UNIVERSITY OF BERGAMO

DEPARTMENT OF MANAGEMENT, ECONOMICS AND QUANTITATIVE METHODS

Working paper n. 1/2017

ricerca_meq@unibg.it

Series Quantitative Methods

Reprojection of the conjugate directions in ABS classes – Part II

Jósef Abaffy

Reprojection of the conjugate directions in ABS classes – Part II

József Abaffy
Óbuda University, Institute of Applied Mathematics
H-1034 Budapest, Bécsi út 96/b, Hungary
abaffy.jozsef@nik.uni-obuda.hu

February 28, 2017

Abstract

In the paper, we use the modification of the Kahan-Parlett "twice is enough" algorithm for the conjugate directions (CD) in the ABS class. In our previous paper we gave the theoretical background. Now, we present an intensive testing of 22 algorithms of the ABS class. The results also show the usefulness of the reprojection technic in CD algorithms.

Keywords— twice is enough, reprojection of conjugate direction methods, ABS methods

Dedico questo articolo alla memoria di Marida Bertocchi con cui ho collaborato in modo piacevole e fecondo per decenni.

1 Introduction

Consider the linear system $Ax = b$, where A is a positive definite n by n symmetric matrix. We want to determine the $p_1, ..., p_n$ A-conjugate directions.

In our earlier paper [2], we gave the necessary theoretical backround for the reprojection of the conjugate direction. In this paper, we show how the 22 chosen algorithms of the ABS class work for a simple randomly generated positive definite symmetric matrix with dimensions between 500–510. Then we test the best of them with the Pascal matrix between 5–50 dimensions. Note that the infimum norm in 50 dimensions of it 5.0446e+028, the rank is 9 in MATLAB 2007/b (should be 50) the two norm is 3.3932e+028 and the max. elements of the matrix is 2.5478e+028 therefore we consider it as a difficult problem. We present the figures of the original Lanczos and Hestenes-Stiefel methods as well. The names of the algorithms are defined our previous paper, here we refer to them with short comments only.

In the figures below the x axis shows the dimension while the y axis represents $y = -\log_{10}(yB)/\|A\|_\infty$ where $yB = \max abs(P^TAP - diag(P^TAP))$ and $\|.\|_\infty$ is the infimum norm and P is the matrix of the computed conjugate directions of matrix A. Because of division with $\|A\|_\infty$ the y residuals can be interpreted as a relative accuracy or the number of correct digits of the conjugate directions. It is important to note that these numbers can be larger than 15.85 because we left out the diagonal elements of the P matrices from the computations, therefore the values of the y axis are only very closely follow the number of correct digits. Note further that all calculations of this paper are carried out using double precision floating point variables and we used MATLAB 2007/b

For all algorithm we present three figures. The first one shows the method without any reprojection. The second one uses the modified ABS-CD-PK algorithm (see below) while the last one shows the case when reprojection is done for all steps.

2 The class of the conjugate direction ABS algorithms (S2)

The properties and the definitions of the examined elements of the S2 subclass were discussed in our earlier paper. Now we repeat those arguments which are important to understand the following. As the matrix update (8.24) of [1] takes an important role in some algorithms therefore we present it now:

$$H_{i+1} = H_i - \frac{H_iA^Tp_ip_i^T}{p^TAp_i} \tag{1}$$

where we used the idempotency of H_i. As for the subclass S2 $v_i = p_i$ the remaining free parameters z_i and w_i were defined as follows.

Case A: The symmetric matrix projection case

Here $w_i = A^Tp_i$ or $w_i = H_iA^Tp_i$ because of the idempotency of H_i.

1) $z_i = r_i$, $w_i = H_iA^Tp_i$ this case is equivalent to the original Hestenes-Stiefel method using the idempotency property of H_i. See page 125 of [1] .(S2HSsz)

2) $z_1 = w_1 = r_1$ and $z_i = w_i = Ap_{i-1}$ it is equivalent to the Lanczos method see page 126 of [1]. (S2Lanczos)

3) $z_i = a_i, \quad w_i = Ap_i$ (S2a) where a_i is the ith row of the coefficient matrix A

4) $z_i = a_i, \quad w_i = H_iAp_i$ (S2asz) where a_i is the ith row of the coefficient matrix A

5) $z_i = r_i \;\; w_i = A^Tp_i$ this case is equivalent to the original Hestenes-Stiefel method (S2rsz)

6 $z_i = e_i \;\; w_i = A^Tp_i$where $e_i \in \Re^n$ is the ith unit vector (S2esz).

7) $z_i = e_i, \quad w_i = H_iAp_i$ and (S2LU)

Finally let z_i and w_i are defined by

8) $z_1 = r_1$ and $z_i = p_{i-1}$ for $i > 1$ and $w_i = H_iA^Tp_i$. (S2psz)

Case B: The non-symmetrical ABS matrix projection case.

We consider different cases which are as follows.

9) $z_i = r_i, \quad w_i^T H_i = p_i^T$ and (1) (S2rp824)

10) $z_i = a_i, \quad w_i = e_i$ and (1) (S2ae) where $e_i \in \Re^n$ is the ith unit vector

11) $z_i = e_i, \quad w_i^T H_i = p_i^T$ and (1) (S2ep824)

12) $z_i = a_i, \quad w_i^T H_i = p_i^T$ and (1) (S2ap824)

13) $z_i = r_i, \quad w_i = r_i$ (S2rr)

14) $z_i = a_i, \quad w_i = a_i$ (S2aa)

15) $z_i = r_i, \quad w_i = a_i$ (S2ra)

16) $z_i = e_i, \quad w_i = e_i$ (S2ee)

17) $z_i = e_i, \quad w_i = a_i$ (S2ea)

18) $z_i = e_i, \quad w_i = r_i$ (S2er)

19) $z_i = a_i, \quad w_i = r_i$ (S2ar)

20) $z_i = r_i, \quad w_i = e_i$ (S2re)

21) $z_i = d_i, \quad v_i = d_i \quad w_i = r_i$ (S2GCD) where $d_i = r_i + \max(abs(r_i))e_i$ This is the method of Dennis and Turner (GCD) see [10]. In this case $r_i^T d_i \neq 0$. The theorems which prove the A conjugacy of d_i are proved in p. 60 and p. 69-72 of [10] for the original algorithm see [5].

22) $z_i = (Ax_i - b)$, $w_i = z_i$ and now let $r_i = A^T(Ax_i - b)$ (S2GCR). This is the so called implicit Generalized Conjugate Residual (GCR) method and the vectors z_i are A conjugate. See [10]

3 Original algorithms

We are implemented the original Hestenes-Stiefel and Lanczos methods as well. Because of the importance of those algorithms we repeat them here.

1) Hestenes -Stiefel method (HS CG original). See in [6] or page 125 of [1].

Algorithm HS CG original

Step 1 Initialize. Choose x_1. Compute $r_1 = Ax_1 - b$. Stop if $r_1 = 0$, otherwise set $p_1 = r_1$ and $i = 1$.

Step 2. Update x_i by

$$x_{i+1} = x_i - \frac{p_i^T r_i}{p_i^T A p_i}$$

Step 3. Compute the residual r_{i+1}. Stop if $r_{i+1} = 0$.

Step 4. Compute the search vector p_{i+1} by

$$p_{i+1} = r_{i+1} - \frac{p_i^T A r_{i+1}}{p_i^T A p_i} p_i$$

Step 5. Increment the index i by one and go to Step 2.

2) Lánczos method (Lanczos original). See [7], [8] or page 126 of [1].

Algorithm Lanczos original

Step 1. Initialize. Choose x_1. Compute $r_1 = Ax_1 - b$. Stop if $r_1 = 0$, otherwise set $p_1 = r_1$, $p_0 = 0$ and $i = 1$.

Step 2. Update the estimate of the residual by

$$x_{i+1} = x_i - \frac{p_i^T r_i}{p_i^T A p_i}$$

Step 3. Compute the residual r_{i+1}. Stop if $r_{i+1} = 0$.
Step 4. Compute the search vector p_{i+1} by

$$p_{i+1} = Ap_i - \frac{p_i^T A^2 p_i}{p_i^T A p_i} p_i - \frac{p_{i-1}^T A p_i}{p_{i-1}^T A p_{i-1}} p_{i-1}$$

Step 5. Increment the index i by one and go to Step 2.

4 Numerical results

In this chapter we test the algorithms chosen from the Subclasses S2. The algorithms were implemented in MATLAB version R2007b. These algorithms are tested with Symmetric Positive Definite (SPD) matrices generated randomly by the MATLAB rand function. The dimensions considered are in the interval 500–510. Similarly the solutions of the linear system of equations are generated randomly (by rand function). After these tests, the well-known Pascal problem is used between 5–50 dimensions for the selected algorithms which gave accurate precision for problem SPD, that is at least 10 relative accuracy in the worst case. We mention that the Pascal problems in these dimensions are non-singular in double precision. After the figures we always describe the maximum norm of the residuals and the number of the reprojections for the ABS-CD-PK figures for all dimensions. When during the reprojection Case 3 happens, which is linear dependency is detected, we count and present them. We also present the number of linear dependency observed by the actual ABS algorithm. These informations together with the figures give the basis for the decisions on which are the best algorithms.

We want to select from the many possible versions the best algorithms.

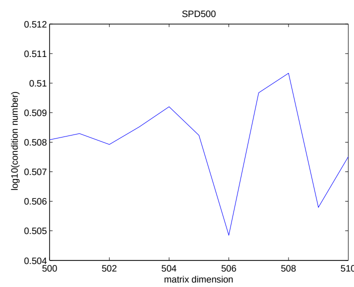
We should note that the titles of the figures contain the problem, the name of the algorithm and identify the reprojection. The algorithm's name exactly defines the algorithm (see above).

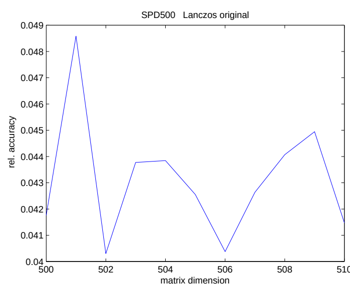
4.1 Test results with the SPD matrix

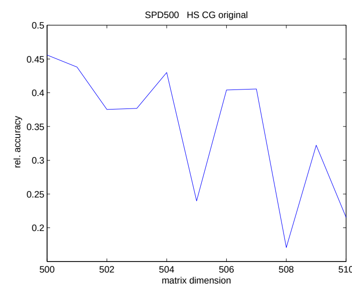
We choose altogether 22 cases from the Subclasses S2. First we show the figure: log10(condition number of SPD in infimum norm) versus dimension.

It can be seen that the log10(cond(SPD)) numbers are not very high. Therefore it is suitable for the selection.

In the figures below the x axis shows the dimension while the y axis represents $y = -\log_{10}(yB)/\left\|A\right\|_\infty$ where $yB = \max abs(P^T AP - diag(P^T AP))$ and $\|.\|_\infty$ is the infimum norm of a matrix. Furthermore when we write down the maxnorm of the residuals it means the maximum absolute value of the residual







vectors of the linear systems that is without divided by any norm of the coefficient matrix A. Because we are interested in how near is the residual to the zero vector.

Before we turn to the cases of the ABS Subclasses we give the figures of the original Lanczos and Hestenes-Stiefel method see ex.[1].

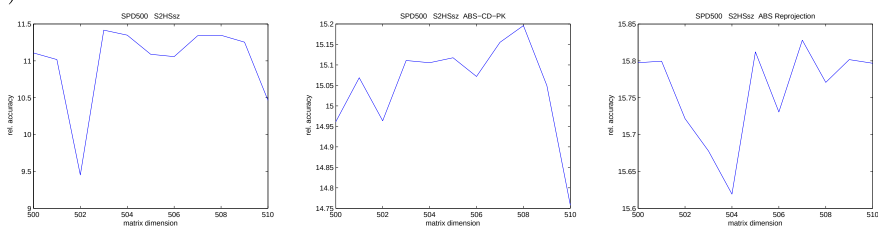
As we can see the relative accuracies are bad. In case Lanczos original NaN happened, because the denominators of the update formulas tended to ∞. Therefore we had to introduce into the original algorithm a stop criteria for the denominators. If they were greater than 1.e200 then stop. It is worthwhile to note that in this case the maximum norm of residuals is 1.199e-011 which is very nice. In case HS original method it was 1.147e-012 and there were no problems in the denominators. As we can see below there are good representations of the Hestenes-Stiefel method which give acceptable precision in the conjugate direction vectors too.

4.1.1 Subclass S2

Now we turn to our methods. For the sake of brevity in the following we give the maximum value of residual's norm and only those other metrics which are represent valuable information. Therefore, if the number of linear independency vector contains only zero elements, we do not write it down. The first figure show the actual algorithm in the ABS, the second one gives the result with ABS-CD-PK reprojection, and the third one the reprojections are done in all steps.

We begin with the algorithms of the symmetric projection matrices.

1) S2HSsz



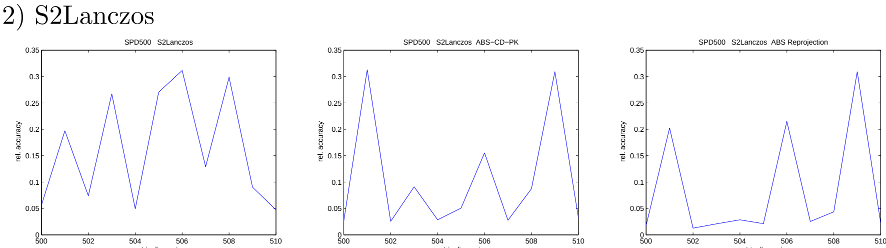
The maxnorm of the residuals in the case without reprojection is 1.306e-011. The number of linear dependency according to ABS algorithm (ABS later) 55 53 68 44 51 58 47 53 56 56 56. This linear dependency in the ABS algorithms is as follows: $if\ norm(H_i A^T p_i) < 4eps$. where eps the machine epsilon. The $4eps$ a reasonable value we did not decrease it even if we know the coefficient matrix A is positive definite symmetric one. Any case this means the number of the zero columns in P. In the later we do not repeat this statement we give the numbers only if they are no zeros.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.264e-011. The numbers of the reprojections are 346 346 353 354 359 356 355 364 365 374 390. The number of linear dependency (ABS) 55 43 47 39 52 57 44 46 45 39 43.

The maxnorm of the residuals in the case of the always reprojection is 1.378e-011. The number of linear dependency (ABS) 52 61 54 40 48 63 48 53 46 51 44

We conclude that the ABS-CD-PK and the always reprojection cases give definitely better results than the original method in the ABS. Furthermore the original version in ABS is a lot better than the original HS CG algorithm. The residuals of the linear systems are also very satisfactory. This algorithm shows the efficiency of the ABS-CD-PK "twice is enough" method.

2) S2Lanczos



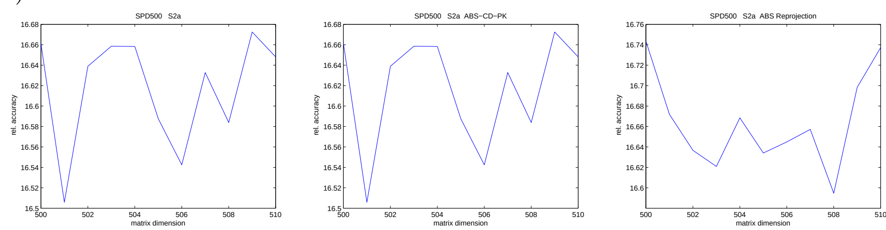
The maxnorm of the residuals in the case of no reprojection is 1.317e-011. In the ABS realization the p_i projection vectors tend to ∞ therefore the earlier condition was introduced for the norm of p_i

The maxnorm of the residuals in the case of the ABS-CD-PK reprojection is 1.342e-011. There were neither need to any reprojection nor any linear dependence happened. That is the P matrix is full.

The maxnorm of the residuals in the case of the always reprojection is 1.361e-011.

We conclude that because of the bad figures the conjugate directions can not be accepted, but the residuals were computed with a good precision.

3) S2a



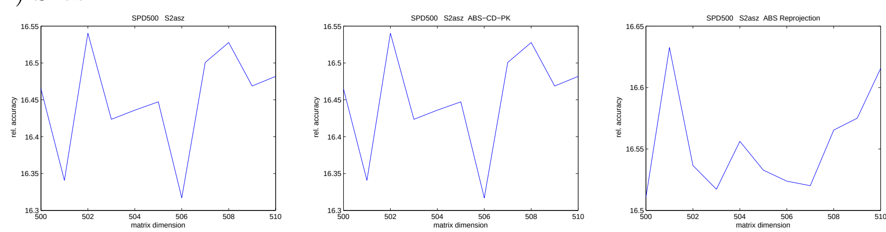
The maxnorm of the residuals in case of the no reprojection is 1.411e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.411e-011. There were no need to any reprojection.

The maxnorm of the residuals in case of the always reprojection is 1.315e-011.

All the three figures are essentially the same and show good accuracy.

4) S2asz



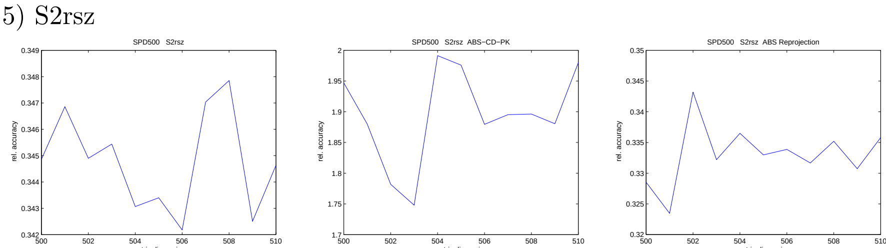
The maxnorm of the residuals in case of the no reprojection is 1.99e-011.

The maxnorm of the residuals in case of the ABS-CD-PK is 1.99e-011. There were no need for any reprojection.

The maxnorm of the residuals in case of the always reprojection is 1.377e-011.

All the three figures are very accurate.

5) S2rsz



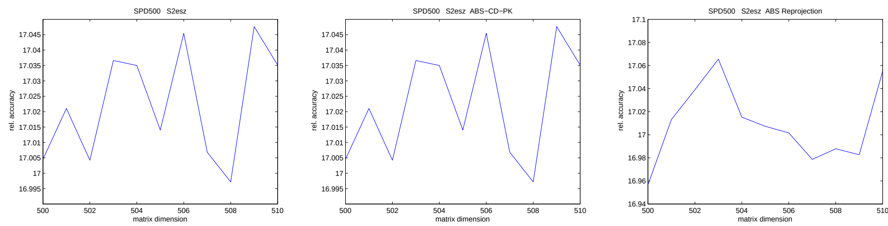
The maxnorm of the residuals in case of no reprojection is 9.018e-007.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 0.01723. The numbers of the reprojections are 1 1 1 1 1 1 1 1 1 1 1. The numbers of the zero columns in the P matrix are 494 495 496 497 498 499 500 501 502 503 504, that is the P matrix practically does not have any good information.

The maxnorm of the residuals in case of the always reprojection is 1.405e-006.

All the three figures are bad because $z_i = r_i$.

6) S2esz

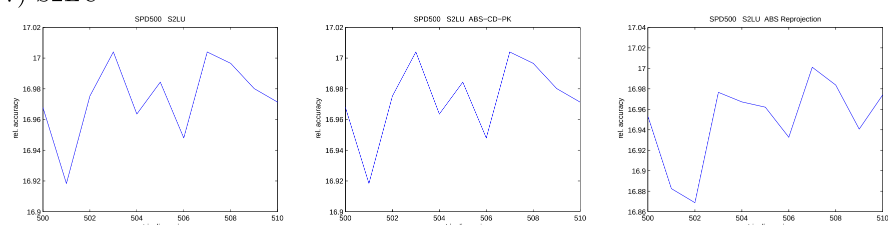


The maxnorm of the residuals in case of no reprojection is 1.225e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.225e-011 the same as above because there were no need to any reprojections.

The maxnorm of the residuals in case of the always reprojection is 1.213e-011. All the three figures are the best so far. The reason is that as $z_i = e_i$ that are no multiplications which would increase the rounding errors in the calculation of the projections vectors p_i.

7) S2LU



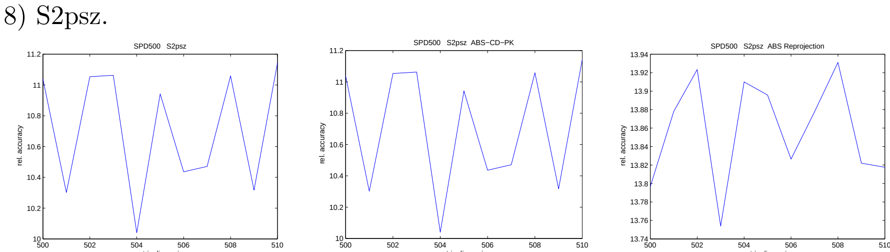
The maxnorm of the residuals in case of no reprojection is 1.253e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.253e-011. The first two figures are equivalent as there were no need for any reprojections because of the high accuracy.

The maxnorm of the residuals in case of the always reprojection is 1.238e-011.

All the three figures are practically equivalent. So the always reprojection in this case is not a reasonable choice. They have similar results because of the very accurate values and the relatively small number of computations.

8) S2psz.



The maxnorm of the residuals in case of no reprojection is 1.391e-011.

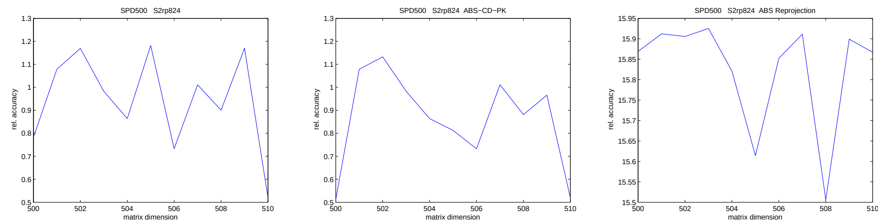
The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.391e-011. The numbers of the reprojections are 1 1 1 1 1 1 1 1 1 1 1.

The maxnorm of the residuals in case of the always reprojection is 5.175e-012.

Here the always reprojection is definitely better than the other two cases.

Now we turn to the non-symmetric cases.

9) S2rp824



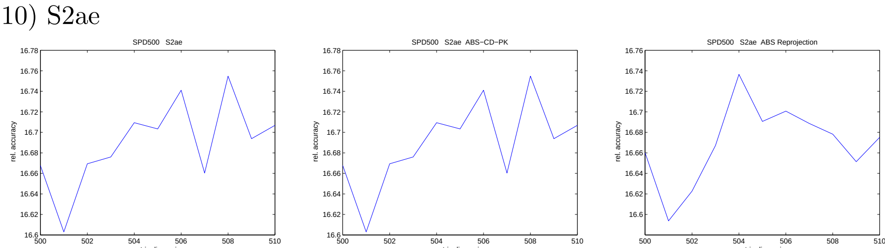
The maxnorm of the residuals in case of the no reprojection is 1.197e-011. The numbers of the linear dependency (ABS) are 235 83 106 110 116 307 176 291 81 58 95 that is the matrix P is not full.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.234e-011. The numbers of the reprojections are 378 343 378 346 341 366 346 385 377 379 374 and the numbers of the linear dependency (ABS) are 57 37 46 35 58 61 24 51 52 43 51.

The maxnorm of the residuals in case of the always reprojection is 1.307e-011. The numbers of linear dependency (ABS) are 54 45 57 37 56 54 48 52 51 50 57.

The reason of the bad figures is again the residual vectors in the computations of the projection vectors. The third figure shows that we should do more research about the possibility of an extra reprojection in certain cases even if the presence of the residual vectors in p_i explains the bad results.

10) S2ae



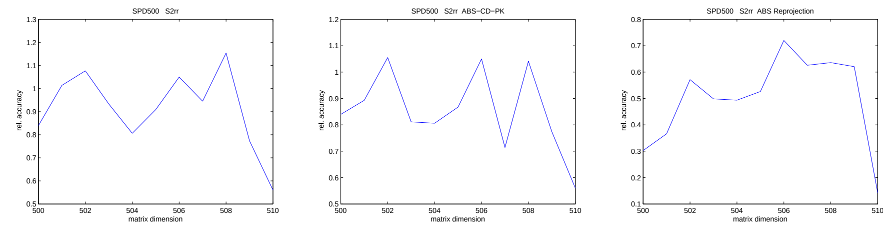
The maxnorm of the residuals in case of the no reprojection is 1.374e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.374e-011.

The maxnorm of the residuals in case of the always reprojection is 1.265e-011.

The first two figures are the same because the results are accurate enough without reprojections.

11) S2rr



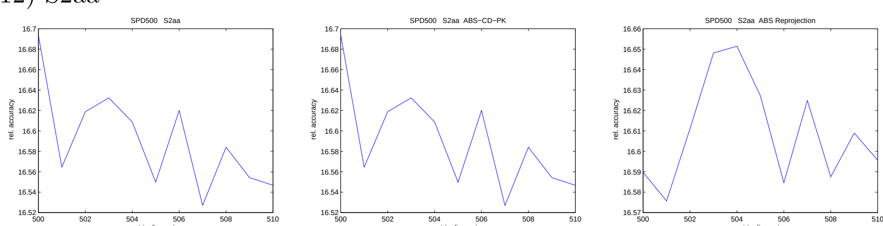
The maxnorm of the residuals in case of the no reprojection is 1.212e-011. The numbers of linear dependency (ABS) are 132 204 207 118 196 160 150 204 126 140 141.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.174e-011. The numbers of the reprojections are 381 368 370 348 347 354 350 385 364 361 357. The number of linear dependency (ABS) are 251 168 225 71 176 202 238 73 105 119 149.

The maxnorm of the residuals in case of the always reprojection is 1.112e-011. The number of linear dependency (ABS) are 132 88 313 93 89 325 329 92 323 404 339.

The reason of the bad figures are evident, the residual vectors in the ABS algorithm.

12) S2aa



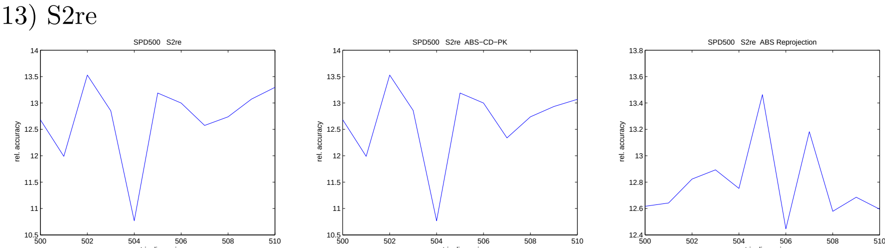
The maxnorm of the residuals in case of the no reprojection is 1.433e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.433e-011.

The maxnorm of the residuals in case of the always reprojection is 1.421e-011

There were no need for any reprojection because of the accurate results.

13) S2re



The maxnorm of the residuals in case of the no reprojection is 1.63e-011. The numbers of linear dependency (ABS) are 0 16 0 7 1 0 11 0 0 0 0.

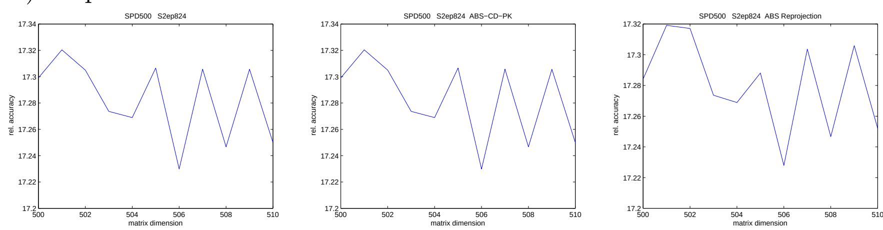
The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.63e-011. The numbers of linear dependency (ABS) are 0 16 0 7 1 0 11 0 0 0

0. The numbers of the reprojections are 3 21 4 12 17 3 13 5 2 3 7.

The maxnorm of the residuals in case of the always reprojection is 1.764e-011. The numbers of linear dependency (ABS) are 1 13 1 3 1 0 5 0 0 0 0.

These are somewhat worse results then above. The reason of that is the presence of the residual vectors in the algorithm.

14) S2ep824



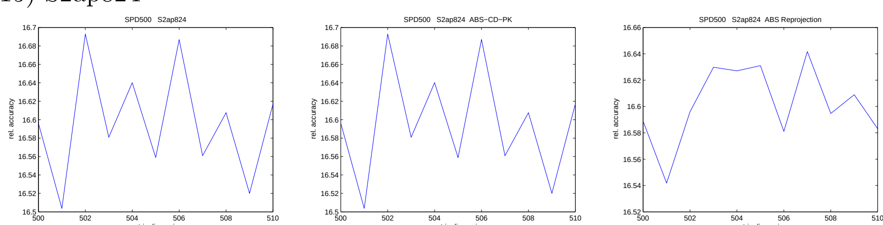
The maxnorm of the residuals in case of the no reprojection is 1.059e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.059e-011.

The maxnorm of the residuals in case of the always reprojection is 1.058e-011. The number of linear dependency (ABS) 1 13 1 3 1 0 5 0 0 0 0.

Comparing these figures with the figures of the S2rp824, the difference is visible that is due to $z_i = e_i$ instead of $z_i = r_i$. Again, the first figure is so accurate that there was no need to any reprojection.

15) S2ap824



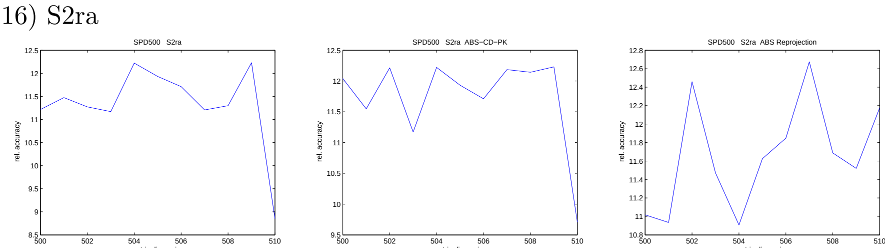
The maxnorm of the residuals in case of the no reprojection is 1.31e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.31e-011.

The maxnorm of the residuals in case of the always reprojection is 1.425e-011.

There were no need to any reprojection, because of the high accuracy without it.

16) S2ra



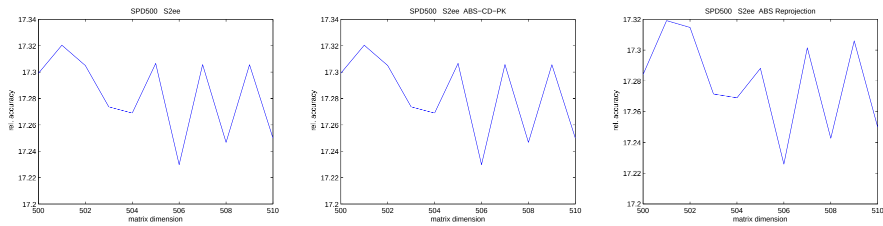
The maxnorm of the residuals in case of the no reprojection is 2.14e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 2.14e-011. The numbers of the reprojections are 7 6 32 26 6 4 3 25 4 12 30.

The maxnorm of the residuals in case of the always reprojection is 2.198e-011.

Here we can show again that when the results without reprojections are not so excellent then how the reprojections improve them.

17) S2ee



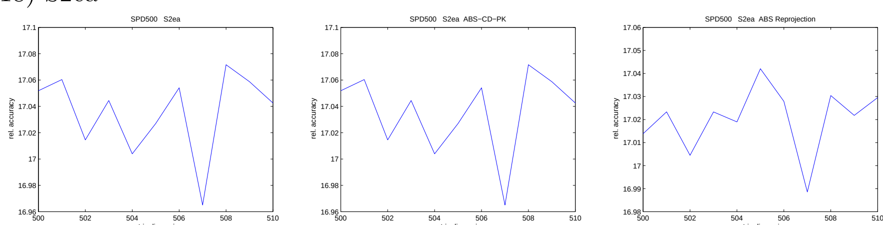
The maxnorm of the residuals in case of the no reprojection is 1.059e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.059e-011.

The maxnorm of the residuals in case of the always reprojection is 1.058e-011.

Observe that, the rounding errors are so small because of the two unit vectors, that the relative accuracy is at least 17.

18) S2ea



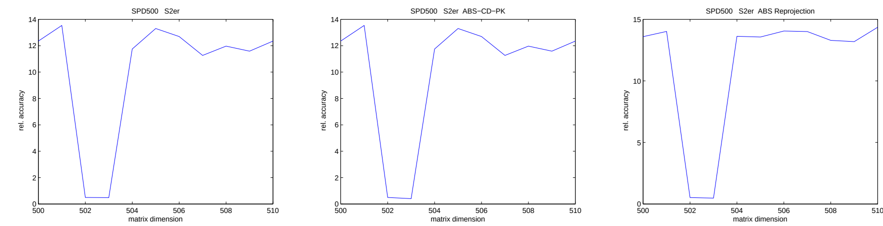
The maxnorm of the residuals in case of the no reprojection is 1.282e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.282e-011.

The maxnorm of the residuals in case of the always reprojection is 1.26e-011

The accuracy without any reprojection is so high that there is no need for any reprojection in case of the ABS-CD-PK. Therefore, there is no sense in using the always reprojection in this case.

19) S2er



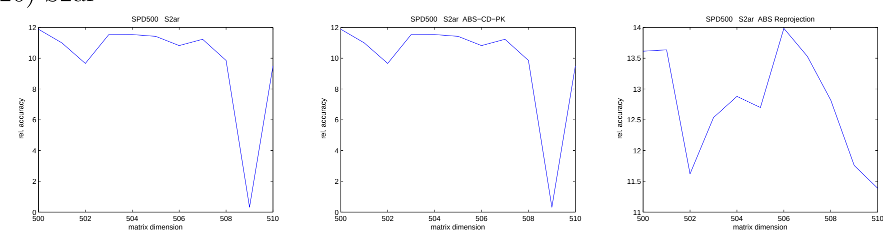
The maxnorm of the residuals in case of the no reprojection is 6.581e-009.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 6.581e-009. The numbers of the zero columns are 0 0 186 0 0 0 0 0 0 0 0 and in dimension 503 (where there are zero columns) NaN happened too.

The maxnorm of the residuals in case always reprojection is 2.372e-010.

The reason of the bad results is again the presence of the residual vectors in the algorithm.

20) S2ar



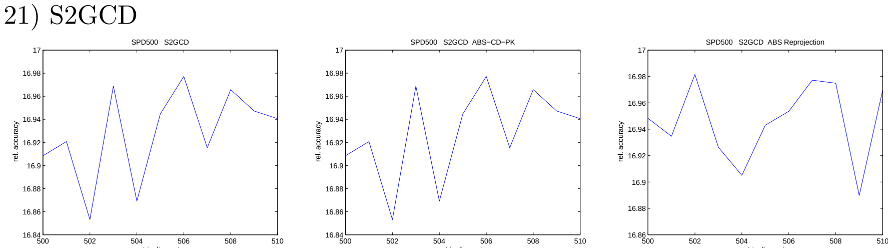
The maxnorm of the residuals in case of the no reprojection is 4.166e-009. The numbers of linear dependency (ABS) are 208 124 258 304 172 210 70 0 259 246 236.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 4.166e-009. The numbers of the reprojections are 0 0 0 0 0 0 1 0 0 0 0 while the numbers of linear dependency (ABS) are 208 124 258 304 172 210 70 0 259 246 236.

The maxnorm of the residuals in case of the always reprojection is 1.691e-009. The numbers of linear dependency (ABS) are 210 176 237 269 149 197 92 0 258 269 266.

Everything as in case S2er.

21) S2GCD



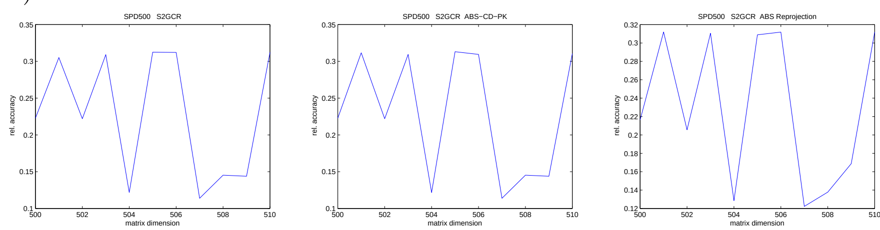
The maxnorm of the residuals in case of the no reprojection is 1.257e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.257e-011.

The maxnorm of the residuals in case of the always reprojection is 1.189e-011.

Again, we observe that when the results without reprojections are so accurate then there is no need to do any reprojections.

22) S2GCR



The maxnorm of the residuals in case of the no reprojection is 1.134e-011.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.241e-011. The numbers of the reprojections are 371 351 345 356 356 367 361 378 393 381 357.

The maxnorm of the residuals in case of the always reprojection is 1.267e-011.

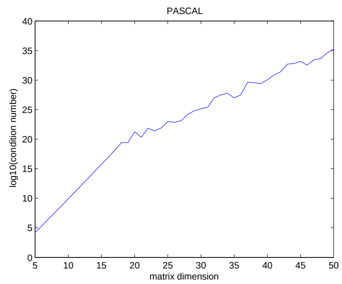
The reason of the bad results are twofold. First, the presence of the residual vectors in the algorithm and second the term $H*(A^T*(A*p))$ in the projection matrix update which cause great rounding errors. This shows that in pathological cases the second term of our Theorem 2 of PART I of the paper can give bad results.

Generally speaking, we can observe that those methods of which one of the free parameters is the residual vector give bad results in the conjugate directions even if the residual of the linear systems are acceptable. The reason of this phenomena is the rounding error of computation of the residual vectors. All the 22 methods give good residuals. Almost all of them have an order of 10^{-11} at least in all components. However 17 algorithms give good results in relative accuracy of the conjugate directions that is 11.0 at least. As we know that the SPD test matrices are positive definite symmetric ones, we chose only those which did not give linear dependency. So we have 11 algorithms only. These have 10 relative accuracies at least. These algorithms will be considered for the PASCAL matrix. Finally we chose the symmetric version of the Hestenes-Stiefel algorithm as well, because it is a well-known method and the ABS version of it is acceptably accurate.

4.2 Results with the PASCAL matrix

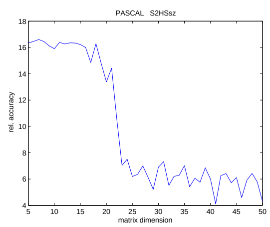
The Pascal problem is well-known as a difficult problem because of the high condition numbers of these matrices computed by the MATLAB function cond(). This can be seen in the following figure.

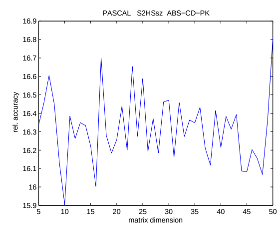
We mention that we present the figures in the same order as before. We have to underline again that the residuals are absolute, that is without the division by any norm of A.

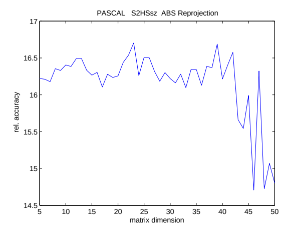


4.2.1 Subclass S2

1) S2HSsz







The maxnorm of the residuals in case of the no reprojection is 9.909e+018.

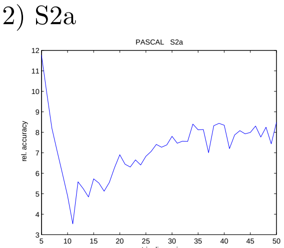
The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 4.063e+012. The numbers of the reprojections are 0 0 0 0 0 0 1 1 2 2 4 4 6 7 8 10 11 12 14 15 12 18 11 11 18 14 15 12 16 8 7 11 8 7 7 9 6 6 6 6 7 5 5 5 8 7. The numbers of linear dependency (ABS) are 0 0 0 0 0 0 0 1 0 1 1 1 1 2 2 2 3 3 1 2 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5 0 7 7 3 8 8 12 9 18 20 18 22 24 25 24 28 29 30 31 31 34 35 36 35 36.

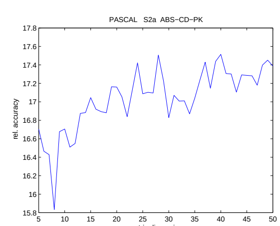
The maxnorm of the residuals in case of the always reprojections is 7.859e+023.

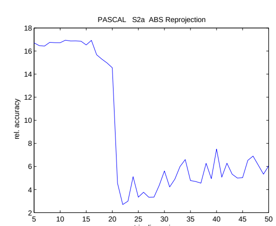
The number of linear dependency (ABS) 0 0 0 0 0 0 0 1 0 1 1 1 1 2 2 2 3 3 1 2 1 0 1 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0.

It is clear that the S2HSsz and ABS-CD-PK algorithm gives acceptable results but with many zeros in the conjugate directions matrix. Therefore, the always reprojection version is acceptable only.

2) S2a







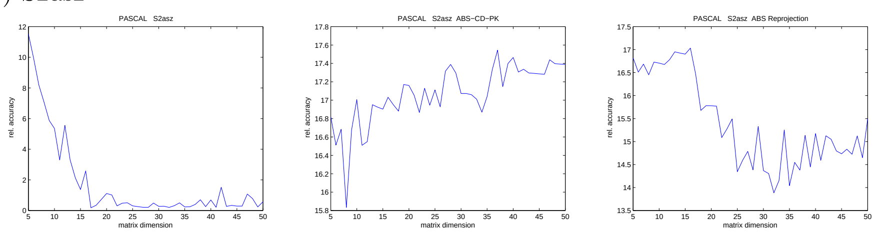
The maxnorm of the residuals in case of the no reprojection is 1.259e+019.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.558e+013. The numbers of the reprojections are 4 5 6 6 7 8 9 9 10 10 11 11 11 11 12 12 12 12 12 12 12 12 11 11 11 12 11 11 11 12 12 12 12 12 12 12 12 12 12 13 13 13 13 12 13 14. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 2 3 3 4 5 6 6 7 8 9 10 11 12 13 15 16 17 17 19 20 21 21 22 23 24 25 26 27 28 29 30 30 31 32 33 35 35 35.

The maxnorm of the residuals in case of the always reprojections is 4.226e+016. The numbers of linear dependency (ABS) are 0 0 0 0 0 0 0 0 1 1 1 2 2 2 2 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0.

The ABS-CD-PK figure seems to be acceptable only, but in this case there are many zero columns in the matrix P. Note that the norm of the Pascal matrices ex. $\|Pascal(50)\|_\infty = 1.9526e+035$.

3) S2asz



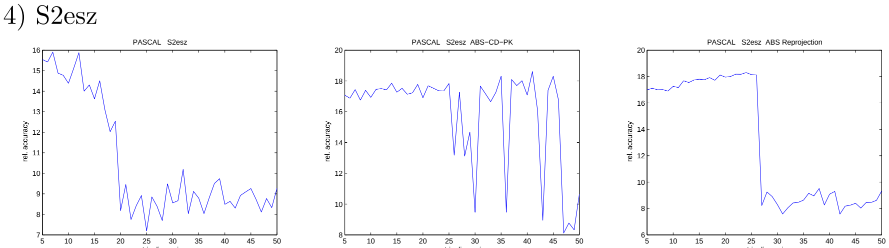
The maxnorm of the residuals in case of the no reprojection is 6.836e+016. The numbers of linear dependency (ABS) are 0 0 0 0 0 0 0 0 0 1 1 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 1.018e+013. The numbers of the reprojections are 4 5 6 6 7 8 9 9 10 10 11 11 11 11 12 12 12 12 12 12 12 12 11 12 11 12 12 11 11 12 12 12 12 12 12 12 12 13 13 13 13 12 13 13 13 13. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 2 3 3 4 5 6 6 7 8 9 10 11 12 13 15 15 17 17 18 20 21 21 22 23 24 25 26 27 28 28 29 30 31 33 33 34 35 36.

The maxnorm of the residuals in case of the always reprojection is 7.174e+020.

Observe that for this pathological case the always reprojection with this algorithm is more efficient than the ABS-CD-PK case where there are many non-zero columns in P.

4) S2esz



The maxnorm of the residuals in case of the no reprojection is 2.195e+018

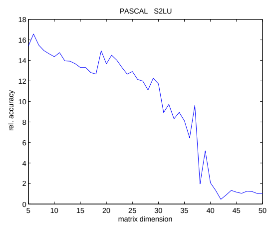
The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 4.279e+017. The numbers of the reprojections are 2 3 3 4 5 6 6 7 8 8 9 10 10 11 12 13 13 14 15 15 16 17 18 17 16 18 16 16 15 15 8 19 11 11 10 10 6 3 27 9

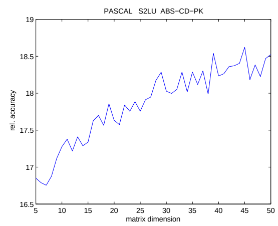
9 7 19 23 21 28. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 3 2 4 5 7 8 15 6 14 14 16 17 22 25 2 21 22 24 0 0 0 6.

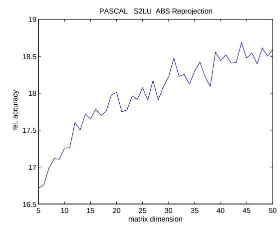
The maxnorm of the residuals in case of the always reprojection is 8.794e+016

This is an important algorithm because it shows how is the accuracy of the conjugate directions in case of the ABS-CD-PK better than the one with the always reprojection.

5) S2LU







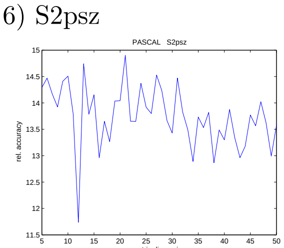
The maxnorm of the residuals in case of the no reprojection is 3.388e+021. The numbers of linear dependency (ABS) are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0.

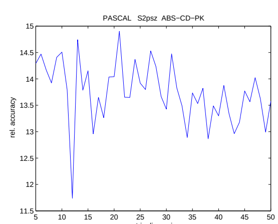
The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 5.607e+019. The numbers of linear dependency (ABS) are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 2 2 2 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 1 1 3 5 6 13 8 13 15 9 15 23 26 26 26 29 21 32 18 22.

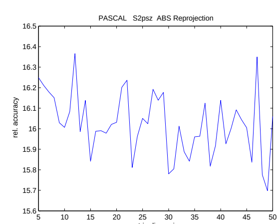
The maxnorm of the residuals in case of the always reprojection is 4.375e+020. The numbers of linear dependency (ABS) are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 1 1 1 1 1 1 2 1 2 2 2 2 2 2 3 2 3 2 3 3 3 4 3 4 4 4 4 5 5 6.

In case of always reprojection it is the bes if the P matrix is almost full. It is interesting to also note that as the dimension increases the relative accuracy is better because the numbers of the zero columns are slightly growing.

6) S2psz







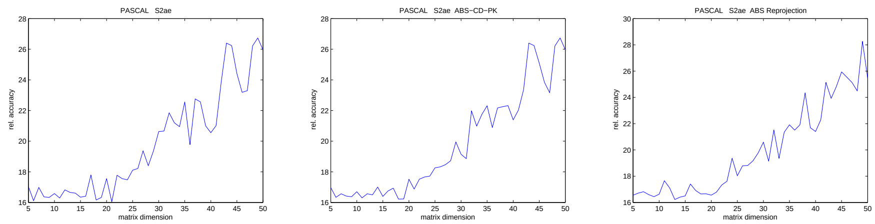
The maxnorm of the residuals in case of the no reprojection is 1.815e+024.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 6.629e+014. The numbers of the reprojections are 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 1 1 2 1 3 2 4 2 2 1 1 3 1 2 1 2 1 1 1 2 1 2 1 1 2 2 2 1 2 2 4. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 4 0 15 20 16 23 24 23 25 28 29 30 29 29 33 34 36 36 36.

The maxnorm of the residuals in case always of the reprojections is 7.122e+021.

Definitely the always reprojection is the best algorithm in this case.

7) S2ae



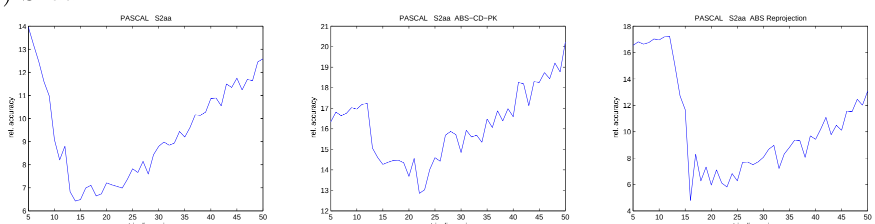
The maxnorm of the residuals in case of the no reprojection is 7.845e+023.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 7.845e+023. The numbers of the reprojections are 1 1 1 1 2 2 3 3 3 4 4 4 5 5 6 6 6 7 7 8 8 8 8 8 6 7 9 1 6 7 6 6 6 6 7 6 4 6 0 2 5 10 8 0 1 7. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0.

The maxnorm of the residuals in case of the always reprojection is 2.043e+025.

All three figures are excellent.

8) S2aa



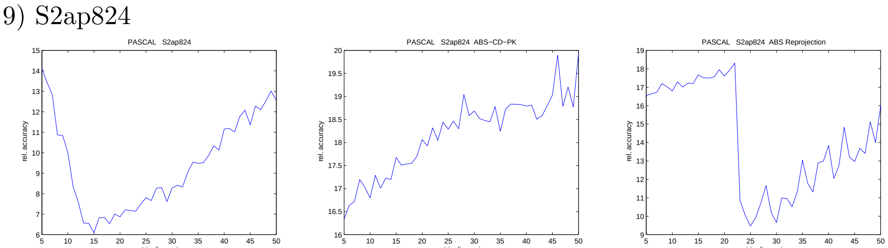
The maxnorm of the residuals in case of the no reprojection is 2.46e+018.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 4.735e+015. The numbers of the reprojections are 3 5 6 7 8 9 10 11 12 12 13 13 13 13 13 14 13 14 14 14 14 14 13 13 14 14 13 13 13 14 13 13 13 14 13 13 12 12 13 12 12 12 12 12 12 11. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 0 0 1 1 2 3 4 5 5 7 7 8 9 10 11 13 14 14 15 17 18 19 19 21 22 23 23 25 26 28 29 29 31 32 33 34 35 36 38.

The maxnorm of the residuals in case of the always reprojection is 4.921e+019.

This case shows that the always reprojection is not always the best algorithm. It depends on the problem and on choice of algorithm.

9) S2ap824



The maxnorm of the residuals in case of the no reprojection is 1.277e+019.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is

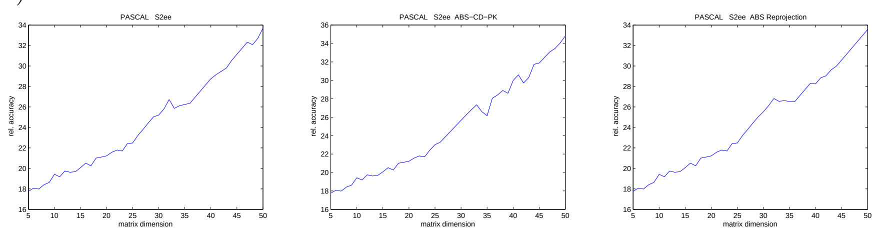
6.352e+012.

The numbers of the reprojections are 3 5 6 7 8 9 10 11 12 12 13 14 14 15 15 15 16 16 16 16 16 17 17 17 18 17 17 18 18 18 18 18 19 18 18 20 18 18 19 19 19 19 19 19 19 18. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 0 1 1 1 2 2 3 4 4 5 6 7 8 8 9 10 10 12 13 13 14 15 16 17 17 19 20 19 22 23 23 24 25 26 27 28 29 31.

The maxnorm of the residuals in case of the always reprojection is 1.622e+021.

Even if the best results is the ABS-CD-PK case, the numbers of the zero columns are too many.

10) S2ee



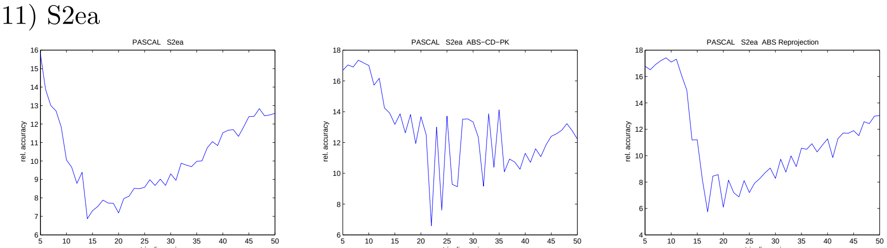
The maxnorm of the residuals in case of the no reprojection is 1.824e+036. The numbers of the zero columns (ABS) are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 8.595e+032. The numbers of the reprojections are 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 19 20 20 21 22 23 24 24 25 27 28 29 30 31 32 32 32 35 36 36 37 37 37 37 37 37. The numbers of the zero columns (ABS) are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 2 2 2 2 2 3 3 2 2 2 2 2 2 3 4 2 2 3 3 4 5 6 7 8.

The maxnorm of the residuals in case of the always reprojection is 4.513e+036.

Obviously, the best algorithm here is the S2ee without any reprojection.

11) S2ea



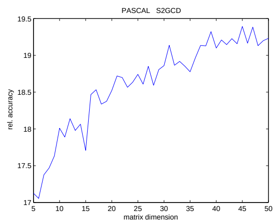
The maxnorm of the residuals in case of the no reprojection is 2.976e+019.

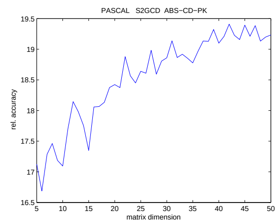
The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 4.865e+019. The numbers of the reprojections are 2 3 3 4 5 6 6 7 8 8 9 8 9 8 8 8 8 9 9 9 7 9 9 8 7 5 5 22 6 7 4 24 8 24 10 27 27 30 30 30 30 33 27 31 34 35. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 1 1 2 2 4 4 5 6 5 7 7 10 9 10 12 13 15 16 1 17 17 20 1 19 3 17 0 1 0 0 0 0 0 5 1 0 0.

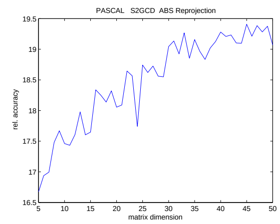
The maxnorm of the residuals in case of the always reprojections is 2.788e+019.

The best result is given by the without reprojections case.

12) S2GCD







The maxnorm of the residuals in case of the no reprojection is 9.357e+015.

The maxnorm of the residuals in case of the ABS-CD-PK reprojection is 4.157e+017. The numbers of the reprojections are 0 2 2 4 7 8 9 9 10 11 12 13 14 14 15 16 17 17 18 19 20 21 21 22 23 24 25 25 26 26 27 29 30 30 32 33 24 35 36 38 38 39 40 40 43 44. The numbers of the zero columns because of the ABS-CD-PK are 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10 0 0 0 0 0 0 0 0 0 0.

The maxnorm of the residuals in case of the always reprojections is 1.179e+016.

All three figures are more or less equal therefore the without any reprojection case is the cheapest algorithm with respect to the number of operations.

Conclusion

In the paper, we considered 22 cases to compute conjugate directions with the new idea of ”twice is enough” technique in the ABS class. All of them give acceptable accuracy with the residual of the considered linear system SPD between 500 and 510 dimensions. These were normal and not very difficult problems. 12 algorithms gave good results in the sense that linear dependency was not found neither in the case of the ABS-CD-PK nor in the always reprojection in the ABS methods. Therefore, for difficult problems like the Pascal matrix 12 algorithms remained. It is very important to underline that 6 cases from the 36 algorithms for Pascal problems had linear dependency according to the ABS algorithm. This phenomena underline that the introduced ABS-CD-PK algorithm has a stronger criteria for the linear dependency. On the other hand, we could also note that the linear dependency condition of the ABS class is correct, see [3]. It shows that we should further our investigations using other difficult problems, however, we cannot expect considerably better result than that of the solutions of the Pascal linear systems, because if we divide the norm of the residuals by the infimum norm of the Pascal matrix (dimension 50 is 5.0446e+028) we get very good values. Among the 36 cases of the Pascal figures there are 5 algorithms in 10 cases where the relative accuracy 14 at least and the P projection matrices are practically full (3 without reprojections, 2 with the ABS-CD-PK and 5 with the always reprojection).

It is important to note the difference between the algorithm pairs (S2HSsz, S2rsz), (S2a, S2asz) and (S2esz, S2LU) with the use of the idempotency property in the w_i vectors. The results show that the using it gives slightly better results, however, this is still an open question.

It is clear that this field of research is not closed with this paper, not even for the basic cases when the matrix A is symmetric positive definite. We did not considered here the Subclasses S6 and S7 which also give conjugate directions (see PART III of our paper). The algorithms of these Subclasses will be compared with the best algorithm used in this PART II of our series. We would like to further note that there are many known variants of the Lánczos and HS algorithms, see for example [4]. We will compare these variants too in a following paper and we deal with cases, when the coefficient matrix not symmetric positive definite as well.

Acknowledgement

I would like to thank my Ph.D. student, Szabolcs Blága for his valuable help in writing this paper.

References

[1] Abaffy, J., and Spedicato, E., "*ABS Projection Algorithms: Mathematical Techniques for Linear and Nonlinear Equations*", Ellis Horwood Limited, John Wiley and Sons, Chichester, England, (1989).

[2] Abaffy, J., "Reprojection of the conjugate directions in ABS classes Part I" Acta Polytechnica Hungarica, Vol 13 No. 3 pp. 7-24 (2016)

[3] Abaffy, J., Fodor, Sz., "Reorthogonalization methods in ABS classes, Acta Polytechnica Hungarica, Vol 12 No. 6 pp. 23-41 (2015)

[4] Broyden, C.G. and Vespucci, M.T. "*Krylov Solvers for Linear Algebraic Systems*", Elsevier, (2004) ISBN 0-444-51474-0

[5] Dennis, J.E. JR and Turner, K. :"Generalized Conjugate Directions", Linear Algebra and its Application Vol 88/89 pp.187-209 (1987)

[6] Hestenes, M.R. and Stiefel, E.: "Methods of Conjugate Gradients for Solving Linear Systems" J. Res.Natlr. Bur. Stand. Vol 49 pp. 409-436 (1952)

[7] Lánczos,C. "An Iteration Method for the residual of the Eigenvalue Problem of Linear Differential and Integral Operators", J. Res.Natlr. Bur. Stand. Vol 45 pp. 255-282 (1950)

[8] Lánczos,C. "Solution of systems of linear equations by minimized iterations", J. Res.Natlr. Bur. Stand. Vol 49 pp. 33-53 (1952)

[9] Parlett, B.N. "*The symmetric Eigenvalue Problem*", Englewood Cliffs, N. J. Prentice-Hall (1980)

[10] Zhang Liwei, Xia Zunquan and Feng Enmin, "*Introduction to ABS Methods in Optimization*", Dalian University of Technology Press, (in chinese) (1998)

Editor

Department of Management, Economics and Quantitative Methods
University of Bergamo
Via dei Caniana n° 2
24127 Bergamo
Italy
Tel. +39 35 2052538
Fax +39 35 2052549

The editorial office has complied with its obligations under Article 1, D.L.L. 31.8.1945, n. 660 and subsequent amendments

Printed 2017
University of Bergamo