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An Investigation of Restarted GMRES Method by Using Flexible Starting Vectors†

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Abstract. We discuss a variant of restarted GMRES method that allows changes of the restarting vector at each cycle of iterations. The merit of the variant is that previously generated information can be utilized to select a new starting vector, such that the occurrence of stagnation be mitigated or the convergence be accelerated. The more appealing utilization of the new method is in conjunction with a harmonic Ritz vector as the starting vector, which is discussed in detail. Numerical experiments are carried out to demonstrate that the proposed procedure can effectively mitigate the occurrence of stagnation due to the presence of small eigenvalues in modulus.

AMS subject classifications: 65F10, 65F15

Key words: Linear systems of equations, Arnoldi process, GMRES, harmonic Ritz vector.

1. Introduction

In this paper, we consider the solution of large sparse linear systems of equations

$$Ax = b, \tag{1.1}$$

where A is an $n \times n$ nonsingular matrix, b is an n dimensional vector. Krylov subspace methods are particularly appealing for this kind of problems and they are widely investigated, see, e.g., [10, 16, 17, 21, 24]. We refer to [22] for a recent survey.

For nonsymmetric matrix A, the GMRES method proposed by Y. Saad and M. H. Schultz [17] is one of the most popular choices. The GMRES method is an iterative method in nature, it generates a sequence of approximations converging to the exact solution to (1.1),

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and the approximations have the property of minimizing the 2-norm of the residual vector over the Krylov subspace involved. However, the optimality of the GMRES comes at a cost. As the computational costs and storage requirements are prohibitive, so the full GMRES is limited for practical applications, the restarted version of the algorithm is proposed in [17]. The idea is that the GMRES method is restarted after fixed number of iterations, say m ($\ll n$ usually), the resulting restarted version algorithm is denoted by GMRES(m). However, since GMRES(m) only keeps the current approximate solution as the new initial guess for the next cycle (the next m iterations), restarting would lose most information obtained from the previous cycle of the iteration and the convergence may slow down and even stagnation occurs. Stagnation means that there is little decrease in the residual norm at the end of a restart cycle, which is often encountered in the GMRES(m), especially in the case that m is small though there are exceptions [8]. In this paper, the occurrence of the stagnation is studied in restarted GMRES method, the result reveals that stagnation of restarted GMRES method occurs if and only if the first row of $\tilde{H}_m$, the projection matrix of the coefficient matrix A in Krylov subspace, is zero.

Techniques for reducing the negative effect of restarting have been investigated in [13, 14, 19]. These methods aim to recovering the superlinear convergence behavior of full GMRES (see, e.g., [21]) by retaining some eigenvector information generated in the former cycle of iterations. M. Eiermann et al. [7] provided an overview of the augmentation strategies and some comparisons are done with some preconditioning approaches [4, 9]. Generalizations of augmenting procedures that aim to retaining information other than approximate subspace are investigated in [2, 5]. Some other equivalent formulations and variants of restarted GMRES method have been proposed in [1, 18, 20, 26]. All these methods take the residual vector at the end of each restart cycle as the starting vector at the new cycle of iterations, continuing the process until convergence. In this paper, after analysis of convergence behavior including stagnation of restarted GMRES algorithm, we present a variant of GMRES(m) that allows change of the restarting vector at every cycle of the iterative process. The flexibility of choosing the starting vector of the new method provides us a frame work of using inner-outer iterations, in which other iterative methods can be used to get the next starting vector. A simple strategy of taking the harmonic vector associated with the smallest harmonic Ritz value as the starting vector is discussed in details. Numerical experiments are done to compare the variant of GMRES(m) combining with this strategy with the original GMRES(m) and show the former superiority.

In Section 2, we give a brief review of restarted GMRES and an analysis of convergence behavior including stagnation of GMRES(m). In Section 3, we present a variant of restarted GMRES and a simple strategy of choosing the restarting vector. Some numerical results are reported in Section 4. The last section gives a brief concluding remarks.

Throughout the paper, by f^* we denote the conjugate transpose of vector f, by $\mathscr{R}^m$ the m-dimensional complex space and by e_j the jth column of the unit matrix whose order is determined from the context. The Euclidean inner product $\langle x, y\rangle = y^*x$ is used and norm $\|\cdot\|$ denotes both the Euclidean vector norm and the subordinate spectral matrix norm.