

M.Sc. Simulation Sciences, Summer Semester 2023

Fast Iterative Solvers

Project 1

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Introduction

For this project, we are utilizing Krylov subspace methods such as (preconditioned) GMRES and the Conjugate Gradient (CG) method to solve a linear system of equations, $Ax = b$. The matrix A is a real square matrix (symmetric positive definite for CG), and b is a predetermined vector. The project's precise instructions have been executed on MATLAB, and you can find the details in the sections below.

GMRES Method

Full GMRES method is implemented both with and without precondition. Left-preconditioning is applied for three different types of preconditioning, namely Jacobi, Gauss-Seidel and ILU(0). On a semi-log scale, Figure 1 displays the relative residual in relation to the iteration index.

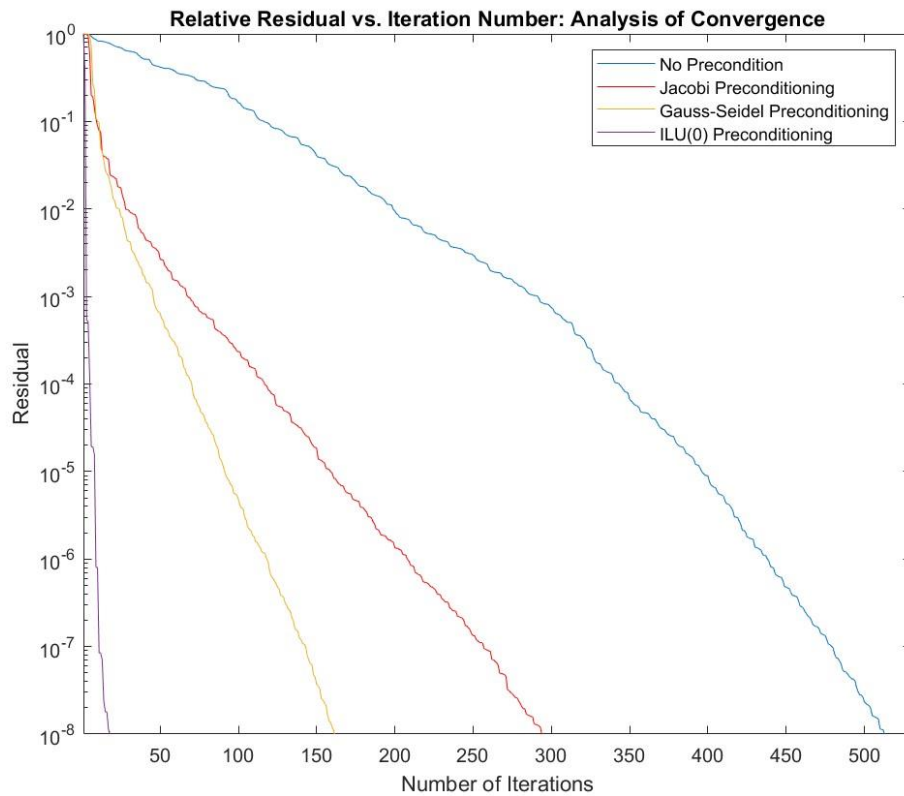


Figure 1: Relative Residual vs. Iteration Number: Analysis of Convergence

The generated number of Krylov vectors for each case is displayed in Table 1.

Table 1: Number of Krylov Vectors Generated for Each Preconditioning Condition

Preconditioning Types	Number of Krylov Vectors Generated
No Preconditioning	512
Jacobi	293
Gauss-Seidel	161
ILU(0)	17

The required number of Krylov has been mentioned earlier, and a restart parameter of 600 has been chosen for GMRES to function as Full GMRES. The computations were halted when the relative residual met the tolerance level, chosen as 10^{-8} , as depicted in Figure 1.

Table 2: Comparison of Runtimes

Without Restart	m=10	m=30	m=50	m=100	m=200
No Preconditioning	0.5507	0.5316	0.4960	0.4863	0.4822
Jacobi	0.1774	0.1737	0.1689	0.1631	0.1666
Gauss-Seidel	0.0924	0.0661	0.0645	0.0646	0.0636
ILU(0)	0.0200	0.0093	0.0106	0.0101	0.0098
With Restart					
No Preconditioning	0.0201	0.0253	0.0342	0.0980	0.1636
Jacobi	0.0202	0.0152	0.0247	0.0559	0.0830
Gauss-Seidel	0.0190	0.0182	0.0325	0.0314	0.0641
ILU(0)	0.0127	0.0100	0.0115	0.0105	0.0099

While full GMRES runs until the desired tolerance is achieved, restarted GMRES performs a fixed number of iterations (m) before restarting and leveraging previous computation results until the tolerance is met. Also, the results indicate that using restarted GMRES leads to reduced computation time compared to the full GMRES method. This improvement is attributed to the fact that restarted GMRES utilizes less memory by not storing all Krylov vectors.

Based on our observations, it appears that the restart method is faster than the full GMRES in all cases except for ILU(0). It seems that setting $m=30$ would be the optimal choice. However, using a low restart parameter may increase the run-time as we will be using fewer Krylov vectors, which require restarting computations every m iteration. On the other hand, this can significantly improve storage efficiency.

Figure 2 shows orthogonality of Krylov Vectors with respect to Iteration number. It appears that with every iteration, there is a decrease in orthogonality. This can be attributed to the presence of round-off errors during the computations of the Gram-Schmidt method.

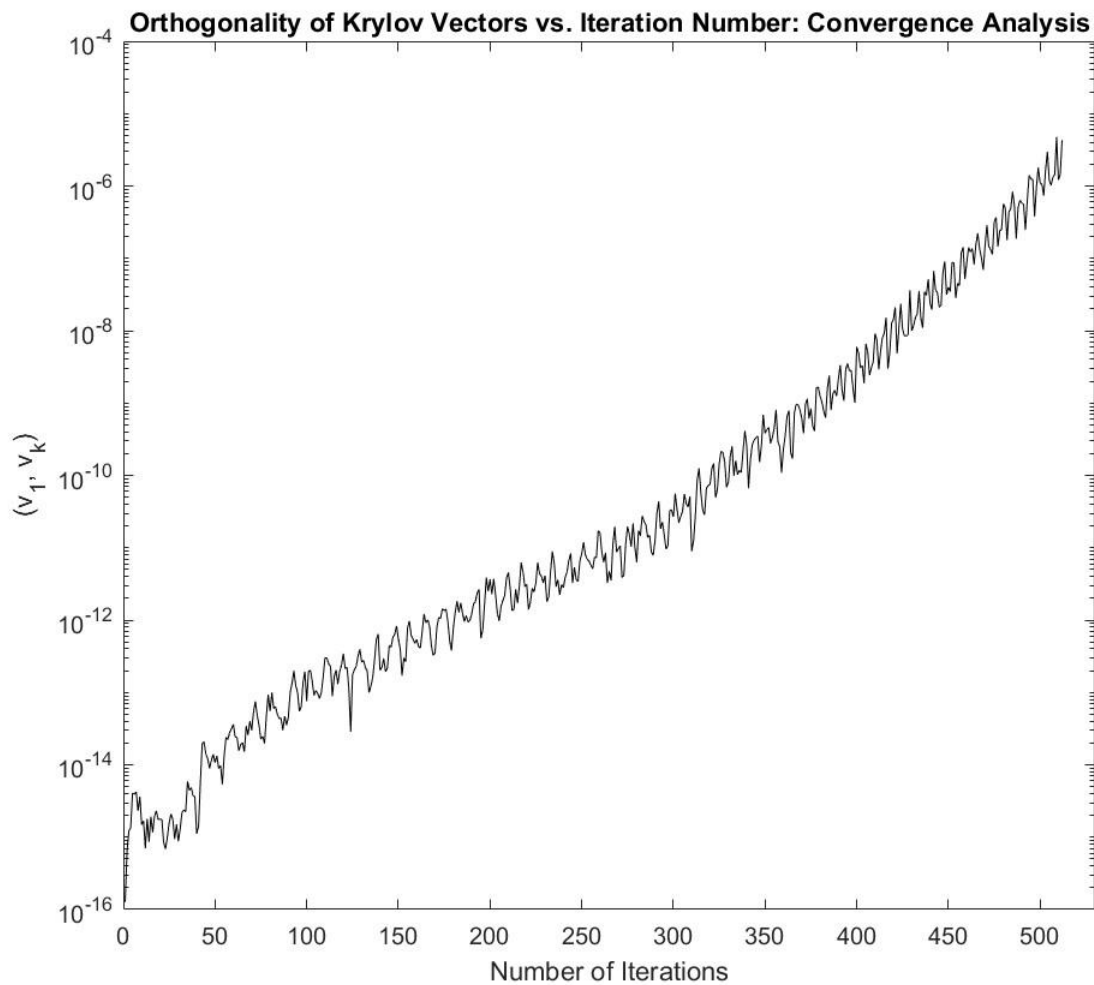


Figure 2: Orthogonality of Krylov Vectors vs. Iteration Number: Convergence Analysis

Solving sparse linear systems resulting from discretized PDEs is a complex task. Direct solvers often have quadratic complexity, which is dependent on geometry. Meanwhile, iterative solvers necessitate problem-dependent preconditioners to ensure efficiency and robustness. It is therefore anticipated that restarting GMRES will generally yield better results.

Conjugate Gradient

For Conjugate Gradient Method, we did not apply any preconditioning. Here, the differences between 2-norm and A-norm are analyzed. Figure 3 shows both of the norms with respect to the number of iterations.

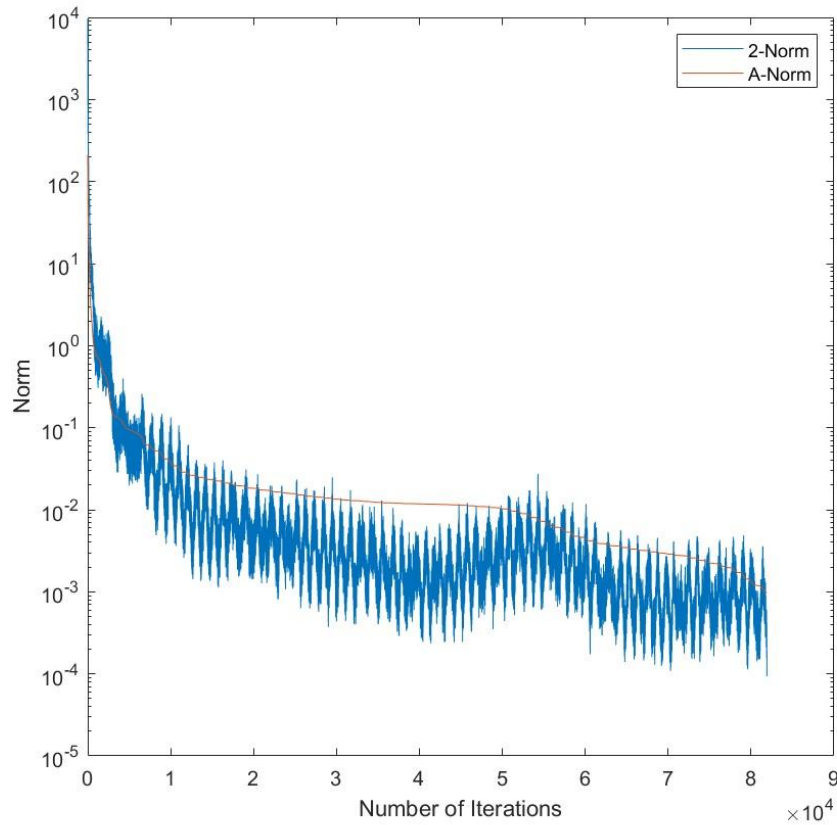


Figure 3: Norms wrt Iteration Numbers

The A-Norm, also known as the error norm, exhibits a monotonic decrease in each iteration of the conjugate gradient method. This behavior can be attributed to the fact that the A-Norm represents the improvement of numerical results as the method progresses. As each iteration of the conjugate gradient method is performed, the A-Norm decreases monotonically, indicating a reduction in the error or deviation from the desired solution.

When using the conjugate gradient method, the 2-Norm, which gauges the size of the solution vector, may display oscillations throughout the iterations. This occurs because the method looks for the solution in varied directions, without reversing previous steps. As a result, the 2-Norm may fluctuate as the process explores various avenues to minimize errors.

To summarize, the A-Norm consistently decreases as it indicates better numerical results and reduced errors. On the other hand, the 2-Norm may exhibit oscillatory patterns due to the conjugate gradient method's exploration of various directions without reversing prior actions.