Condition Number Estimation in a Solution Process of a Large and Sparse Linear System

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1 INTRODUCTION

A system of linear equations $A\boldsymbol{x} = \boldsymbol{b}$ having a large sparse coefficient matrix $A \in \mathbb{R}^{N\times N}$ often arises in a wide range of applications. In these applications, the Krylov subspace iterative methods such as the Conjugate Gradient (CG) method are typically used to solve the linear system. In the iterative method, we continuously refine an approximate solution vector until a given convergence criterion is satisfied. The relative residual norm is typically used for the criterion. Accordingly, we obtain an approximate solution vector, whose relative residual norm is less than a preset threshold. However, from application viewpoints, the (relative) error norm is more important than the residual norm, which more directly represents the accuracy of an approximate solution vector. Although it is difficult to calculate the relative error norm, it can be bounded by the product of the condition number of A and the relative residual norm. Consequently, if we can estimate the condition number of A in the iterative solution process, it can be useful to evaluate the error of the obtained (approximate) solution vector to the true solution.

2 RESEARCH PURPOSE AND METHOD

The purpose of the present research is to evaluate two condition number estimation methods in the following scenario. We solve a linear system with a large sparse symmetric positive-definite matrix using a (parallel) ICCG solver. In the solution process, we also calculate the largest and the smallest eigenvalues of the coefficient matrix to estimate the condition number.

One of the estimation methods is the Lanczos method, which gives the computation of both the largest and smallest eigenvalues. The other method is based on the error vector sampling (ES) [2], which can be used for finding the smallest eigenvalue. In this method, the largest eigenvalue is calculated by using the power method.

We conduct numerical tests and compare the above methods from the viewpoints of the accuracy of the obtained condition number and the additional computational time dedicated to the condition number estimation.

3 NUMERICAL RESULTS

We conducted a numerical test using 9 test matrices from the SuiteSparse Matrix Collection [1]. All matrices are real symmetric positive definite and have more than 500,000 dimensions. We used a computational node having two Intel Xeon Gold 6148 processors. We run our programs with 40 threads. The Localized IC preconditioning method was used for parallelization of the ICCG solver.

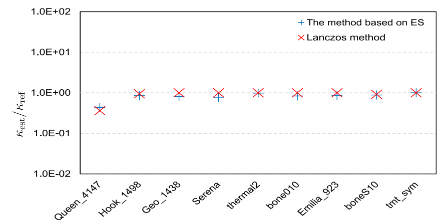

Figure 1: Evaluate the accuracy

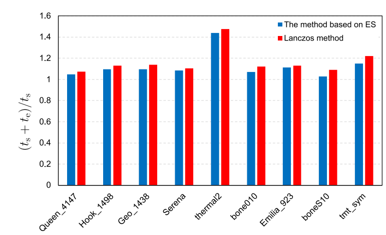

Figure 2: Evaluate the execution time

Figure 1 shows the ratio of the estimated condition number κ_{est} to its reference value κ_{ref}. To calculate the reference value, we used the inverse iteration and the power methods, which give accurate results but demand large computational cost. Figure 1 indicates that two methods (Lanczos and ES-based) are comparable in terms of the accuracy of the condition number estimation result. Figure 2 shows the ratio of $t_s + t_e$ to t_s, where t_s is the time for the solution process and t_e is the additional time for the condition number estimation. Figure 2 indicates that the ES-based method is slightly faster than the Lanczos method. However, for most of the test matrices, both methods could estimate the condition number in 10 - 20 % of the solution time. We conclude that both methods can be used for the condition number estimation with a solution process of a linear system.

REFERENCES

[1] Timothy A. Davis and Yifan Hu. 2011. The University of Florida Sparse Matrix Collection. *ACM Trans. Math. Software* 38, 1 (Dec. 2011), 1:1–1:25.

[2] Takeshi Iwashita, Kota Ikehara, Takeshi Fukaya, and Takeshi Mifune. 2023. Convergence acceleration of preconditioned conjugate gradient solver based on error vector sampling for a sequence of linear systems. *NLAA* (2023), e2512.