Homework I
Iterative methods for sparse matrices

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1 Abstract

When solving $\|\mathbf{Ax}-\mathbf{b}\|$ for very large $\mathbf{A}$ the memory requirements do not allow it to let the `GMRES` algorithm iterate until convergence, as memory and computational cost increases with each step. Therefore a modified version of `GMRES` called restarted `GMRES(m)` has been proposed by Saad and Schultz in their original paper[1]. After a fixed amount of iterations `m` the algorithm is restarted using $\mathbf{x}_m$ as initial condition for the next run. This changed version avoids memory problems at the cost of convergence. One would expect that the larger m is chosen the better the convergence properties of the restarted would be. However this is not always the case. In this report this curious behavior will be investigated following the paper "The Tortoise and the Hare, Restart GMRES"[2] by Marc Embree.

2 Results

2.1 Experiments done in the paper

Embree considers two examples in his paper, the first one using

$$\mathbf{A} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} 2 \\ -4 \\ 1 \end{pmatrix}. \tag{1}$$

The second being

$$\mathbf{B} = \begin{pmatrix} 1 & 2 & -2 \\ 0 & 2 & 4 \\ 0 & 0 & 3 \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} 3 \\ 1 \\ 1 \end{pmatrix} \tag{2}$$

Using series expressions as provided in the paper the convergence plots for `GMRES(1)` and `GMRES(2)` have been computed, the results shown in figure 1 resemble plots one and three

[1] A Generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM J. Sci. Stat. Comput. Vol 7, No.3 1986

[2] SIAM Rev., 45(2), 259266. (8 pages) The Tortoise and the Hare Restart GMRES, Marc Embree, `http://epubs.siam.org/doi/abs/10.1137/S003614450139961`

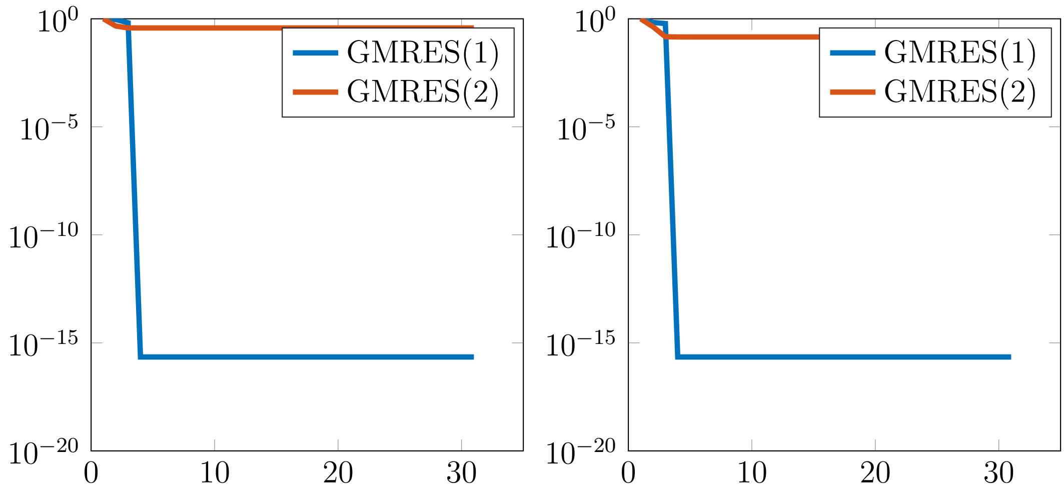

Figure 1: Convergence plot of GMRES(1) and GMRES(2). As seen in figure 1 and three of Embree's paper.

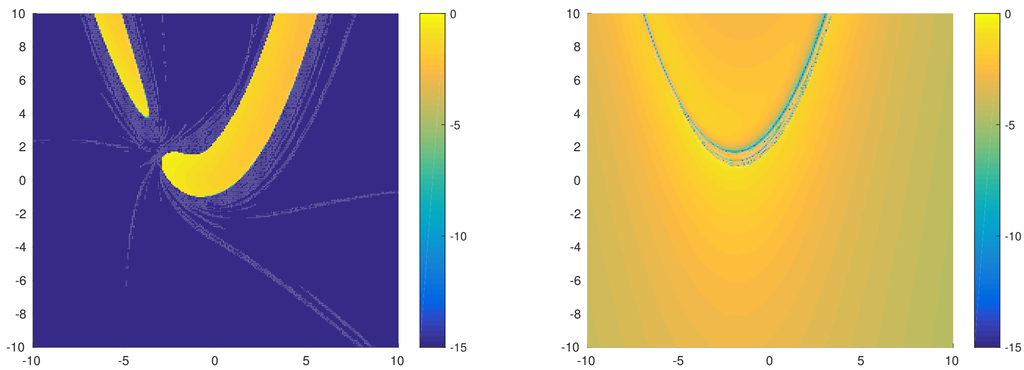

Figure 2: Plot as seen in the Embree paper GMRES(1)(left) and GMRES(2)(right) in figure two.

in the paper. However to truly understand the gravity of the phenomenon $\mathbf{b}$ has been replaced with

$$\mathbf{r_0} = \begin{pmatrix} \xi \\ \eta \\ 1 \end{pmatrix}. \tag{3}$$

If ξ and $\eta \in [-10, 10]$ the plots shown in figures 2 and 3. Can be computed, which are the same as figure 2 and 4, if the different coloring is neglected. These plots show the residual of the two schemes after 30 iterations on a logarithmic scale. Blue ares indicate convergence.

2.2 Additional experiments

If $A - 0.35 * \mathbf{I}$ is considered the condition number changes from $\kappa(\mathbf{A}) = 14.2950$ to $\kappa(\mathbf{A} - 0.35 * \mathbf{I}) = 39.1873$. At the same time the convergent area of `GMRES(1)` shown in figure 4, shrinks considerably in comparison to the plot 2. Additionally as the conditioning worsened the white foggy areas without convergence grew significantly.

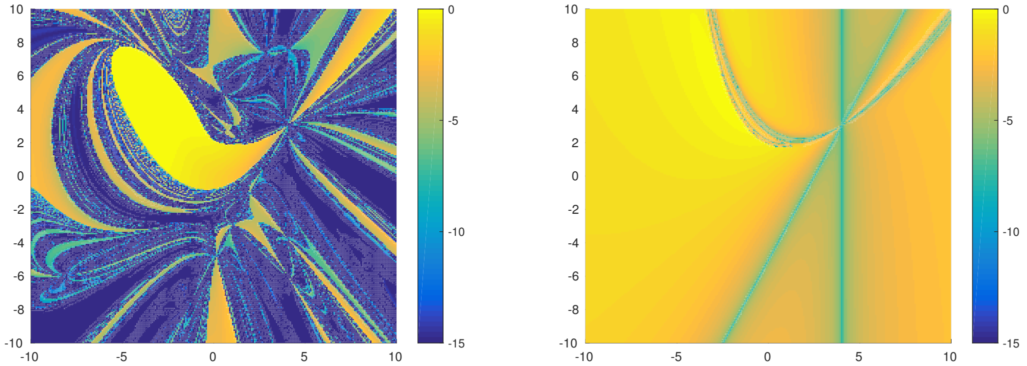

Figure 3: Plot as seen in the Embree paper for GMRES(1)(left) and GMRES(2)(right) in figure 4.

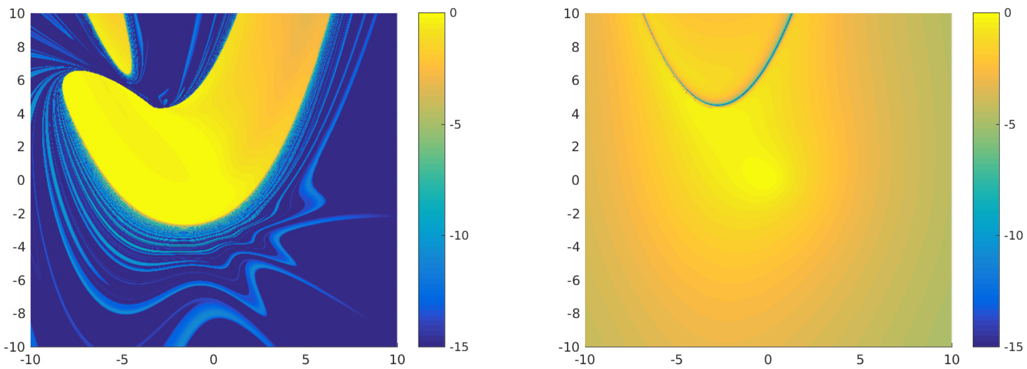

Figure 4: `GMRES(1)` and `GMRES(2)` convergence on $\mathbf{A} - 0.35 \cdot \mathbf{I}$.

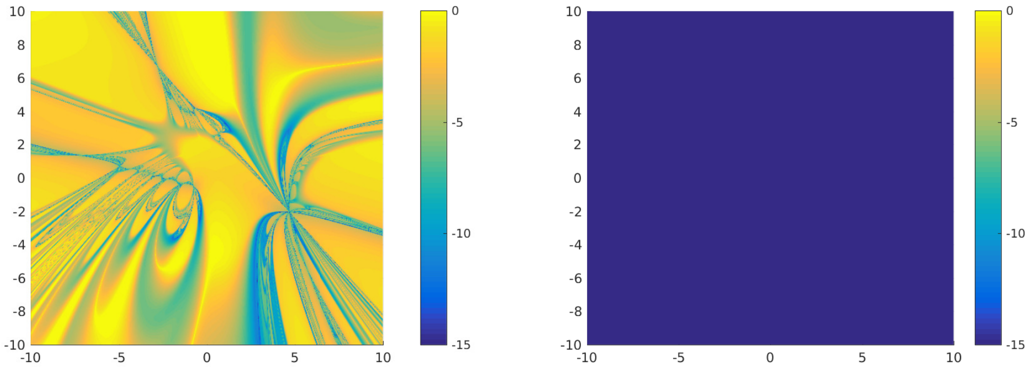

Figure 5: Convergence of `GMRES(1)` (left) and `GMRES(2)` (right) for the random matrix $\mathbf{R}$.

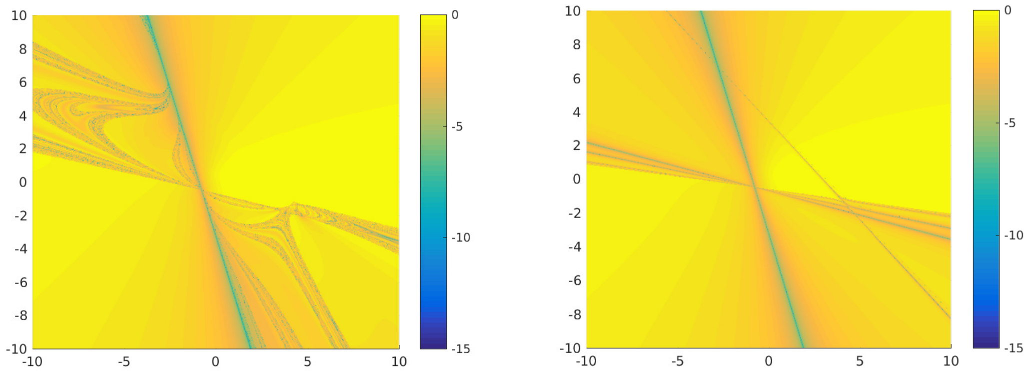

Figure 6: Convergence results for $\mathbf{R} + 2\mathbf{I}$

In a second series of experiments, designed to further investigate the effect of changed conditioning, $\mathbf{A}$ will be filled with entries drawn from the standart normal distribution ($\mu = 0$, $\sigma^2 = 1$). The values turned out to be:

$$\mathbf{R} = \begin{pmatrix} -0.3034 & 0.8884 & -0.8095 \\ 0.2939 & -1.1471 & -2.9443 \\ -0.7873 & -1.0689 & 1.4384 \end{pmatrix} \tag{4}$$

Results for `GMRES(1)` and `GMRES(2)`. Are shown in figure 5. Here it can be observed, that `GMRES(2)`, converges for all possible right hand sides $\mathbf{b}$, while `GMRES(1)` does not. This is probably the more common, but mathematically less interesting case. Often convergence improves significantly if the identity matrix is added to A. Unfortunately the condition number got worse by adding one multiple of the identity. It increased from $\kappa(\mathbf{R}) = 5.1025$ to $\kappa(\mathbf{R} + \mathbf{I}) = 32.4770$. Adding two dimes the identity matrix makes matters even worse as $\kappa(\mathbf{R} + 2\mathbf{I}) = 77.5446$, with results shown in figure 6. Finally adding three times the identity leads to $\kappa(\mathbf{R} + 3\mathbf{I}) = 6.4262$ and complete convergence for both algorithms figure 7. However the conditioning is still worse then it was originally, which indicates that conditioning alone can not be used to predict `GMRES(m)` convergence.

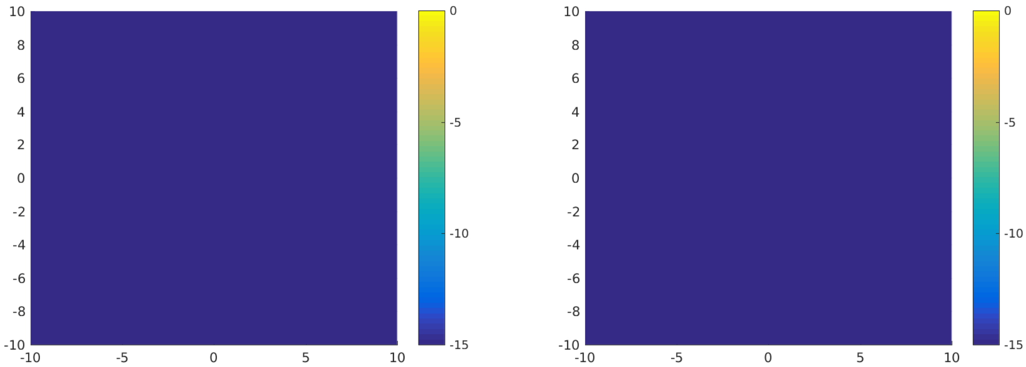

Figure 7: Convergence results for $\mathbf{R} + 3\mathbf{I}$

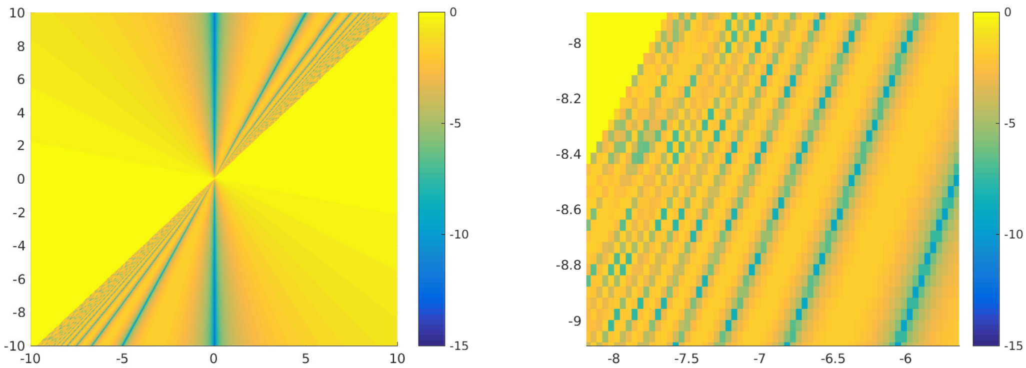

Figure 8: A plot of the convergence plain for the matrix proposed at the end of Embree's paper. With zoom on an interesting region.

2.3 Two-Dimensional case

At the end of the paper Embree proposes to take a closer look at:

$$\mathbf{C} = \begin{pmatrix} 1 & -2 \\ 0 & 1 \end{pmatrix} \tag{5}$$

This matrix displays similar noisy residuals in the bottom and top corners as where observed for `GMRES(1)` in figure 3.

3 Conclusion

In this report the results of Embree's paper "The Tortoise and the Hare, Restart GMRES "have been successfully reproduced. Just like in the tortoise the hare in the fairytale `GMRES(1)` is able to beat (`GMRES(2)`) if specific matrices are considered. As to why this is remains unknown. Additional experiments confirmed the link between `GMRES(m)` convergence and the conditioning of the problem that was already observed in the first report. However this report showed clearly that the initial condition plays a key role as well.