MGMRES: A Generalization of GMRES for Solving Large Sparse Nonsymmetric Linear Systems

by

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We are concerned with the solution of the linear system (1): $Au = b$, where A is a real square nonsingular matrix which is large, sparse and nonsymmetric. We consider the use of Krylov subspace methods. We first choose an initial approximation $u^{(0)}$ to the solution $\bar{u} = A^{-1}b$ of (1). We also choose an auxiliary matrix Z which is nonsingular. For $n = 1, 2, \ldots$ we determine $u^{(n)}$ such that $u^{(n)} - u^{(0)} \epsilon K_n(r^{(0)}, A)$ where $K_n(r^{(0)}, A)$ is the (Krylov) subspace spanned by the Krylov vectors $r^{(0)}, Ar^{(0)}, \ldots, A^{n-1}r^{(0)}$ and where $r^{(0)} = b - Au^{(0)}$. If ZA is SPD we also require that $(u^{(n)} - \bar{u}, ZA(u^{(n)} - \bar{u}))$ be minimized. If, on the other hand, ZA is not SPD, then we require that the Galerkin condition, $(Zr^{(n)}, v) = 0$, be satisfied for all $v \epsilon K_n(r^{(0)}, A)$, where $r^{(n)} = b - Au^{(n)}$.

With the GMRES method, which was developed by Saad and Schultz [1986], and which has for many years been used extensively for solving large sparse nonsymmetric systems one lets $Z = A^T$. One generates a set of mutually orthogonal vectors $w^{(0)}, w^{(1)}, \ldots w^{(n)}$ such that $w^{(0)} = r^{(0)}$ and such that $Sp(w^{(0)}, w^{(1)}, \ldots, w^{(k-1)}) = K_k(r^{(0)}, A)$ for $k = 0, 1, 2, \ldots, n$. To do this, for each k we let $w^{(k)}$ be a linear combination of $Aw^{(k-1)}, w^{(k-1)}, \ldots, w^{(0)}$. Next, for each n we choose $c_o^{(n)}, c_1^{(n)}, \ldots, c_{n-1}^{(n)}$ so that $u^{(n)} = u^{(0)} + c_o^{(n)} w^{(0)} + \ldots + c_{n-1}^{(n)} w^{(n-1)}$ and so that $(r^{(n)}, r^{(n)})$ is minimized. The $c_i^{(n)}$ are determined by solving a related system of linear equations in the least squares sense. This is done in a stable manner using Givens rotations.

In this paper we consider a generalization of GMRES. This generalized method, which we refer to as "MGMRES", is very similar to GMRES except that we let $Z = A^T Y$ where Y is a nonsingular matrix which is symmetric but not necessarily SPD. We require that the $w^{(i)}$ be mutually orthogonal

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with respect to Y. Of course if Y is not SPD it is possible that the process of generating the $w^{(i)}$ may break down. Also, unless Y is SPD we must replace the minimization condition on $(r^{(n)}, r^{(n)})$ by a Galerkin condition which requires that $(Zr^{(n)}, w^{(i)}) = 0$ for $i = 0, 1, \ldots, n-1$. The determination of the coefficients $c_i^{(n)}$ can be carried out using Givens rotations, as in the case of GMRES, though the overall procedure is somewhat more complicated. It can, however be shown that, for given n^* and $u^{(0)}$, one can uniquely determine $u^{(1)}, u^{(2)}, \ldots, u^{(n*)}$ provided that the process of computing $w^{(0)}, w^{(1)}, \ldots, w^{(n^*-1)}$ does not break down and provided that for $n = 1, 2, \ldots, n^*$ there actually exists a unique vector $u^{(n)}$ such that $u^{(n)} - u^{(0)} \varepsilon K_n(r^{(0)}, A)$ and such that the Galerkin condition is satisfied.

The MGMRES algorithm is considerably simplified if YA as well as Y is symmetric. Under this assumption one can determine $w^{(n)}$ in terms of $w^{(n-1)}$ and $w^{(n-2)}$ instead of in terms of $w^{(n-1)}, w^{(n-2)}, \ldots, w^{(0)}$ as would be required in the general case. The determination of the coefficients $c_i^{(n)}$ which are involved in the Galerkin condition is also considerably simplified. An example of a case where Y and YA are symmetric is the "double system" which corresponds to the Lanczos method for solving (1). Thus given the linear system (1) one can consider the double system $\{A\}\{u\} = \{b\}$ where for some $\tilde{b}$ and $\tilde{u}$ we have

$$\{A\} = \begin{pmatrix} A & 0 \\ 0 & A^T \end{pmatrix}, u = \begin{pmatrix} u \\ \tilde{u} \end{pmatrix}, b = \begin{pmatrix} b \\ \tilde{b} \end{pmatrix} \tag{1}$$

We also choose

$$\{Y\} = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \tag{2}$$

Evidently $\{Y\}$ and $\{Y\}\{A\}$ are symmetric. The application of MGMRES with $Y = \{Y\}$ to the double system yields the "LANGMRES" method given by Young and Chen [1994].

An important feature of the GMRES algorithm is that one can determine $(r^{(n)}, r^{(n)})$ for a given n and test for convergence without actually carrying out the complete GMRES process to determine $u^{(n)}$. Thus, one can compute $(r^{(n)}, r^{(n)})$ for each iteration and only actually compute $u^{(n)}$ when $(r^{(n)}, r^{(n)})$ is smaller than a prescribed tolerance level. We describe a similar procedure for MGMRES. For each n we first compute the residual $\bar{r}^{(n)}$ for ORTHORES

(Y) by determining the scaling factor c_n such that $\tilde{r}^{(n)} = c_n w^{(n)}$. The residual $r^{(n)}$ for MGMRES can be determined from $\tilde{r}^{(n)}$ by a short series of elementary vector operations. No matrix-vector operations or inner products are required to get $r^{(n)}$.

References

[1] Saad, Youcef and Schultz, Martin H. [1986], "GMRES, A Generalized Minimum Residual Algorithm for Solving Non Symmetric Linear Systems", *SIAM J. Sci. Stat. Comput.* **7**, 856-869.

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