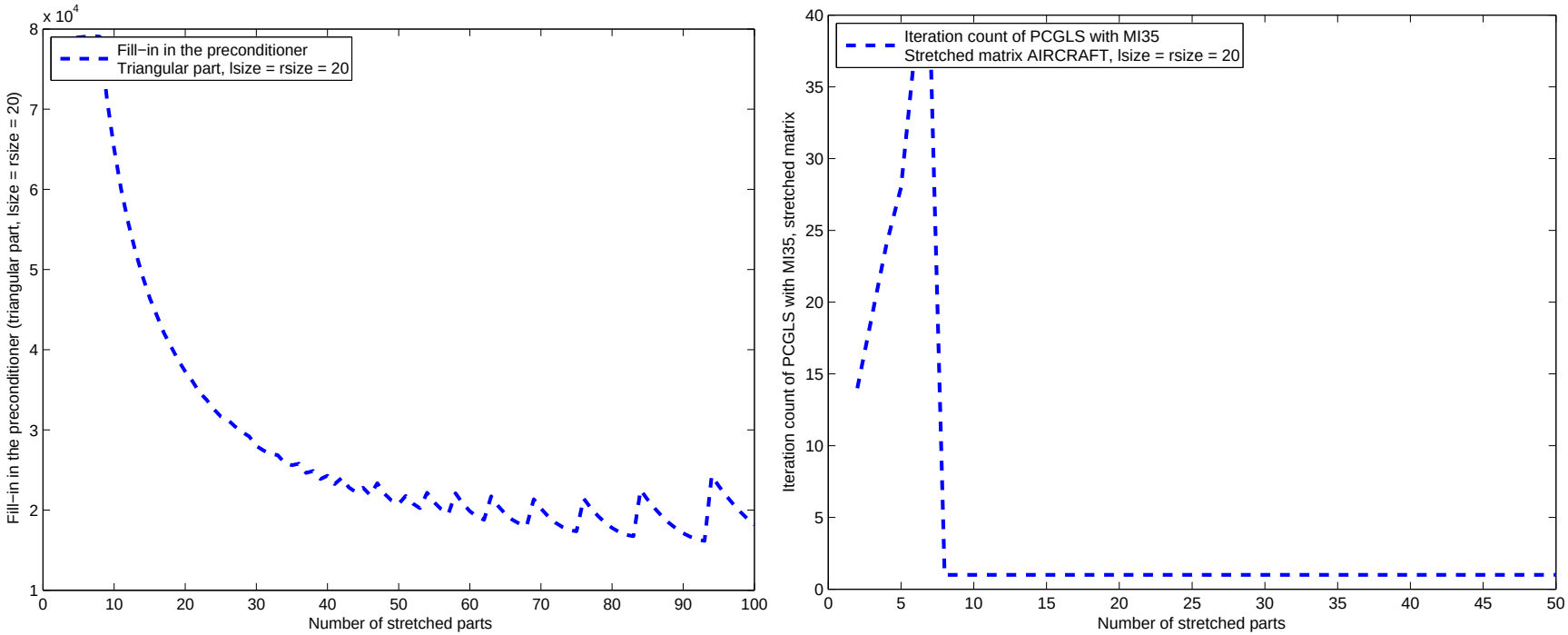

Figure: Stretching only for the bridge. Fill in $A^T A$ (left), iteration count (right)

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- Solving linear least squares problems where A has a number of dense rows.
- A new approach that processes the dense rows separately within a conjugate gradient method
- Not all the formulas above work in practice !!!! In our case, the best has been the simplest one.
  - Dense rows must be treated separately
  - Dense rows must be considered
  - Problem of zero columns in A_s solved by limited use of the stretching.

Last but not least

Thank you for your attention!