M.Sc. Simulation Sciences, Summer Semester 2023

Fast Iterative Solvers

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Project 3

Due: September 12, 2023, 23.59pm

Summary

Implement a Lanczos method to approximate maximum eigenvalues of a s.p.d. matrix A, and compare to a pure power iteration. The methods were discussed in class. You should make sure to write an efficient implementation of both schemes.[1]

Step 1

Implement a power iteration.

- Test with the matrix `power_test_msr` (stored in MSR format), which can be found on the moodle page for project 3.
- Note that this matrix is symmetric positive definite
- Use the initial guess $\mathbf{x} = \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)^T$
- Stop the iteration when $|\lambda^{(k)} - \lambda^{(k-1)}| < 10^{-8}$
- report the approximation for the eigenvalue that you obtained
- Plot the convergence $|\lambda^{(k)} - \lambda^{(k-1)}|$ against iteration index k on a semilog scale (linear in k)

Step 2

Implement a Lanczos method to find the largest eigenvalue of the matrix `cg_test_msr` from the first project.

Note: As part of the Lanczos method you need to numerically compute the eigenvalues of the small triangular matrix that you generate as part of the algorithm. It is ok to use a power iteration to get the maximum eigenvalue of that matrix. However, you should use a lower tolerance, depending on the size of the Krylov space. (See below.)

Use the vector $\mathbf{x} = \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)^T$ as initial guess, where n is the dimension of the problem.

[1] In particular, it should be noted that the algorithms given in class are not necessarily meant to be copied verbatim. They were optimized for readability, not for efficiency. Here, the power iteration should take no more that one matrix-vector product per iteration.

We compare the maximum eigenvalue that we obtain with the maximum eigenvalue obtained from the pure power iteration (see step 1). For that purpose, you should re-run the power iteration with the matrix `cg_test_msr`. For timing (see below) you should run both the Lanczos method and the power iteration with the same compilation options, and possibly suppress output to make results as comparable as possible. You should also exclude the setup time, e.g. I/O operations, from the timing.

Instructions:

- For the pure power iteration, plot the error against both iteration index and runtime on a semi-log scale (linear in time)
- For the matrix `cg_test_msr`, the largest eigenvalue is $\lambda_1 = 9.5986080894852857E + 03$
- Run the Lanczos method for $m = 30, 50, 75, 100$, where m is the dimension of the Krylov space
- Use a power iteration to compute the maximum eigenvalue of the triangular Lanczos matrix.
- For the power iteration you can use a convergence criterion $|\theta^{(k)} - \theta^{(k-1)}| < tol$, where $\theta^{(k)}$ is the approximation to the maximum eigenvalue of the Lanczos matrix at iteration k. For the tolerance tol you can use 10^{-2} $(m = 30)$, 10^{-4} $(m = 50)$, 10^{-6} $(m = 75)$, 10^{-10} $(m = 100)$.
- You may optionally try to optimize the tolerances for the Lanczos method yourself.
- Record the final error and overall runtime for each m and generate a plot on a semi-log scale (linear in time). Compare to the pure power iteration.