M.Sc. Simulation Sciences, Summer Semester 2023

Fast Iterative Solvers

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Project 1

Due: June 6, 2023, 11.59pm

Overview

Implement the following Krylov subspace methods:

- (preconditioned) GMRES,
- the Conjugate Gradient (CG) method,

to solve a linear system

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

where A is a real square matrix (symmetric positive definite in the case of CG), and $\mathbf{b}$ is a given vector.

General Instructions

Download the matrices

- `gmres_test_msr` (non-symmetric and indefinite)
- `cg_test_msr` (symmetric positive definite)

from the project page on Moodle. These matrices are stored in *modified compressed sparse row* (MSR) format, as discussed in class. Some annotation to help read the files are provided along with the assignment. For all tests, you should use the following setup:

- Prescribe the solution vector $\mathbf{x} = (1, 1, \ldots, 1)$, and determine the corresponding right-hand side $\mathbf{b} = A\mathbf{x}$.
- Use the initial guess $\mathbf{x}_0 = \mathbf{0}$.
- Use a tolerance of $||\mathbf{r}_k||_2/||\mathbf{r}_0||_2 = 10^{-8}$ to establish convergence.[1] Whenever the relative residual drops below this value, we consider the iteration to be converged.

As we determine the right-hand-side $\mathbf{b}$ such that it corresponds to a known solution $\mathbf{x}$, we can also compute the error $\mathbf{e}_k = \mathbf{x}_k - \mathbf{x}$ at each iteration k.

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).

[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. For restarted GMRES, the iteration index k is the cumulative iteration index, i.e., the total number of Krylov vectors generated.

Specific Instructions

GMRES

- The GMRES algorithm should be implemented in *restarted* formulation GMRES(m). Full GMRES can be tested by choosing the restart parameter large enough. (For the present project, $m = 600$ will be enough.)
- The Hessenberg matrix which you compute as part of the GMRES method can be stored in dense storage format.
- Apply *left* pre-conditioning to the GMRES procedure. Implement the following options:
  1. Jacobi preconditioning;
  2. Gauss-Seidel preconditioning;
  3. ILU(0) preconditioning.
- For the full GMRES method (with and without preconditioning), plot the relative residual against iteration index on a semi-log scale. How many Krylov vectors do you need to solve the problem with and without preconditioning?
- In an effort to try and find a good restart parameter, try $m = 30$, $m = 50$, $m = 100$, and compare the runtime 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.) What factors, other than runtime, may provide motivation to use restarts, as opposed to full GMRES?
- For full GMRES (without preconditioning): 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.

CG

- The conjugate gradient method should be implemented as discussed in class. You don't have to implement preconditioning.
- Plot the error in A-norm, i.e., $||\mathbf{e}||_A = \sqrt{(A\mathbf{e}, \mathbf{e})}$, as well as the residual in standard 2-Norm, i.e., $||\mathbf{r}||_2 = \sqrt{(\mathbf{r}, \mathbf{r})}$, against iteration index on a semi-log scale.
- Compare qualitatively the difference in convergence between $||\mathbf{e}||_A$ and $||\mathbf{r}||_2$. Give an explanation for what you observe!

Report

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