ON A WEIGHTED QUASI-RESIDUAL MINIMIZATION STRATEGY OF QMR FOR SOLVING COMPLEX SYMMETRIC SHIFTED LINEAR SYSTEMS

Tomohiro Sogabe, Shao-Liang Zhang
Department of Computational Science and Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464-8603, Japan
e-mail: {sogabe,zhang}@na.cse.nagoya-u.ac.jp

Keywords: shifted linear systems, complex symmetric matrices, QMR

Abstract

We consider the solutions of complex symmetric shifted linear systems of the form

$$(A + \sigma_k I)\boldsymbol{x}^{(k)} = \boldsymbol{b}, \quad k = 1, 2, \ldots, m, \tag{1}$$

where $A + \sigma_k I$ is a nonsingular n-by-n complex symmetric matrix with scalar shifts $\sigma_k \in C$, and $\boldsymbol{x}^{(k)}, \boldsymbol{b}$ are complex vectors of length n. The systems (1) arise in large-scale electronic structure calculation, e.g. [3], and there is a strong need for the fast solutions of the systems.

In this talk, to solve the systems (1) efficiently, we will derive an iterative method (referred to as shifted QMR_SYM) from the combination of the two important results given in [1, 2]. Since we found that the most time consuming part of shifted QMR_SYM was to update approximate solutions when the number of systems m in (1) was large enough, we will present a weighted quasi-residual minimization strategy of shifted QMR_SYM and give a specific weight such that it reduces the computational cost of recurrence formulas for updating approximate solutions. To show the efficiency of the present strategy, we will report the results of some numerical experiments.

References

[1] R. W. Freund, *Conjugate gradient-type methods for linear systems with complex symmetric coefficient matrices*, SIAM J. Sci. Stat. Comput., 13 (1992), pp. 425–448.

[2] R. W. Freund, *Solution of shifted linear systems by quasi-minimal residual iterations, Numerical Linear Algebra*, L. Reichel, A. Ruttan and R. S. Varga eds., W. de Gruyter, (1993), pp. 101–121.

[3] R. Takayama, T. Hoshi, T. Sogabe, S.-L. Zhang, and T. Fujiwara, *Linear algebraic calculation of Green's function for large-scale electronic structure theory*, Phys. Rev. B 73, 165108 (2006), pp. 1–9.