M.Sc. Simulation Sciences, Summer Semester 2021

Fast Iterative Solvers

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Project 3

Due: September 14, 2021, 6pm

Summary

You will 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 `nos6.mtx`, which can be found in the `Matrix Market` repository
- 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 `s3rmt3m3.mtx`.

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.

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

[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.

with the matrix `s3rmt3m3.mtx`. Measure the execution time of both approaches. You should run both the Lanczos method and the power iteration with the same compilation options, and possibly suppress output for the timing runs 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 power method, plot the error against both iteration index and runtime
- (For the matrix `s3rmt3m3.mtx`, the largest eigenvalue is reported on the corresponding matrix-market website!)
- 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 plot the error against runtime. Compare to the power iteration.