M.Sc. Simulation Sciences, Summer Semester 2020

Fast Iterative Solvers

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Project 1

Due: June 19, 2020, 6pm

We use several iterative methods to solve linear systems of the type

$$A\mathbf{x} = \mathbf{b}.$$

where A is a real square matrix, and $\mathbf{b}$ is a given vector. Implement the following methods:

- (preconditioned) GMRES method
- Conjugate Gradient method

The goal is to gain some insight into the inner workings of each method, and also carry out a comparison.

Download the matrices

- `ORSIRR 1` (non-symmetric and indefinite)
- `s3rmt3m3` (symmetric positive definite)

from the `MatrixMarket` repository (`https://math.nist.gov/MatrixMarket/`). We use these matrices to test the algorithms. For all tests, you should use the following setup

- We *prescribe* the solution vector $\mathbf{x}^* = (1, 1, \dots, 1)$, and determine the corresponding right-hand side $\mathbf{b} = A\mathbf{x}^*$.
- Use the initial guess $\mathbf{x}_0 = \mathbf{0}$.
- A tolerance of $||\mathbf{r}_k||_2/||\mathbf{r}_0||_2 = 10^{-8}$ will be used to establish convergence[1]. This means, whenever the relative residual at the k^{th} iteration drops below this value, we consider the iteration to be converged. (Here $\mathbf{r}_0 := \mathbf{b} - A\mathbf{x}_0$ is the residual corresponding to the initial guess.)

Because we determine the right-hand-side $\mathbf{b}$ such that it corresponds to a known solution $\mathbf{x}^*$, we can compute the error $\mathbf{e}_k = \mathbf{x}_k - \mathbf{x}^*$, where k is the iteration number.

The two test matrices should be stored in `CSR` format. (Note: The Hessenberg matrix which you compute as part of the GMRES method can be stored in dense storage format.) More tips and hints will be provided for each method individually.

[1] For preconditioned GMRES this will be the "preconditioned" residual, $\mathbf{r}_k = M^{-1}(\mathbf{b} - A\mathbf{x}_k)$, where M is the preconditioner.

GMRES

The GMRES algorithm should be implemented in *restarted* formulation GMRES(m). In this way, full GMRES can be implemented simply by choosing the restart parameter large enough. Make sure you integrate the Givens rotations with the Gram-Schmidt procedure, as discussed in class.

Apply *left* pre-conditioning to the GMRES procedure. Implement two options:

1. Jacobi preconditioning
2. Gauss-Seidel preconditioning

You should test with the matrix `ORSIRR 1` from matrix market.

Conjugate Gradients

The conjugate gradient method should be implemented as discussed in class. You should test with the matrix `s3rmt3m3` from matrix market.

Points to investigate

- General remark: In the following, a plot in semi-log scale always means logarithmic y-axis (value to be plotted), and linear x-axis (usually iteration index, time, etc.)
- For all methods you should plot the relative residual against iteration index[2] on a semi-log scale.
- For the *full* GMRES method: How many Krylov vectors do you need to solve the problem with and without preconditioning? (Hint: should be less than 600 vectors even without preconditioning.)
- For the *restarted* GMRES method: In an effort to try and find a good restart parameter, try m=10, m=30, m=50, m=100, and compare the runtime for these runs to full GMRES. Is restarted faster than full GMRES for some, or all values of m? If yes, why do you think this is? (You may optionally do more fine-grained tests to find the 'best' restart parameter, but for the purposes of answering the question, a few tests are enough). What factors other than runtime may provide motivation to use restart, as opposed to full GMRES?
- For the preconditioned GMRES method: Compare the *true* absolute residual $\mathbf{r} := \mathbf{b} - A\mathbf{x}$ with the residual of preconditioned system. Does the *relative* residual reduction depend on which residual you monitor? (Why would one rather not monitor the true residual during the computation of the solution?)
- For full GMRES: check the orthogonality of the Krylov vectors! Plot the computed values of $(\mathbf{v}_1, \mathbf{v}_k)$ against k on a *semi-log* scale.
- For the conjugate gradient method: Plot both the error in A-norm, i.e. $||\mathbf{e}||_A = \sqrt{(A\mathbf{e}, \mathbf{e})}$, and the residual in standard 2-Norm, i.e. $||\mathbf{r}||_2 = \sqrt{(\mathbf{r}, \mathbf{r})}$ against the iteration index on a semi-log scale. Compare qualitatively the difference in convergence behavior. (i.e. the difference between the two norms). Is there an explanation for what you observe?

Report

You should write a short report that addresses all the points raised in the previous section.

[2]For the restarted GMRES method, this should be the cumulative iteration index.