

AN ALGORITHM FOR SYMMETRIC INDEFINITE SYSTEMS OF LINEAR EQUATIONS

SUCHEOL YI

Abstract

It is shown that a new Krylov subspace method for solving symmetric indefinite systems of linear equations can be obtained. We call the method as the projection method in this paper. The residual vector of the projection method is maintained at each iteration, which may be useful in some applications.

1. Introduction. The k th Krylov subspace $K_k(r_0, A)$ generated by an initial residual vector $r_0 = b - Ax_0$ and A is defined by

$$(1) \quad K_k(r_0, A) \equiv \text{span}\{r_0, Ar_0, \dots, A^{k-1}r_0\}.$$

Iterative methods that choose corrections from the space $K_k(r_0, A)$ at each iteration are called Krylov subspace methods. The GMRES method [7] is a Krylov subspace method for solving systems of linear equations

$$(2) \quad Ax = b, \quad \text{where } A \in R^{n \times n} \text{ is nonsingular.}$$

The k th iterate of GMRES can be characterized as $x_k = x_0 + z_k$ for a given initial guess $x_0 \in R^n$ and the correction z_k is chosen to minimize the norm of the residual vector $r(z) = r_0 - Az$ over the k th Krylov subspace $K_k(r_0, A)$ at each iteration, i.e.,

$$(3) \quad \|r_0 - Az_k\|_2 = \min_{z \in K_k(r_0, A)} \|r_0 - Az\|_2.$$

If the Arnoldi process is applied with $v_1 = Ar_0/\|Ar_0\|_2$ to generate a basis for the Krylov subspace $K_k(r_0, A)$, simpler GMRES implementations of Walker and Zhou [8] are obtained and the Arnoldi process is summarized as follows:

Algorithm 1.1 Arnoldi process

Initialize: Choose an initial guess v_1 with $\|v_1\|_2 = 1$.

Iterate: For $k = 1, 2, \dots$, do:

$$h_{i,k} = v_i^T Av_k, \quad i = 1, 2, \dots, k,$$

$$\tilde{v}_{k+1} = Av_k - \sum_{i=1}^k h_{i,k} v_i.$$

Set $h_{k+1,k} = \|\tilde{v}_{k+1}\|_2$.

If $h_{k+1,k} = 0$, stop; otherwise,

$$v_{k+1} = \tilde{v}_{k+1}/h_{k+1,k}.$$

Key words: GMRES, MINRES, SYMMLQ, symmetric QMR, and Krylov subspace method.
AMS subject classification. 65F10

Without loss of generality we may assume the initial residual vector is nonzero. The initial Arnoldi vector $v_1 = Ar_0/\|Ar_0\|_2$ is then well-defined, since A is a nonsingular matrix. Setting $\rho_{1,1} = \|Ar_0\|_2$ gives the equation

$$(4) \quad Ar_0 = \rho_{1,1}v_1,$$

and the following equation is satisfied by the Arnoldi process:

$$(5) \quad Av_{k-1} = \sum_{i=1}^k \rho_{i,k}v_i \text{ for unique } \rho_{i,k} \text{ s with } \rho_{k,k} > 0 \text{ for } k > 1.$$

From the equations (4) and (5) we have the following relation:

$$(6) \quad AU_k = V_kR_k,$$

where $U_k = (r_0, v_1, \dots, v_{k-1})$, $V_k = (v_1, \dots, v_k)$, and

$$R_k = \begin{pmatrix} \rho_{1,1} & \cdots & \rho_{1,k} \\ & \ddots & \vdots \\ & & \rho_{k,k} \end{pmatrix}.$$

Then the relation (6) reduces the least-squares problem (3) directly to an upper triangular least-squares problem by decomposing the initial residual vector r_0 as $r_0 = \Pi_k^\perp r_0 + V_kV_k^T r_0$ for each k , where Π_k^\perp is the orthogonal projection onto the orthogonal complement of the space $K_k(v_1, A)$.

We introduce another approach to Krylov subspace methods for solving symmetric indefinite linear systems, which is called the projection method in this paper. The projection method is closely related to the simpler GMRES method in that the projection and simpler GMRES methods use the same initial basis vector $v_1 = Ar_0/\|Ar_0\|_2$ in applying the symmetric Lanczos and Arnoldi processes, respectively, and, in the symmetric case, the projection method can be derived from the simpler GMRES method by finding a search direction p_k such that $Ap_k = v_k$ for each k . Both simpler GMRES and the projection method maintain orthonormal bases of the space $AK_k(r_0, A)$, which permit residual minimization through projection of the residual onto $AK_k(r_0, A)^\perp$. With simpler GMRES, the k th approximate solution is obtained by solving a $k \times k$ upper triangular system. This is also done with the projection method, but only implicitly. Because the projection method is based on the short recurrence symmetric Lanczos process, the triangular system is tridiagonal and, therefore, one can update the approximate solution using a three-term short recurrence formula. In contrast to simpler GMRES, the usual GMRES implementation maintains an orthonormal basis of $K_k(r_0, A)$ through the Arnoldi process, and, consequently, achieves residual minimization through the solution of an upper Hessenberg least-squares problem. MINRES [6] can be viewed as a specialization of the usual GMRES approach to the symmetric case, in which the short recurrence symmetric Lanczos process is used to generate an orthonormal basis of $K_k(r_0, A)$. The upper Hessenberg system is tridiagonal, and so

solution of the upper Hessenberg least-squares problem is done implicitly in MINRES by implementing a three-term short recurrence formula for updating the approximate solution. In the symmetric indefinite case without preconditioning, symmetric QMR [2] is obtained using the same approach as MINRES. However, in solving the systems of the preconditioned system

$$(7) \quad A'x' = b', \quad \text{where } A' = M_1^{-1}AM_2^{-1}, \quad x' = M_2x, \quad \text{and } b' = M_1^{-1}b,$$

symmetric QMR is implemented by solving a quasi-minimization problem. Thus the approach of the projection method is similar to that of simpler GMRES, while standard GMRES, MINRES, and symmetric QMR follow an alternative approach. In section 2, we give a derivation of the projection method and also present the results of numerical experiments in section 3.

2. A derivation of the projection method. By applying the Arnoldi process starting with $v_1 = Ar_0/\|Ar_0\|_2$ we can have a set $\{v_1, \dots, v_k\}$ of orthonormal basis vectors of the space $K_k(v_1, A)$. Suppose we have a vector p_k such that $Ap_k = v_k$ for each k . Then the k th residual vector r_k in the simpler GMRES method is

$$(8) \quad \begin{aligned} r_k &= r_{k-1} - (r_{k-1}^T v_k) v_k \\ &= r_0 - Az_{k-1} - (r_{k-1}^T v_k) Ap_k \\ &= r_0 - A[z_{k-1} + (r_{k-1}^T v_k) p_k]. \end{aligned}$$

By the last expression in equation (8) it is natural to define the k th iterate x_k of the projection method as $x_k = x_{k-1} + (r_{k-1}^T v_k) p_k$. Setting $P_k = (p_1, \dots, p_k)$ and $V_k = (v_1, \dots, v_k)$ we need to have $AP_k = V_k$ by the requirement of $Ap_k = v_k$ for each k . By the relation $AU_k = V_k R_k$ in (6), the equation $AP_k = V_k$ is equivalent to

$$(9) \quad U_k = P_k R_k.$$

The search direction p_k is then defined as

$$p_k = \begin{cases} r_0/\rho_{1,1} & \text{if } k = 1 \\ \frac{1}{\rho_{k,k}}(v_{k-1} - \rho_{1,k}p_1 - \dots - \rho_{k-1,k}p_{k-1}) & \text{if } k > 1. \end{cases}$$

Then we have a long recursion formula to generate p_k in general.

If A is symmetric, then an orthonormal basis $\{v_1, \dots, v_k\}$ of the space $K_k(v_1, A)$ can be generated by the symmetric Lanczos process. Then the upper triangular matrix R_k in (6) can be reduced to the form of

$$\begin{pmatrix} \rho_{1,1} & \rho_{1,2} & \rho_{1,3} & 0 & \cdots & 0 \\ 0 & \rho_{2,2} & \rho_{2,3} & \rho_{2,4} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \rho_{k-2,k} \\ \vdots & & & \ddots & \ddots & \rho_{k-1,k} \\ 0 & \dots & \dots & \dots & 0 & \rho_{k,k} \end{pmatrix}.$$

Therefore, we have a short recursion formula for p_k by (9), i.e.,

$$p_k = \frac{1}{\rho_{k,k}}(v_{k-1} - \rho_{k-1,k}p_{k-1} - \rho_{k-2,k}p_{k-2}) \quad \text{for } k > 1,$$

where $\rho_{k-2,k} = v_{k-2}^T A v_{k-1}$, $\rho_{k-1,k} = v_{k-1}^T A v_{k-1}$, $\rho_{k,k} = \|\tilde{v}_k\|_2$, and $\tilde{v}_k = A v_{k-1} - \rho_{k-1,k}v_{k-1} - \rho_{k-2,k}v_{k-2}$.

Note that we may wish to apply the projection method for solving nonsymmetric linear systems using the nonsymmetric Lanczos process to get a short recursion formula for a search direction p_k . However, we found that the projection method with the nonsymmetric Lanczos process is very unstable for solving nonsymmetric linear systems. Therefore, we consider only symmetric indefinite systems in this paper. It is known that there exists a symmetric positive definite matrix S such that $M = S^2$ for a given symmetric positive definite matrix M . Therefore, the MINRES, SYMMLQ, and projection methods can be applied to the following system:

$$(10) \quad \tilde{A}\tilde{x} = \tilde{b}, \quad \text{where } \tilde{A} = S^{-1}AS^{-1}, \quad \tilde{x} = Sx, \quad \text{and } \tilde{b} = S^{-1}b.$$

With symmetric positive definite preconditioners M , the projection method for a symmetric matrix A can be summarized as follows:

Algorithm 2.1 Projection method (symmetric A)

Initialize: Choose x_0 and set $r_0 = b - Ax_0$,
 $z = M^{-1}r_0$, $u_1 = Az$, $w_1 = M^{-1}u_1$, and $\alpha_1 = \sqrt{u_1^T w_1}$.
 Update $u_1 \leftarrow u_1/\alpha_1$ and $w_1 \leftarrow w_1/\alpha_1$.
 Compute $\beta_1 = r_0^T w_1$.
 Set $r_1 = r_0 - \beta_1 u_1$, $p_1 = z/\alpha_1$, and set $x_1 = x_0 + \beta_1 p_1$.
 Iterate: For $k = 2, 3, \dots$, do:
 Set $u_k = A w_{k-1}$.
 For $i = \max\{k-2, 1\}, \dots, k-1$, do:
 Set $\bar{\alpha}_i = u_k^T w_i$.
 Update $u_k \leftarrow u_k - \bar{\alpha}_i w_i$.
 Set $w_k = M^{-1}u_k$ and $\alpha_k = \sqrt{u_k^T w_k}$.
 Update $u_k \leftarrow u_k/\alpha_k$ and $w_k \leftarrow w_k/\alpha_k$.
 Compute $\beta_k = r_{k-1}^T w_k$ and set $r_k = r_{k-1} - \beta_k w_k$.
 Set $p_k = \frac{1}{\alpha_k} \left(w_{k-1} - \sum_{i=\max\{k-2, 1\}}^{k-1} \bar{\alpha}_i w_i \right)$ and set
 $x_k = x_{k-1} + \beta_k p_k$.

3. Numerical Experiments. We present numerical experiments that show the performance of the Krylov subspace methods for symmetric indefinite systems discussed in the previous sections. In our experiments, we also include the SYMMLQ method [6] for solving symmetric indefinite linear systems. Basically, the k th iterate x_k of SYMMLQ can be obtained by orthogonalizing the residual vector $r(z) = r_0 - Az$ against $K_k(r_0, A)$, whereas that of MINRES is obtained by minimizing the residual vector

over the space $K_k(r_0, A)$ for each k . For a symmetric positive definite preconditioner M , it can be shown that algorithms for the SYMMLQ, MINRES, symmetric QMR, and projection method can be implemented with only one matrix-vector multiplication with A and one preconditioner-vector solve with M at each iteration if $M_1^T = M_2$ in implementing symmetric QMR. However, in implementing a preconditioner-vector solve of the form $Mw = r$, factorizing the preconditioner M first, i.e., $M = M_1M_2$, we may save floating-point operations by solving two preconditioning solves of the form $M_1u = r$ and $M_2w = u$ instead of performing a preconditioner-vector solve with M . Besides matrix-vector multiplication with A , two M_1 and M_2 preconditioning solves or one preconditioner-vector solve with M , algorithms for the symmetric QMR, MINRES, SYMMLQ, and projection methods use approximately $7n$, $10n$, $11n$, and $12n$ multiplications and divisions, respectively.

We use a discretization of

$$\begin{aligned}\Delta u + cu &= f \quad \text{in } D, \\ u &= 0 \quad \text{on } \partial D,\end{aligned}$$

for a test problem involving a symmetric linear system, where $D = [0, 1] \times [0, 1]$, and c is a constant. The usual centered difference approximations were used in the discretization. We set $f \equiv x(1-x) + y(1-y)$ and used $m = 64$, where m is the number of equally spaced interior points on each side of D , so that the resulting system has dimension 4096. For a preconditioner we used $-M + I$, which is symmetric positive definite, where M is the discretized Laplacian matrix. In experiments of the SYMMLQ, MINRES, symmetric QMR, and projection methods, we used Cholesky decomposition of the preconditioner. Also, we used the vector $(1, 1, \dots, 1)^T \in R^n$ for the initial guess and used double precision on Sun Microsystems workstations in all experiments. The true residual norms $\|b - Ax_k\|_2$ are monitored in assessing the comparative performance.

In the following Figure 1, the true residual norm curves generated by the MINRES, SYMMLQ, symmetric QMR, and projection methods are monitored using values of $c = 100$ and $m = 64$. As shown in Figure 1, we could see that there were some differences in the limits of reduction of the true residual norms. We regard these differences as insignificant, since the differences are small relative to that of the satisfactory limit of residual norms. The projection method is as numerically sound as MINRES, SYMMLQ, symmetric QMR in all our experiments.

In the following Figure 2, we plotted the true residual norm reduction versus floating-point operation counts for the MINRES, SYMMLQ, symmetric QMR, and projection methods. We ran the algorithms for 80 iterations. Figure 2 shows that the symmetric QMR, MINRES, projection methods need about the same number of operations to reach around the 10^{-10} level of residual norm reduction, although symmetric QMR needs slightly fewer number of operations than the MINRES and projection methods do. Figure 2 also shows that SYMMLQ requires approximately 10% more operations relative to that of the other three methods for 10^{-10} level of residual norm reduction.

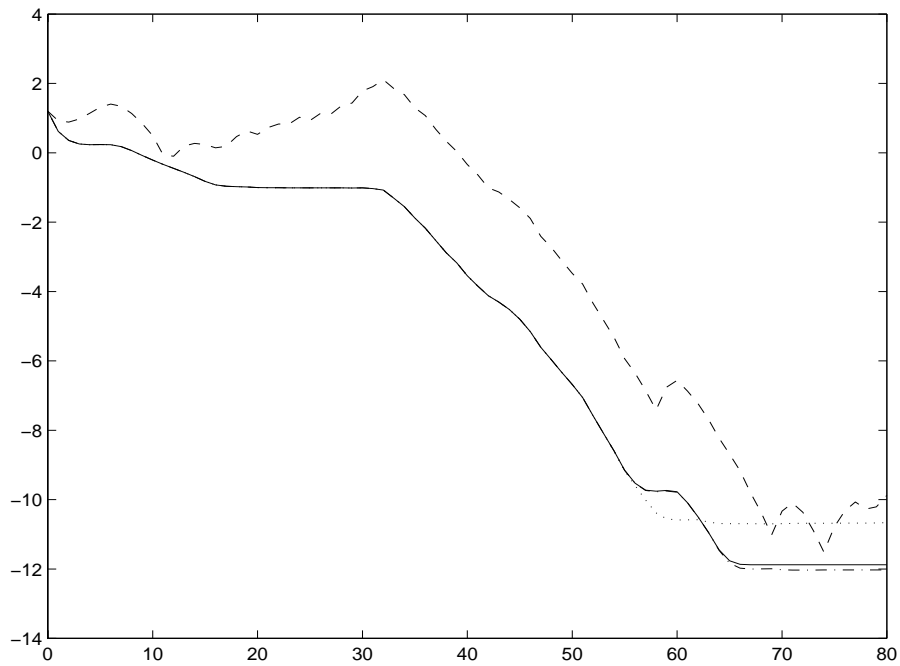


Figure 1: Log_{10} of the true residual norms vs. the number of iterations; $c = 100$ with preconditioner $-M + I$, where M is the discretized Laplacian matrix. Solid curve: MINRES; dashdot curve: symmetric QMR; dotted curve: algorithm 2.1; dashed curve: SYMMLQ; $m = 64$.

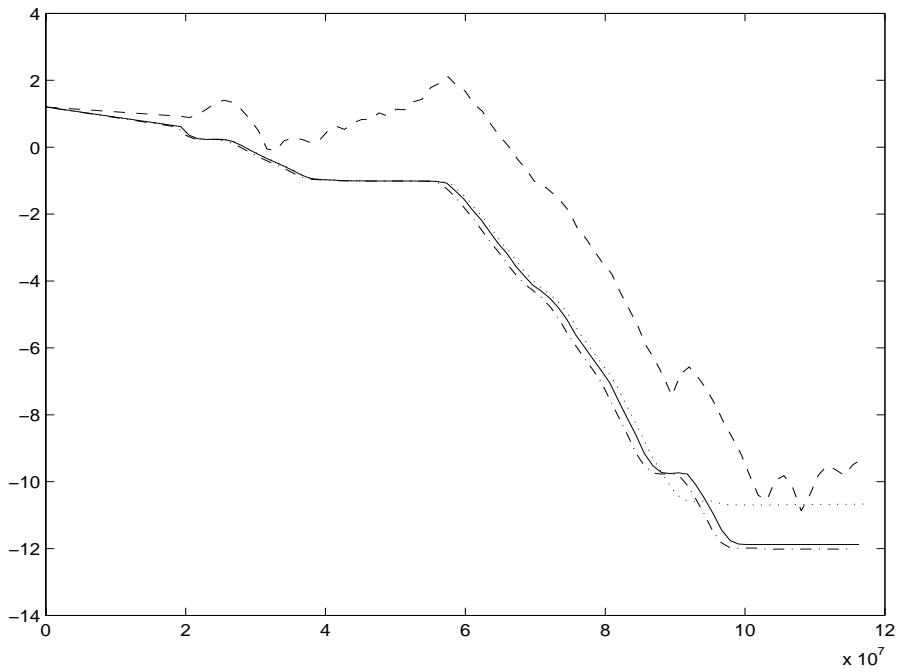


Figure 2: Log_{10} of the true residual norms vs. the number of floating-point operations; $c = 100$ with preconditioner $-M + I$, where M is the discretized Laplacian matrix. Solid curve: MINRES; dashdot curve: symmetric QMR; dotted curve: algorithm 2.1; dashed curve: SYMMLQ; $m = 64$.

4. Conclusion. In this paper, we have considered Krylov subspace methods for solving large symmetric indefinite linear systems and have introduced a new approach for solving them, which is called the projection method in this paper. Our numerical experiments showed that the projection method is as numerically sound as the MINRES, SYMMLQ, and symmetric QMR methods. Furthermore, these methods require roughly similar effort to achieve comparable residual norm reduction, although symmetric QMR is most efficient and SYMMLQ is mostly cost by a slight margin. However, only the symmetric QMR method allows use of arbitrary nonsingular symmetric indefinite preconditioners, which is an advantage of this method over the other methods. The symmetric QMR and projection methods have also an advantage over MINRES and SYMMLQ in easier programming.

REFERENCES

- [1] R. W. FREUND, AND N. M. NACHTIGAL, *QMR: a quasi-minimal residual method for non-Hermitian linear systems*, Numer. Math., 60 (1991), pp. 315-339.
- [2] R. W. FREUND, AND N. M. NACHTIGAL, *A new Krylov subspace method for symmetric indefinite linear systems*, ORNL/TM-12754 (1994).
- [3] R. W. FREUND, AND T. SZETO, *A quasi-minimal residual squared algorithm for non-Hermitian linear systems*, Tech. Rep. 91-26, Research Institute for Advanced Computer Science, NASA, Ames Research Center (1991).
- [4] R. W. FREUND, AND H. ZHA, *Simplifications of the nonsymmetric Lanczos process and a new algorithm for Hermitian indefinite linear systems*, Murray Hill Bell Labs (1994).
- [5] G. H. GOLUB, AND C. F. VAN LOAN, *Matrix Computations*, 2nd ed., The Johns Hopkins University press, Baltimore MD, (1989).
- [6] C. C. PAGE, AND M. A. SAUNDERS, *Solution of sparse indefinite systems of linear equations*, SIAM J. Numer. Anal., 12 (1975), pp. 617-629.
- [7] Y. SAAD, AND M. H. SCHULTZ, *GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems*, SIAM J. Sci. Stat. Comput., 7 (1986), pp. 856-869.
- [8] H. F. WALKER, AND L. ZHOU, *A simpler GMRES*, Numer. Lin. Alg. Appl., 1 (1994), pp. 571-581.

Department of Applied Mathematics
 Changwon National University
 9 Sarim-dong, Changwon,
 Kyongnam, 641-773, Korea.
 E-mail: scyi@sarim.changwon.ac.kr