Exercise 3: - a Report

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Introduction

The following is a report, discussing the results we obtained for the three tasks of exercise 1, as a part of the lecture 360.242 Numerical Simulation and Scientific Computing I.

Task 1: Benchmark Vector Triad 1

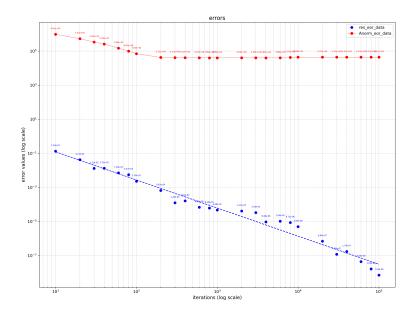


Figure 1: Plot $\frac{\|r_k\|_2}{\|r_0\|_2}$ and $\|e_k\|_A$ as a function of the iteration number for the matrix BCSSTK13 [1]

In the first task, we discuss our findings from two plotted errors as a function of iteration numbers of the conjugate gradients (CG) algorithm. The algorithm for iteratively solving Ax = b, where A should be symmetric positive definite. The input vector starts from an initial guess $x_0 = [0, ..., 0]$.

Algorithm 1 CG algorithm

- 1: $x_0 = 0$, $r_0 = b$, $p_0 = r_0$
- 2: **for** k = 1, 2, ... **do** 3: $\alpha_k = \frac{r_{k-1}^T r_{k-1}}{p_{k-1}^T A p_{k-1}}$ 4: $x_k = x_{k-1} + \alpha_k p_{k-1}$

- $r_{k} = r_{k-1} \alpha_{k} A p_{k-1}$ $\beta_{k} = \frac{r_{k}^{T} r_{k}}{r_{k-1}^{T} r_{k-1}}$ $p_{k} = r_{k} + \beta_{k} p_{k-1}$
- 7:
- 8: end for
- 9: return x_k

Residual: $r_0 = b - A \cdot 0$ is the residual of the initial not converged result. r_k is the residual of the approximation of the k-th iteration. Then $\frac{||r_k||_2}{||r_0||_2}$ is a metric of the approximation accuracy over k iterations. As shown in figure 1, the CG method reduces the metric almost linearly in the log-log scale. We can conclude that the CG method finds appropriate descent directions and moves x_k closer to the true result $x^* = [1, ..., 1]$ as expected.

A-norm error: The error on A-norm is defined by:

$$\|e_k\|_A = \|x^* - x_k\|_A = \sqrt{e_k^T A e_k}$$

 $e_k = x_k - x^*$ is the error between the approximation of the k-th iteration and the true result. $\sqrt{e_k^T A e_k}$ reflects the method's convergence in the Krylov subspace. The behavior of the convergence is shown in figure 1. The trend becomes stable when k > 200, which means the result converges since then. However, the error value is rather large because the metric incorporates elements from A.

References

 $[1] \quad BCSSTK13 \ matrix. \ {\tt https://math.nist.gov/MatrixMarket/data/Harwell-Boeing/bcsstruc1/bcsstk13.html}.$