VARIABLE METRIC CONJUGATE GRADIENT METHODS*

TERI BARTH † AND THOMAS MANTEUFFEL ‡

1. Introduction.

1.1. Motivation. In this paper we present a framework that includes many well known iterative methods for the solution of nonsymmetric linear systems of equations,

$$A\underline{x} = \underline{b}.$$

The purpose of this framework is that it provides a basis for analyzing and comparing methods.

Section 2 begins with a brief review of the conjugate gradient method. Next, we describe a broader class of methods, known as projection methods, to which the conjugate gradient (CG) method and most conjugate gradient-like methods belong. The concept of a method having either a fixed or a variable metric is introduced. Methods that have a metric are referred to as either fixed or variable metric methods. Some relationships between projection methods and fixed (variable) metric methods are discussed. The main emphasis of the remainder of this paper is on variable metric methods.

In Section 3 we show how the biconjugate gradient (BCG), and the quasi-minimal residual (QMR) methods fit into this framework as variable metric methods. By modifying the underlying Lanczos biorthogonalization process used in the implementation of BCG and QMR, we obtain other variable metric methods. These, we refer to as generalizations of BCG and QMR.

A consequence of this variable metric property is that, like CG, these methods all produce direction vectors, $\underline{p}_n$'s, and residual vectors, $\underline{r}_n$'s, that satisfy

$$\underline{p}_n \perp_B \mathcal{K}_n(\underline{r}_0, A), \qquad A^{-1}\underline{r}_n \perp_B \mathcal{K}_n(\underline{r}_0, A),$$

where B is a Hermitian positive definite (HPD), inner product matrix, and

$$\mathcal{K}_n(\underline{r}_0, A) = \mathrm{sp}\{\underline{r}_0, A\underline{r}_0, ..., A^{n-1}\underline{r}_0\}$$

is the Krylov subspace of dimension n generated by the initial residual, $\underline{r}_0$, and the matrix A. Since $\underline{p}_n$, $\underline{r}_n \in \mathcal{K}_{n+1}(\underline{r}_0, A)$, they can be expressed as

$$\underline{p}_n = \phi_n(A)\underline{r}_0, \qquad \underline{r}_n = \rho_n(A)\underline{r}_0,$$

where ϕ_n and ρ_n are referred to as the B-orthogonal polynomials and the residual polynomials respectively, associated with the corresponding method. Section 4 reviews the properties of these polynomials and describes how their roots can be used to obtain approximations of the spectrum of A. We conclude with a brief summary.

* This work was sponsored by the Department of Energy under grant number DE-FG03-93ER25165 and by the National Science Foundation under grant number DMS–8704169.

† Department of Mathematics, University of Colorado at Denver, Los Alamos National Laboratory

‡ Department of Mathematics, University of Colorado at Boulder, Los Alamos National Laboratory

1.2. Notation. We will make use of the following notation throughout this paper.

$\mathcal{R}^n, \mathcal{C}^n$	–	Vector spaces of real and complex $n-$ tuples.
$\mathcal{R}^{n\times m}, \mathcal{C}^{n\times m}$	–	Vector spaces of real and complex $n \times m$ matrices.
$\mathcal{P}_k$	–	Space of polynomials of degree at most k.
$\mathcal{P}_k^o$	–	Space of polynomials, $p_k(\lambda) \in \mathcal{P}_k$ such that, $p_k(0) = 1$.
$\mathcal{K},\ \mathcal{V}, \ldots$	–	Other calligraphic letters denote subspaces of $\mathcal{R}^n$ or $\mathcal{C}^n$.
$A, B, \ldots$	–	Upper case Roman and Greek letters denote matrices.
$\underline{x}, \underline{p}, \ldots$	–	Underlined lower case Roman and Greek letters denote vectors.
$\alpha, \beta, \ldots$	–	Lower case Roman and Greek letters denote scalars.
$\langle \cdot, \cdot \rangle,\ \|\cdot\|$	–	Euclidean inner product on $\mathcal{C}^n$ and induced norm.
$\langle B\cdot, \cdot \rangle,\ \|\cdot\|_B$	–	$B-$inner product on $\mathcal{C}^n$ and induced $B-$norm.
A^*	–	Euclidean adjoint of A, $A^* = \bar{A}^T$.
$A^\dagger$	–	$B-$adjoint of A.
$sp\{\underline{x}_j\}$	–	The linear span of the vectors $\underline{x}_j$.
$\Sigma(A)$	–	Spectrum of A.
$\mathcal{H}(A)$	–	Convex hull of $\Sigma(A)$.
$\mathcal{F}_B(A)$	–	$B-$Field of values of A.

2. A framework for conjugate gradient-like methods.

2.1. The conjugate gradient method. Given a Hermitian positive definite (HPD) inner product matrix, B, and an initial guess, $\underline{x}_0$, a conjugate gradient (CG) method for the solution of the $N \times N$ linear system

$$A\underline{x} = \underline{b}, \tag{2.1}$$

produces iterates that are uniquely defined by two conditions:

$$\begin{array}{lcll} \underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1}, & \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A), \\ \underline{e}_n & \perp_B & \underline{z}, & \forall \underline{z} \in \mathcal{K}_n(\underline{r}_0, A), \end{array} \tag{2.2}$$

where,

$$\mathcal{K}_n(\underline{r}_0, A) = \mathrm{sp}\{\underline{r}_0, A\underline{r}_0, ..., A^{n-1}\underline{r}_0\},$$

is the Krylov subspace of dimension n generated by the initial residual, $\underline{r}_0$, and the matrix A, $\underline{e}_n = \underline{x} - \underline{x}_n$, is the error at step n, and $\perp_B$ represents orthogonality in the B-inner product, that is, $\langle B\underline{e}_n, \underline{z}\rangle = 0$. (c.f. [AMS90])

For an HPD matrix B, the orthogonality condition given in (2.2) is equivalent to a minimization property, (see [JoMa90]). That is, choosing $\underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A)$ such that $\underline{e}_n \perp_B \underline{z}$, $\forall \underline{z} \in \mathcal{K}_n(\underline{r}_0, A)$ is equivalent to minimizing $\|\underline{e}_n\|_B$ over $\mathcal{K}_n(\underline{r}_0, A)$. This is known as the optimality property of the conjugate gradient method.

We denote by CG(B, A), a conjugate gradient method which is defined with respect to an inner product matrix, B, and the matrix A. CG(B, A) is implemented via the construction of a B-orthogonal basis $\{\underline{p}_j\}_{j=0}^{n-1}$ for $\mathcal{K}_n(\underline{r}_0, A)$. The $\underline{p}_j$'s are called direction vectors. There are several algorithms for CG(B, A), for example; Orthodir, Orthomin, Orthores, and GMRES. The Orthodir algorithm is given by

$$\begin{array}{rcl}\underline{r}_0 &=& \underline{b} - A\underline{x}_0, \\ \underline{p}_0 &=& \underline{r}_0, \\ &\vdots& \\ \underline{x}_{n+1} &=& \underline{x}_n + \alpha_n \underline{p}_n, \\ \underline{p}_{n+1} &=& A\underline{p}_n - \sum_{j=0}^{n} \sigma_{n,j} \underline{p}_j,\end{array}$$

where,

$$\langle B\underline{p}_n, \underline{p}_j \rangle = 0, \quad n \neq j \;\Rightarrow\; \sigma_{n,j} = \frac{\langle BA\underline{p}_n, \underline{p}_j \rangle}{\langle B\underline{p}_j, \underline{p}_j \rangle}.$$

In general, full recursions for the direction vectors are necessary in order to implement CG(B,A). The work and storage requirements needed to do this quickly become prohibitive, making CG(B,A) impractical to run in the general case.

In 1984 it was proven that, except for a few anomalies, the class of matrices for which a conjugate gradient method can be implemented via a single, short (s-term) recursion for the direction vectors is limited to matrices that are B-normal(s-2) [FaMa84]. Thus, a practical CG(B,A) algorithm is available for only a small class of matrices.

Generalizations of the conjugate gradient method for B-normal matrices to non-normal matrices are often referred to as conjugate gradient-like methods. The CG method along with most CG-like methods belong to a more general class of methods known as projection methods.

2.2. Projection methods. A projection method is an iterative method, where given an initial guess, $\underline{x}_0$, it produces iterates that are defined by two conditions:

$$\begin{array}{rcll}\underline{x}_n &=& \underline{x}_{n-1} + \underline{z}_{n-1}, & \underline{z}_{n-1} \in \mathcal{V}_n, \\ \underline{e}_n &\perp& \underline{y}, & \forall \underline{y} \in \mathcal{Y}_n, \\ & \text{or} & & \\ \underline{e}_n &\perp& \mathcal{Y}_n & \end{array} \tag{2.3}$$

where, $\mathcal{Y}_n$ $(\mathcal{V}_n)$ are referred to as left (right) subspaces, and $\perp$ represents orthogonality in the standard Euclidean sense. We say that the projection method breaks down at step n if the iterate, $\underline{x}_n$, does not exist or is not unique.

For the remainder of this section we will assume that

$$\dim(\mathcal{Y}_n) = \dim(\mathcal{V}_n) = n, \qquad \forall n,$$

and denote by

$$Y_n = \begin{bmatrix} | & | & & | \\ \underline{y}_0 & \underline{y}_1 & \cdots & \underline{y}_{n-1} \\ | & | & & | \end{bmatrix}, \quad V_n = \begin{bmatrix} | & | & & | \\ \underline{v}_0 & \underline{v}_1 & \cdots & \underline{v}_{n-1} \\ | & | & & | \end{bmatrix},$$

as the matrices whose columns span $\mathcal{Y}_n$ $(\mathcal{V}_n)$. From this it follows that (2.3) can be rewritten as

$$\begin{array}{rcll}\underline{x}_n &=& \underline{x}_{n-1} + V_n \underline{\gamma}, & \underline{\gamma} \in \mathcal{C}^n, \\ \underline{e}_n &=& \underline{e}_{n-1} - V_n \underline{\gamma}. & \end{array}$$

Multiplying the error equation through on the left by Y_n^* and using the orthogonality condition given in (2.3) yields

$$\underline{0} = Y_n^* \underline{e}_n = Y_n^* \underline{e}_{n-1} - Y_n^* V_n \underline{\gamma}.$$

If $Y_n^* V_n$ is nonsingular, then

$$\underline{\gamma} = (Y_n^* V_n)^{-1} Y_n^* \underline{e}_{n-1},$$

and explicit forms for the iterates and the error are given by

$$\begin{aligned} \underline{x}_n &= \underline{x}_{n-1} + V_n (Y_n^* V_n)^{-1} Y_n^* \underline{e}_{n-1}, \\ \underline{e}_n &= [I - V_n (Y_n^* V_n)^{-1} Y_n^*] \underline{e}_{n-1}. \end{aligned} \tag{2.4}$$

The name projection method comes from recognizing $[I - V_n (Y_n^* V_n)^{-1} Y_n^*]$ as a projection operator. From the above discussion, we see that the projection method breaks down if and only if $Y_n^* V_n$ is singular.

For every n, a map from the right subspace to the left subspace can be constructed to yield

$$\mathcal{Y}_n = \mathcal{B}_n^*(\mathcal{V}_n). \tag{2.5}$$

To see how this is done, choose any bases for $\mathcal{Y}_n$ and $\mathcal{V}_n$, and let Y_n and V_n be the corresponding matrices whose columns are the basis vectors. It follows that

$$B_n^* = Y_n (V_n^* V_n)^{-1} V_n^*$$

satisfies (2.5).

If there exists a fixed square matrix B, such that

$$Y_n = B^* V_n, \qquad \forall n, \tag{2.6}$$

we call the projection method stationary. Although B is fixed for every iteration, it may still depend on the initial guess, $\underline{x}_0$. Using (2.6), we can rewrite the orthogonality condition

$$\underline{e}_n \perp \mathcal{Y}_n \;\Leftrightarrow\; \underline{e}_n \perp_B \mathcal{V}_n,$$

where we mean a one-sided orthogonality with respect to the bilinear form matrix, B; that is, $\langle B\underline{e}_n, \underline{z}\rangle = 0, \;\; \forall \underline{z} \in \mathcal{V}_n$. If B is also HPD, the bilinear form is an inner product, and

$$\underline{e}_n \perp_B \mathcal{V}_n \;\Leftrightarrow\; \text{minimizing } \|\underline{e}_n\|_B \text{ over } \mathcal{V}_n,$$

and the projection method has an error minimization property or a metric. When B is independent of the initial guess, we call the metric fixed; otherwise, B is dependent on $\underline{x}_0$ and the metric is called variable. Thus, these methods are referred to as either fixed or variable metric methods. A projection method whose right subspace, $\mathcal{V}_n$, is the Krylov subspace, $\mathcal{K}_n(\underline{r}_0, A)$, is called a polynomial or Krylov projection method. We refer to fixed (variable) metric methods that are also polynomial methods as fixed (variable) metric conjugate gradient methods.

Definition 2.1: Fixed (variable) metric conjugate gradient methods are iterative methods whose iterates are uniquely defined by the following conditions:

$$
\begin{array}{lllll}
(2.7) \qquad & \underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1} & \qquad \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A), \\
& \underline{e}_n & \perp_B & \underline{z}, & \qquad \forall \underline{z} \in \mathcal{K}_n(\underline{r}_0, A),
\end{array}
$$

for $B(\underline{x}_0)$ an HPD matrix. If B is independent of $\underline{x}_0$, we have a fixed metric conjugate gradient method, or just a conjugate gradient method. Otherwise, we have a variable metric conjugate gradient method.

For more information about projection methods and their properties, see ([Sa81],[Sa82],[JoMa90]). In Section 3 we will show how the biconjugate gradient (BCG) and the quasi-minimal residual (QMR) methods fit into this framework as variable metric CG methods. Before demonstrating these specific cases, we first discuss some general relationships between variable metric methods and projection methods.

LEMMA 2.1. *Every fixed (variable) metric conjugate gradient method is a projection method.*

Proof. The iterates from a fixed (variable) metric conjugate gradient method are defined by the following:

$$
\begin{array}{llll}
\underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1}, & \qquad \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A) \\
\underline{e}_n & \perp_B & \underline{z}, & \qquad \forall \underline{z} \in \mathcal{K}_n(\underline{r}_0, A),
\end{array}
$$

where $B(\underline{x}_0)$ is an HPD matrix. Let

$$
\mathcal{V}_n = \mathcal{K}_n(\underline{r}_0, A), \qquad \mathcal{Y}_n = B\mathcal{K}_n(\underline{r}_0, A),
$$

then it follows that

$$
\begin{array}{llll}
\underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1}, & \qquad \underline{z}_{n-1} \in \mathcal{V}_n, \\
\underline{e}_n & \perp & \underline{y}, & \qquad \forall \underline{y} \in \mathcal{Y}_n,
\end{array}
$$

which is the definition for the iterates generated by a projection method. □

Given a nested sequence of subspaces

$$
\mathcal{V}_1 \subset \mathcal{V}_2 \subset \cdots \subset \mathcal{V}_N, \quad \dim(\mathcal{V}_i) = i, \quad \forall i,
$$

we say that $\{\underline{v}_i\}_{i=0}^{N-1}$ is an *ascending basis* for $\{\mathcal{V}_i\}_{i=1}^{N}$ if

$$
\begin{array}{lll}
\mathcal{V}_1 & = & \mathrm{sp}\{\underline{v}_0\} \\
\mathcal{V}_2 & = & \mathrm{sp}\{\underline{v}_0, \underline{v}_1\} \\
& \vdots & \\
\mathcal{V}_N & = & \mathrm{sp}\{\underline{v}_0, \underline{v}_1, \ldots, \underline{v}_{N-1}\}.
\end{array}
$$

LEMMA 2.2. *If $\{\underline{v}_i\}_{i=0}^{N-1}$ is an ascending basis for $\{\mathcal{V}_i\}_{i=1}^{N}$ and $\{\hat{\underline{v}}_i\}_{i=0}^{N-1}$ is any other ascending basis for $\{\mathcal{V}_i\}_{i=1}^{N}$ then*

$$
\hat{V}_N = V_N T_N,
$$

where,

$$\hat{V}_N = \begin{bmatrix} | & | & & | \\ \hat{\underline{v}}_0 & \hat{\underline{v}}_1 & \cdots & \hat{\underline{v}}_{N-1} \\ | & | & & | \end{bmatrix}, \quad V_N = \begin{bmatrix} | & | & & | \\ \underline{v}_0 & \underline{v}_1 & \cdots & \underline{v}_{N-1} \\ | & | & & | \end{bmatrix},$$

and T_N is a nonsingular, upper triangular matrix.

Proof: Since $\{\underline{v}_i\}_{i=0}^{N-1}$ and $\{\hat{\underline{v}}_i\}_{i=0}^{N-1}$ are ascending bases for $\{\mathcal{V}_i\}_{i=1}^{N}$, at each step k, we must have that $\mathrm{sp}\{\underline{v}_0, ..., \underline{v}_{k-1}\} = \mathrm{sp}\{\hat{\underline{v}}_0, ..., \hat{v}_{k-1}\} = \mathcal{V}_k$. This is true if and only if we can write each $\hat{\underline{v}}_{k-1} = \sum_{j=0}^{k-1} \alpha_{j,k-1}\underline{v}_j$, where $\alpha_{k-1,k-1} \neq 0$, since if $\alpha_{k-1,k-1} = 0$, we would have that $\mathrm{sp}\{\hat{\underline{v}}_0, ..., \hat{\underline{v}}_{k-1}\} = \mathrm{sp}\{\underline{v}_0, ..., \underline{v}_{k-2}\}$. Now, $\hat{\underline{v}}_{k-1} = \sum_{j=0}^{k-1} \alpha_{j,k-1}\underline{v}_j$, where $\alpha_{k-1,k-1} \neq 0, \;\; \forall k \leq N$ implies that

$$\hat{V}_N = V_N T_N, \quad \text{where} \quad (T_N)_{j,k-1} = \begin{cases} \alpha_{j,k-1} & j \leq k-1 \\ 0 & j > k-1 \end{cases}.$$

Since $\alpha_{k-1,k-1} \neq 0$, T_N is a nonsingular upper triangular matrix. $\square$

For the next lemma, let

$$\{\mathcal{V}_i\}_{i=1}^{N}, \quad \{\mathcal{Y}_i\}_{i=1}^{N}$$

be nested sequences of subspaces with ascending bases

$$\{\underline{v}_i\}_{i=0}^{N-1} \quad \text{for} \quad \{\mathcal{V}_i\}_{i=1}^{N},$$

$$\{\underline{y}_i\}_{i=0}^{N-1} \quad \text{for} \quad \{\mathcal{Y}_i\}_{i=1}^{N},$$

such that

$$\dim(\mathcal{V}_i) = \dim(\mathcal{Y}_i) = i, \quad \forall i \leq N.$$

Denote by V_i and Y_i, the matrices whose j'th columns are $\underline{v}_j$ and $\underline{y}_j$ respectively, and assume that $(Y_i^* V_i)$ is nonsingular $\forall i \leq N$.

Define a *stationary map* B^* from

$$\{\mathcal{V}_i\}_{i=1}^{N} \;\rightarrow\; \{\mathcal{Y}_i\}_{i=1}^{N},$$

to be a map such that

$$B^*(\mathcal{V}_i) = \mathcal{Y}_i, \quad \forall i \leq N.$$

LEMMA 2.3. *All possible stationary maps from $\{\mathcal{V}_i\}_{i=1}^{N} \rightarrow \{\mathcal{Y}_i\}_{i=1}^{N}$,* for $i \leq N$, *are of the form*

$$B^* = Y_N T_N V_N^{-1}, \tag{2.8}$$

where T_N is a nonsingular, upper triangular matrix.

Proof: There exists a stationary map from $\{\mathcal{V}_i\}_{i=1}^N \rightarrow \{\mathcal{Y}_i\}_{i=1}^N$, $\forall i \leq N$, given by

$$B^* = Y_N V_N^{-1}.$$

Let $\hat{B}^*$ be any other stationary map and let $\hat{\underline{y}}_i = \hat{B}^* \underline{v}_i$. Then $\{\underline{\hat{y}_i}\}_{i=0}^{N-1}$ is an ascending basis for $\{\mathcal{Y}_i\}_{i=1}^N$. Thus, $\hat{B}^*$ may be written

$$\hat{B}^* = \hat{Y}_N V_N^{-1}. \tag{2.9}$$

By Lemma 2.2, we know there exists a nonsingular, upper triangular matrix, T_N, such that

$$\hat{Y}_N = Y_N T_N. \tag{2.10}$$

Substituting (2.10) into (2.9) yields

$$\hat{B}^* = Y_N T_N V_N^{-1}.$$

Thus, any stationary map can be written in the form given by (8). Finally, note that any map of the form given by (2.8) is a stationary map. □

We remark here that the assumption that

$$Y_i^* V_i \quad \text{is nonsingular } \forall i, \tag{2.11}$$

is an assumption about the spaces, $\{\mathcal{V}_i\}_{i=1}^N$ and $\{\mathcal{Y}_i\}_{i=1}^N$, since if (2.11) is true for one pair of bases, it is true for every pair of bases. We will refer to (2.11) as: $\mathcal{V}_i^* \mathcal{Y}_i$ is nonsingular for every i.

THEOREM 2.4. *Any projection method based on nested subspaces $\{\mathcal{V}_i\}_{i=1}^N$ and $\{\mathcal{Y}_i\}_{i=1}^N$, where $\dim(\mathcal{V}_i) = \dim(\mathcal{Y}_i) = i$, $\forall i \leq N$, and where $\mathcal{V}_i^* \mathcal{Y}_i$ is nonsingular for every $i \leq N$, has a metric, which is unique up to an arbitrary positive, diagonal matrix.*

Proof: Let $\{\underline{v}_i\}_{i=0}^{N-1}$ and $\{\underline{y}_i\}_{i=0}^{N-1}$ be ascending bases for the nested sequences of subspaces, $\{\mathcal{V}_i\}_{i=1}^N$ and $\{\mathcal{Y}_i\}_{i=1}^N$ respectively. Denote by V_i and Y_i, the matrices whose j'th columns are $\underline{v}_j$ and $\underline{y}_j$ respectively. It follows from Lemma 2.3 that all possible stationary maps are of the form

$$B^* = V_N^{-*}(V_N^* Y_N) T_N V_N^{-1}. \tag{2.12}$$

By hypothesis, $V_i^* Y_i$ is nonsingular for every $i \leq N$ and it follows that all the principal majors of $V_N^* Y_N$ are nonsingular. Thus, an LU- decomposition of $V_N^* Y_N$ can be performed without pivoting, yielding

$$V_N^* Y_N = L_N U_N.$$

Let $T_N = U_N^{-1} \Omega_N L_N^*$, where $\Omega_N = \mathrm{diag}(\cdots \omega_i \cdots)$ and $\omega_i > 0$ is arbitrary. Making these substitutions for T_N and $(V_N^* Y_N)$ into (2.12) yields an HPD B given by

$$B = V_N^{-*} L_N \Omega_N L_N^* V_N^{-1}, \tag{2.13}$$

where we see that B is unique up to a positive diagonal matrix, Ω_N. Thus, we have a stationary, HPD B, such that $BV_i = Y_i$ for every $i \leq N$. By definition, the projection method is either a fixed or a variable metric method. Notice that any B of the form given by (2.13), in a fixed or variable metric method, will produce the same sequence of iterates. $\Box$

Define

$$P_N = V_N L_N^{-*}, \tag{2.14}$$

where V_N and L_N are the matrices given in Theorem 2.4. Since L_N^{-*} is a nonsingular, upper triangular matrix, it follows from Lemma 2.2 that the columns of P_N, $\{\underline{p}_i\}_{i=0}^{N-1}$, form an ascending basis for $\{\mathcal{V}_i\}_{i=1}^{N}$. It is easy to see from (2.13) and (2.14) that $\{\underline{p}_i\}_{i=0}^{N-1}$ are mutually B-orthogonal. Corollary 2.5 shows an equivalent way to write all possible metrics for these methods. This form may be more useful since the information needed to write the metric in this form is often readily available.

COROLLARY 2.5. *Suppose we have any fixed or variable metric method. Let $\hat{P}_N$ be any matrix whose columns, $\{\underline{\hat{p}}_i\}_{i=0}^{N-1}$, form a B-orthogonal, ascending basis for $\{\mathcal{V}_i\}_{i=1}^{N}$. Then, the metric, B, given by (2.13) in Theorem 2.1, can be written in the form*

$$B = \hat{P}_N^{-*} \hat{\Omega}_N \hat{P}_N^{-1}, \tag{2.15}$$

where $\hat{\Omega}_N$ is an arbitrary positive, diagonal matrix.

Proof: From the above discussion we see that substitution of (2.14) into (2.13) yields

$$B = P_N^{-*} \Omega_N P_N^{-1}, \tag{2.16}$$

where the columns of P_N, $\{\underline{p}_i\}_{i=0}^{N-1}$, form an ascending, B-orthogonal basis for $\{\mathcal{V}_i\}_{i=1}^{N}$. This B-orthogonal basis is unique up to scale. That is,

$$\{\hat{p}_i\}_{i=0}^{N-1} = \{\alpha_i \underline{p}_i\}_{i=0}^{N-1}$$

is another B-orthogonal, ascending basis for $\{\mathcal{V}_i\}_{i=1}^{N}$ if $\alpha_i \neq 0$ for every $i \leq N-1$. Thus, we can write

$$\hat{P}_N = P_N \Delta_N, \text{ where } \Delta_N = \operatorname{diag}(\cdots \alpha_i \cdots) \text{ and } \alpha_i \neq 0. \tag{2.17}$$

Using (2.16) and (2.17), it follows that B can also be written as:

$$B = P_N^{-*} \Omega_N P_N^{-1} = P_N^{-*} \Delta_N^{-*} \hat{\Omega}_N \Delta_N^{-1} P_N^{-1} = \hat{P}_N^{-*} \hat{\Omega}_N \hat{P}_N^{-1},$$

where

$$\hat{\Omega}_N = \Delta_N^{*} \Omega_N \Delta_N$$

is also an arbitrary positive, diagonal matrix. Therefore, it follows from Theorem 2.4 that all possible metrics are given by:

$$B = \hat{P}_N^{-*} \hat{\Omega}_N \hat{P}_N^{-1},$$

where the columns of $\hat{P}_N$ form any B-orthogonal, ascending basis for $\{\mathcal{V}_i\}_{i=1}^N$, and $\hat{\Omega}_N$ is an arbitrary positive, diagonal matrix. □

Recall the definition for the iterates generated by a fixed (variable) metric method:

$$\begin{array}{lclll} \underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1}, & & \underline{z}_{n-1} \in \mathcal{V}_n, \\ \underline{e}_n & \perp_B & \underline{z}, & & \forall \underline{z} \in \mathcal{V}_n. \end{array} \tag{2.18}$$

It follows that

$$\underline{e}_n = \underline{e}_{n-1} - \underline{z}_{n-1}. \tag{2.19}$$

Let $\underline{z}_j \in \mathcal{V}_{n-1}$. Since $\mathcal{V}_{n-1} \subset \mathcal{V}_n$, it follows from (2.19) and the orthogonality condition given in (2.18) that

$$0 = \langle B\underline{e}_n, \underline{z}_j \rangle = \langle B\underline{e}_{n-1}, \underline{z}_j \rangle - \langle B\underline{z}_{n-1}, \underline{z}_j \rangle = 0 - \langle B\underline{z}_{n-1}, \underline{z}_j \rangle.$$

Therefore, we must have $\langle B\underline{z}_{n-1}, \underline{z}_j \rangle = 0,\ j < n-1$. Since a B-orthogonal, ascending basis is unique up to scale, it follows that

$$\underline{z}_{n-1} = \beta_{n-1}\underline{p}_{n-1}, \quad \text{for some scalar } \beta_{n-1}.$$

If $\beta_{n-1} \neq 0,\ \forall n$, then $\{\underline{z}_n\}_{n=0}^{N-1}$ form a B-orthogonal, ascending basis for $\{\mathcal{V}_n\}_{n=1}^N$, and it follows from Corollary 2.5 that all possible metrics, B, can be written in the form:

$$B = Z_N^{-*}\Omega_N Z_N^{-1},$$

where Z_N denotes the matrix whose columns are $\{\underline{z}_n\}_{n=0}^{N-1}$, and where $\Omega_N = \mathrm{diag}(\cdots\omega_n\cdots)$ and $\omega_n > 0$ is arbitrary.

Convergence bounds:

For any fixed or variable metric CG method, we can establish convergence bounds. Since for any of these methods, the error is minimized at each step with respect to the B norm, we can write

$$\frac{\|\underline{e}_n\|_B}{\|\underline{e}_0\|_B} = \min_{p_n \in \mathcal{P}_n^\circ} \frac{\|p_n(A)\underline{e}_0\|_B}{\|\underline{e}_0\|_B}.$$

We can bound $\frac{\|\underline{e}_n\|}{\|\underline{e}_0\|}$ by noting that

$$\begin{aligned} \|\underline{e}_n\|_B &= \min_{p_n \in \mathcal{P}_n^\circ} \|p_n(A)\underline{e}_0\|_B = \min_{p_n \in \mathcal{P}_n^\circ} \|B^{1/2}p_n(A)\underline{e}_0\| \\ &\leq \|B^{1/2}\| \min_{p_n \in \mathcal{P}_n^\circ} \|p_n(A)\underline{e}_0\|, \end{aligned} \tag{2.20}$$

and

$$\|\underline{e}_n\| = \|B^{-1/2}B^{1/2}\underline{e}_n\| \leq \|B^{-1/2}\|\ \|B^{1/2}\underline{e}_n\| = \|B^{-1/2}\|\ \|\underline{e}_n\|_B. \tag{2.21}$$

Multiplying (2.20) on the left by $\|B^{-1/2}\|$ and using (2.21) yields:

$$\|\underline{e}_n\| \le \|B^{-1/2}\|\ \|B^{1/2}\| \min_{p_n \in \mathcal{P}_n^\circ} \|p_n(A)\underline{e}_0\|. \tag{2.22}$$

Since B is HPD, $\|B^{-1/2}\|\ \|B^{1/2}\| = \mathcal{C}(B^{1/2}) = \mathcal{C}(B)^{1/2}$ (the square root of the condition number of B). By dividing (2.22) through by $\|\underline{e}_0\|$ we obtain a bound for the relative error:

$$\frac{\|\underline{e}_n\|}{\|\underline{e}_0\|} \le \mathcal{C}(B)^{1/2} \min_{p_n \in \mathcal{P}_n^\circ} \frac{\|p_n(A)\underline{e}_0\|}{\|\underline{e}_0\|}. \tag{2.23}$$

For a variable metric CG method, B is dependent upon the initial guess and the particular algorithm. For this bound to be meaningful, we need to bound $\mathcal{C}(B)$. An ideal result would be to find some class of matrices and some algorithm for which

$$\mathcal{C}(B(\underline{x}_0)) \le K, \quad \forall \underline{x}_0.$$

As far as we know, such results are essentially nonexistent. We also recall from Theorem 2.4 that B is not unique. Any positive, diagonal matrix, Ω_N in (2.13), will produce the same sequence of iterates. However, it may be possible to choose Ω_N so that B has a smaller condition number, yielding a tighter bound on the relative error.

3. Examples of variable metric methods.

In this section we will show that BCG and QMR are variable metric conjugate gradient methods. First we need to say a few words about Lanczos biorthogonalization which is used in the implementation of both BCG and QMR.

3.1. Lanczos biorthogonalization.

Lanczos biorthogonalization is a process that constructs a pair of ascending bases

$$\{\underline{v}_j\}_{j=0}^{n-1} \quad \text{for} \quad \{\mathcal{K}_j(\underline{v}_0, A)\}_{j=1}^{n},$$

$$\{\underline{w}_j\}_{j=0}^{n-1} \quad \text{for} \quad \{\mathcal{K}_j(\underline{w}_0, A^*)\}_{j=1}^{n},$$

such that

$$\underline{w}_i^* A^p \underline{v}_j = \begin{cases} \delta_i & i = j, \\ 0 & i \ne j, \end{cases} \tag{3.1}$$

where p is any nonnegative integer. The $\underline{v}$'s ($\underline{w}$'s) are called right (left) Lanczos vectors. When $p = 0$, the Lanczos vectors are biorthogonal, and when $p = 1$, they are biconjugate. Lanczos vectors are often normalized to have unit length. Denote, $\underline{v}_n$ ($\underline{w}_n$), as the normalized Lanczos vectors, and let

$$\begin{aligned} \tilde{\underline{v}}_n &= \eta_n \underline{v}_n, & \eta_n &= \|\tilde{\underline{v}}_n\|, \\ \tilde{\underline{w}}_n &= \xi_n \underline{w}_n, & \xi_n &= \|\tilde{\underline{w}}_n\|. \end{aligned}$$

This process is implemented via a 2-sided Gram-Schmidt process

$$\begin{aligned} \eta_n \underline{v}_n &= A\underline{v}_{n-1} - \textstyle\sum_{j=0}^{n-1} \sigma_{n-1,j}\underline{v}_j, \\ \xi_n \underline{w}_n &= A^*\underline{w}_{n-1} - \textstyle\sum_{j=0}^{n-1} \tilde{\sigma}_{n-1,j}\underline{w}_j, \end{aligned}$$

where,

$$\sigma_{n-1,j} = \frac{\langle A^{p+1}\underline{v}_{n-1}, \underline{w}_j\rangle}{\langle A^p \underline{v}_j, \underline{w}_j\rangle}, \quad \tilde{\sigma}_{n-1,j} = \frac{\langle A^* \underline{w}_{n-1}, A^p \underline{v}_j\rangle}{\langle \underline{w}_j, A^p, \underline{v}_j\rangle}.$$

These recurrences naturally truncate to three terms, that is, $\sigma_{n-1,j},\ \tilde{\sigma}_{n-1,j} = 0$, for $j < n-2$. This yields

$$\begin{aligned}
\eta_n \underline{v}_n &= A\underline{v}_{n-1} - \sigma_{n-1,n-1}\underline{v}_{n-1} - \sigma_{n-1,n-2}\underline{v}_{n-2}, \\
\xi_n \underline{w}_n &= A^*\underline{w}_{n-1} - \tilde{\sigma}_{n-1,n-1}\underline{w}_{n-1} - \tilde{\sigma}_{n-1,n-2}\underline{w}_{n-2}.
\end{aligned}$$

This process is subject to breakdowns. For example, if the denominator of $\sigma_{n-1,n-1}$ is zero for nonzero Lanczos vectors, $\underline{v}_{n-1}$, $\underline{w}_{n-1}$, breakdown results. Fortunately, most breakdowns can be avoided by using look-ahead variants of this algorithm, which we briefly discuss below.

Let V_n (W_n) denote the matrices whose columns are the normalized right (left) Lanczos vectors resulting from n steps of the Lanczos iteration. The recurrences for the Lanczos vectors can be rewritten in matrix notation as follows:

$$AV_n = V_{n+1}H_{n+1,n}, \qquad A^*W_n = W_{n+1}\tilde{H}_{n+1,n}. \tag{3.2}$$

For the right Lanczos vectors, this is written explicitly as:

$$A\begin{bmatrix} | & & | \\ \underline{v}_0 & \cdots & \underline{v}_{n-1} \\ | & & | \end{bmatrix} = \begin{bmatrix} | & & | & | \\ \underline{v}_0 & \cdots & \underline{v}_{n-1} & \underline{v}_n \\ | & & | & | \end{bmatrix} \begin{bmatrix} \sigma_{0,0} & \sigma_{1,0} & 0 & \cdots & 0 \\ \eta_1 & \sigma_{1,1} & \sigma_{2,1} & \ddots & \vdots \\ 0 & \eta_2 & \sigma_{2,2} & \ddots & 0 \\ \vdots & \ddots & \eta_3 & \ddots & \sigma_{n-1,n-2} \\ \vdots & & \ddots & \ddots & \sigma_{n-1,n-1} \\ 0 & \cdots & \cdots & 0 & \eta_n \end{bmatrix},$$

where $H_{n+1,n}$ is a tridiagonal, upper Hessenberg matrix. Similarly, the orthogonality condition can be written as

$$W_n^* A^p V_n = D_n = \begin{bmatrix} \delta_0 & & & \\ & \delta_1 & & \\ & & \ddots & \\ & & & \delta_{n-1} \end{bmatrix}, \tag{3.3}$$

a diagonal matrix.

To avoid most breakdowns that can occur in the standard Lanczos iteration, methods such as BCG and QMR are often implemented with look-ahead variants of this process, such as the look-ahead Lanczos (LAL) algorithm of [FrGuNa91]. Breakdowns are avoided by relaxing the orthogonality condition, (3.1). By grouping the right and left Lanczos vectors into blocks, where the first vector in each block is called a regular vector, and all other vectors in the block are called inner vectors, the Lanczos vectors generated by the LAL algorithm satisfy a block orthogonality condition

$$\hat{W}_i^* A^p \hat{V}_j = \begin{cases} [\hat{D}_i]_{d_i,d_j} & \text{if } i = j \\ [0]_{d_i,d_j} & \text{if } i \neq j \end{cases} \quad i,j = 1, \ldots, \ell, \tag{3.4}$$

where $\hat{V}_j$ is the matrix whose columns are the right Lanczos vectors from the j'th block, and $\hat{W}_i$ is the matrix of left Lanczos vectors from the i'th block. The number of columns in $\hat{V}_j$ and $\hat{W}_i$ are denoted by d_j and d_i, and ℓ refers to the current block.

This block orthogonality condition can also be accomplished with short recurrences for the right and left Lanczos vectors. Instead of these recurrences involving only two previous Lanczos vectors, the LAL version involves the two previous blocks of these vectors. The matrix equations for these recurrences can still be written in the form given by (3.2), except that the matrices $H_{n+1,n}$, $\tilde{H}_{n+1,n}$, are block tridiagonal, upper Hessenberg. Similarly, the matrix equation for the orthogonality condition, (3.4), yields a block diagonal matrix, D_n. The reader is referred to [FrGuNa91] for details.

When BCG and QMR are implemented via a look-ahead version of the Lanczos iteration, the material in the previous section on projection methods can be extended in order to be applicable. In particular, consider nested sequences of subspaces, $\{\mathcal{V}_k\}_{k=1}^{\ell}$, where each $\mathcal{V}_k$ may differ from the previous subspace, $\mathcal{V}_{k-1}$, by possibly more than the span of a single vector. In the next section, we will see that both BCG and QMR are projection methods, where the right subspaces, $\{\mathcal{V}_k\}_{k=1}^{\ell}$ are spanned by the right Lanczos vectors. When the LAL version is used in the implementation, $\mathcal{V}_k$ differs from $\mathcal{V}_{k-1}$ by the span of the k'th block of right Lanczos vectors.

Let $\{\mathcal{V}_k\}_{k=1}^{\ell}$ and $\{\mathcal{Y}_k\}_{k=1}^{\ell}$ be nested sequences of right and left subspaces such that $\dim(\mathcal{V}_k) = \dim(\mathcal{Y}_k) = d_{(k)}$, $\forall k \leq \ell$. Denote V_ℓ and Y_ℓ as the matrices whose columns span $\mathcal{V}_\ell$ and $\mathcal{Y}_\ell$. Consider the partitioning

$$V_\ell = [\hat{V}_1, \hat{V}_2, ..., \hat{V}_\ell], \quad Y_\ell = [\hat{Y}_1, \hat{Y}_2, ..., \hat{Y}_\ell],$$

where, for $k = 1, ..., \ell$, $\hat{V}_k$ is the matrix whose n_k columns are the right Lanczos vectors from the k'th block, $\{\underline{v}_{1,k}, \underline{v}_{2,k}, ..., \underline{v}_{n_k,k}\}$. A stationary map from $\{\mathcal{V}_k\}_{k=1}^{\ell} \rightarrow \{\mathcal{Y}_k\}_{k=1}^{\ell}$ is given by

$$B^* = Y_\ell (Y_\ell^* V_\ell)^{-1} Y_\ell^*.$$

This can be viewed as a blockwise mapping, since for every block, k,

$$B^* \hat{V}_k = \hat{Y}_k.$$

It follows that Lemmas 2.1 through 2.3, and Theorem 2.4 can be extended to include blockwise maps, and thus look-ahead versions of BCG and QMR.

For simplicity of this presentation, we have chosen to present the BCG and QMR methods without a look-ahead implementation of the Lanczos process. We will assume there is no breakdown in the Lanczos iteration and that $d(\underline{v}_0, A) = d(\underline{w}_0, A^*) = N$, where $d = d(\underline{z}, A)$ is the dimension of the maximal Krylov subspace generated by the vector, $\underline{z}$, and the matrix, A. Except for rare cases of incurable breakdown, see [FrGuNa91], breakdowns can be avoided with look-ahead variants of this algorithm, and the results that follow can be extended to cover these cases. We can also extend these results to include cases where $d < N$ by restricting all operators to the appropriate subspaces.

3.2. The biconjugate gradient (BCG) method. The BCG method produces iterates that are defined by two conditions:

$$
\begin{array}{rcll}
\underline{x}_n &=& \underline{x}_{n-1} + \underline{z}_{n-1}, & \qquad \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A), \\
\underline{r}_n &\perp& \mathcal{K}_n(\underline{w}_0, A^*), & \\
 & \text{or} & & \\
\underline{e}_n &\perp& A^*\mathcal{K}_n(\underline{w}_0, A^*). &
\end{array} \tag{3.5}
$$

By letting

$$
\begin{array}{rcl}
\mathcal{V}_n &=& \mathcal{K}_n(\underline{r}_0, A), \\
\mathcal{Y}_n &=& A^*\mathcal{K}_n(\underline{w}_0, A^*),
\end{array}
$$

it is clear that BCG is a projection method.

BCG is implemented via Lanczos biorthogonalization, with $p = 1$, which produces a pair of ascending bases

$$
\begin{array}{ccc}
\{\underline{v}_i\}_{j=0}^{N-1} & \text{for} & \{\mathcal{K}_i(\underline{v}_0, A)\}_{i=1}^{N}, \\[2ex]
\{\underline{w}_i\}_{i=0}^{N-1} & \text{for} & \{\mathcal{K}_i(\underline{w}_0, A^*)\}_{i=1}^{N},
\end{array}
$$

such that

$$
\underline{w}_j^* A \underline{v}_i = \left\{ \begin{array}{ll} \delta_i & \quad i = j \\ 0 & \quad i \neq j \end{array} \right. .
$$

For every i, denote by V_i and W_i, the matrices whose columns are these ascending basis vectors for $\mathcal{K}_i(\underline{v}_0, A)$, and $\mathcal{K}_i(\underline{w}_0, A^*)$ respectively. By choosing $\underline{v}_0 = \underline{r}_0/\|\underline{r}_0\|$, and $\underline{w}_0$ arbitrary (usually $\underline{w}_0$ is chosen to be $\underline{v}_0$), we see that

$$
\begin{array}{lcl}
\{\underline{v}_i\}_{i=0}^{N-1} & \text{is an ascending basis for} & \{\mathcal{K}_i(\underline{r}_0, A)\}_{i=1}^{N}, \\[2ex]
\{\underline{A}^*\underline{w}_i\}_{i=0}^{N-1} & \text{is an ascending basis for} & \{A^*\mathcal{K}_i(\underline{w}_0, A^*)\}_{i=1}^{N}.
\end{array}
$$

It follows that the columns of V_i span $\mathcal{V}_i$ and the columns of A^*W_i span $\mathcal{Y}_i$. Since we are assuming there is no breakdown, and $d(\underline{v}_0, A) = d(\underline{w}_0, A^*) = N$, it follows that $\dim(\mathcal{V}_i) = \dim(\mathcal{Y}_i) = i$, $\forall i \leq N$, and $W_i^*AV_i$ is nonsingular $\forall i \leq N$. From Theorem 2.4, we know the method has a metric; thus, there exists an HPD B such that $\mathcal{B}(\mathcal{V}_i) = \mathcal{Y}_i$, $\forall i$. One possible choice of an HPD B is given by:

$$
B = A^* W_N D_N^{-*} D_N^{-1} W_N^* A. \tag{3.6}
$$

This can be seen by using (3.3), with $p = 1$, and noting that for every i,

$$
B\underline{v}_i = A^* W_N D_N^{-*}(D_N^{-1} W_N^* A \underline{v}_i) = A^* W_N D_N^{-1} \underline{\epsilon}_i = \frac{1}{\delta_i} A^* \underline{w}_i,
$$

where $\underline{\epsilon}_i$ is the i'th canonical basis vector, and where $\{\frac{1}{\delta_i} A^* \underline{w}_i\}_{i=0}^{N-1}$ is another ascending basis for $\{\mathcal{Y}_i\}_{i=1}^{N}$.

Substituting $D_N = W_N^* A V_N$ into (3.6) shows that B may also be written as

$$
B = V_N^{-*} V_N^{-1}. \tag{3.7}
$$

Since the first column of V_N is $\underline{r}_0/||\underline{r}_0||$, it is clear that B is dependent upon $\underline{r}_0$, and thus upon $\underline{x}_0$. Also, note that for every n, $\mathcal{V}_n = \mathcal{K}_n(\underline{r}_0, A)$. We see that BCG fits into the framework outlined earlier as a variable metric conjugate gradient method. For B given by (3.7), it is clear that the right Lanczos vectors form a B-orthogonal basis for $\{\mathcal{V}_i\}_{i=1}^N$. Therefore, B is of the form given by Corollary 2.5. Furthermore, it follows from Corollary 2.5 that all possible metrics, B, can be written in the form:

$$B = V_N^{-*}\Omega_N V_N^{-1}, \tag{3.8}$$

for an arbitrary positive, diagonal matrix, Ω_N. Thus, any B of the form given by (3.8) will produce the same sequence of iterates. We may recast the definition for the BCG iterates as:

$$\begin{array}{lcll} \underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1}, & \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A), \\ \underline{e}_n & \perp_B & \underline{z}, & \forall \underline{z} \in \mathcal{K}_n(\underline{r}_0, A), \end{array} \tag{3.9}$$

where,

$$B = A^* W_N D_N^{-*}\Omega_N D_N^{-1} W_N^* A = V_N^{-*}\Omega_N V_N^{-1}, \tag{3.10}$$

for any positive, diagonal matrix, Ω_N, and where V_N and W_N are the matrices of biconjugate Lanczos vectors.

3.3. The quasi-minimal residual (QMR) method. The iterates generated by the QMR method are given by

$$\underline{x}_n = \underline{x}_0 + \underline{z}_{n-1}, \qquad \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A), \tag{3.11}$$

where, $\underline{z}_{n-1}$ is chosen to satisfy a quasi-minimal residual property [FrNa91] which will be described below. QMR is implemented via Lanczos biorthogonalization, with $p = 0$, to construct a pair of ascending bases

$$\{\underline{v}_i\}_{i=0}^{N-1} \quad \text{for} \quad \{\mathcal{K}_i(\underline{v}_0, A)\}_{i=1}^N,$$

$$\{\underline{w}_i\}_{i=0}^{N-1} \quad \text{for} \quad \{\mathcal{K}_i(\underline{w}_0, A^*)\}_{i=1}^N,$$

such that

$$\underline{w}_j^* \underline{v}_i = \begin{cases} \delta_i & i = j \\ 0 & i \neq j \end{cases}.$$

The first right Lanczos vector, $\underline{v}_0$, is chosen to be $\underline{r}_0/||\underline{r}_0||$, so that $\mathcal{K}_n(\underline{v}_0, A) = \mathcal{K}_n(\underline{r}_0, A)$. The starting left Lanczos vector is arbitrary, but often chosen to be $\underline{v}_0$. Denote V_n as the matrix whose n columns are the first n right Lanczos vectors. Since these vectors form a basis for $\mathcal{K}_n(\underline{r}_0, A)$, we can rewrite the QMR iterates in the form

$$\underline{x}_n = \underline{x}_0 + V_n\underline{\gamma}, \qquad \underline{\gamma} \in \mathcal{C}^n.$$

The residuals have the form

$$\underline{r}_n = \underline{b} - A\underline{x}_n = \underline{b} - A(\underline{x}_0 + V_n\underline{\gamma}) = \underline{r}_0 - AV_n\underline{\gamma}. \tag{3.12}$$

Let $\eta_0 = ||\underline{r}_0||$, and note that $\underline{r}_0 = \eta_0\underline{v}_0$, or equivalently,

$$\underline{r}_0 = V_N \begin{pmatrix} \eta_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_N. \tag{3.13}$$

From (3.2) it follows that

$$AV_n\underline{\gamma} = AV_N \begin{pmatrix} \underline{\gamma} \\ \underline{0} \end{pmatrix}_N = V_N H_N \begin{pmatrix} \underline{\gamma} \\ \underline{0} \end{pmatrix}_N, \tag{3.14}$$

where $\underline{\gamma}$ is a vector of length n, so that together, $\begin{pmatrix} \underline{\gamma} \\ \underline{0} \end{pmatrix}$ has length N. Substituting (3.13) and (3.14) into (3.12) yields

$$\underline{r}_n = V_N \left[\begin{pmatrix} \eta_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_N - H_N \begin{pmatrix} \underline{\gamma} \\ 0 \\ \vdots \\ 0 \end{pmatrix}_N \right]. \tag{3.15}$$

Minimizing $\|\underline{r}_n\|$ at each step is expensive, so instead, QMR chooses $\underline{\gamma}_n$ to satisfy

$$\min_{\underline{\gamma}\in\mathcal{C}^n} \left\| \begin{pmatrix} \eta_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} - H_N \begin{pmatrix} \underline{\gamma} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \right\|.$$

This is referred to as the quasi-minimal residual property [FrNa91]. This is implemented via a least squares problem, i.e., at each step we solve

$$H_{n+1,n}\underline{\gamma}_n \approx \begin{pmatrix} \eta_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{n+1},$$

or equivalently, using QR decomposition of $H_{n+1,n}$, solve

$$Q_{n+1,n+1} \begin{bmatrix} R_{n,n} \\ \underline{0}^T \end{bmatrix} \underline{\gamma}_n \approx \begin{pmatrix} \eta_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{n+1}.$$

For details, see [FrNa91].

It follows from (3.3) that $D_N = W_N^* V_N$, so multiplying both sides of (3.15) by $D_N^{-1} W_N^*$ yields

$$(D_N^{-1} W_N^* A)\underline{e}_n = \left[\begin{pmatrix} \eta_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} - H_N \begin{pmatrix} \underline{\gamma} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \right],$$

and we see that QMR is choosing $\underline{\gamma}_n$ to minimize

$$\|D_N^{-1} W_N^* A\underline{e}_n\|.$$

By definition, this is the same as

$$\langle D_N^{-1} W_N^* A \underline{e}_n, D_N^{-1} W_N^* A \underline{e}_n \rangle^{1/2} = \langle B \underline{e}_n, \underline{e}_n \rangle^{1/2} = \|\underline{e}_n\|_B,$$

where,

$$B = (D_N^{-1} W_N^* A)^* (D_N^{-1} W_N^* A) = A^* W_N D_N^{-*} D_N^{-1} W_N^* A.$$

Again, using (3.3), we see that $D_N^{-1} W_N^* A = V_N^{-1} A$, and it follows that B can be written equivalently in the form

$$B = A^* V_N^{-*} V_N^{-1} A.$$

Since the first column of V_N is the normalized initial residual, B depends upon $\underline{r}_0$. Also, we have that $\{\mathcal{V}_i\}_{i=1}^N = \{\mathcal{K}_i(\underline{r}_0, A)\}_{i=1}^N$, so that QMR can be viewed as a variable metric conjugate gradient method. We redefine the iterates generated by the QMR iteration by:

$$\begin{array}{rcll} \underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1}, & \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A), \\ \underline{e}_n & \perp_B & \underline{z}, & \forall \underline{z} \in \mathcal{K}_n(\underline{r}_0, A), \end{array} \tag{3.16}$$

where,

$$\begin{array}{rcl} B & = & A^* W_N D_N^{-*} D_N^{-1} W_N^* A, \\ & \text{or} & \\ B & = & A^* V_N^{-*} V_N^{-1} A, \end{array} \tag{3.17}$$

and V_N and W_N denote the matrices of biorthogonal Lanczos vectors.

At step N, the recurrences for the right Lanczos vectors are written in matrix notation as

$$A V_N = V_N H_N.$$

Multiplying through from the left, and again from the right by V_N^{-1} yields

$$V_N^{-1} A = H_N V_N^{-1} = Q_N R_N V_N^{-1}, \tag{3.18}$$

where the second equality follows from a QR factorization of H_N. Substituting (3.18) into (3.17) shows that B may also be written in the form:

$$B = V_N^{-*} R_N^* R_N V_N^{-1}. \tag{3.19}$$

Denote $P_N = V_N R_N^{-1}$, with columns $\{\underline{p}_j\}_{j=0}^{N-1}$. We recall from [FrNa91] that the $\underline{p}_j$'s are the step directions for the QMR iteration. Since the columns of V_N form an ascending basis for $\{\mathcal{V}_i\}_{i=1}^N$ and R_N is a nonsingular, upper triangular matrix, it follows that the columns of P_N also form an ascending basis for $\{\mathcal{V}_i\}_{i=1}^N$. Using (3.19), it is easy to see that $\{\underline{p}_j\}_{j=0}^{N-1}$ are a B-orthogonal basis. Therefore, Corollary 2.5 shows that all possible metrics, B, can be written in the form:

$$B = V_N^{-*} R_N^* \Omega_N R_N V_N^{-1} = P_N^{-*} \Omega_N P_N^{-1}, \tag{3.20}$$

for an arbitrary positive, diagonal matrix, Ω_N. This means that any B of the form given by (3.20) will produce the same sequence of iterates.

3.4. Generalizations of BCG and QMR. Recall that Lanczos biorthogonalization can be implemented with three term recursions for any nonnegative integer, p, yielding a pair of ascending bases

$$\{\underline{v}_{i(p)}\}_{i=0}^{N-1} \qquad \text{for} \qquad \{\mathcal{K}_i(\underline{r}_0, A)\}_{i=1}^{N},$$

$$\{\underline{w}_{i(p)}\}_{i=0}^{N-1} \qquad \text{for} \qquad \{\mathcal{K}_i(\underline{w}_0, A^*)\}_{i=1}^{N},$$

such that

$$\underline{w}_{j(p)}^* A^p \underline{v}_{i(p)} = \begin{cases} \delta_{i(p)} & i = j \\ 0 & i \neq j \end{cases}.$$

Denote the $N \times N$ matrices with columns $\underline{v}_{i(p)}$, and $\underline{w}_{i(p)}$, as $V_{(p)}$ and $W_{(p)}$ respectively. Also, recall from Lanczos the matrix notation for the recursions and orthogonality condition:

$$AV_{(p)} = V_{(p)} H_{(p)}, \qquad A^* W_{(p)} = W_{(p)} \tilde{H}_{(p)}, \tag{3.21}$$

$$W_{(p)}^* A^p V_{(p)} = D_{(p)} = \operatorname{diag}(\cdots \delta_{i(p)} \cdots). \tag{3.22}$$

Define BCG(p), for $p \geq 1$, as the family of methods whose iterates are defined by:

$$\begin{array}{rcll} \underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1}, & \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A), \\ \underline{e}_n & \perp & (A^*)^p \mathcal{K}_n(\underline{w}_0, A^*). & \end{array}$$

Notice that BCG(1) is the same as standard BCG, and that BCG(0) is not defined since it's implementation at each step, n, involves the unknown quantity, $\underline{e}_n$. These methods are all implemented via the Lanczos process with the corresponding power, p. Analogous derivations to that for BCG(1) shows that they all may be recast as variable metric conjugate gradient methods; that is, the iterates can be defined equivalently by:

$$\begin{array}{rcll} \underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1}, & \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A), \\ \underline{e}_n & \perp_B & \underline{z}, & \forall \underline{z} \in \mathcal{K}_n(\underline{r}_0, A), \end{array} \tag{3.23}$$

where,

$$B_{\mathrm{BCG}(p)} = (A^*)^p W_{(p)} D_{(p)}^{-*} \Omega_N D_{(p)}^{-1} W_{(p)}^* A^p = V_{(p)}^{-*} \Omega_N V_{(p)}^{-1}, \tag{3.24}$$

and again, Ω_N is an arbitrary positive diagonal matrix.

Likewise, we can generalize the QMR method by implementing it via the Lanczos iteration with different powers, p. This yields a family of methods we denote by QMR(p).

Define QMR(p), for $p \geq 0$, as the family of methods whose iterates satisfy:

$$\begin{array}{rcll} \underline{x}_n & = & \underline{x}_{n-1} + \underline{z}_{n-1}, & \underline{z}_{n-1} \in \mathcal{K}_n(\underline{r}_0, A), \\ \underline{e}_n & \perp_B & \underline{z}, & \forall \underline{z} \in \mathcal{K}_n(\underline{r}_0, A), \end{array} \tag{3.25}$$

where,

$$
\begin{aligned}
B_{\mathrm{QMR}(p)} &= (A^*)^{p+1} W_{(p)} D_{(p)}^{-*} D_{(p)}^{-1} W_{(p)}^* A^{p+1} = A^* V_{(p)}^{-*} V_{(p)}^{-1} A \\
&= V_{(p)}^{-*} R_{(p)}^* R_{(p)} V_{(p)}^{-1}.
\end{aligned} \tag{3.26}
$$

Note that QMR(0) is standard QMR. Again, any B of the form

$$B_{\mathrm{QMR}(p)} = V_{(p)}^{-*} R_{(p)}^* \Omega_N R_{(p)} V_{(p)}^{-1}, \tag{3.27}$$

where Ω_N is an arbitrary positive, diagonal matrix, will yield the same iterates.

From above, we can obtain a relationship between the metrics for BCG(p) and QMR(p). If we let $\Omega_N = I$ in both cases, we obtain

$$B_{\mathrm{QMR}(p)} = A^* B_{\mathrm{BCG}(p)} A.$$

Since BCG(0) is not defined, we can't directly relate QMR(0) (standard QMR) to a BCG method in terms of their metrics.

In Figure 3.1 we compare the convergence plots of QMR(0), QMR(1), and BCG(1) run on a real nonnormal annulus matrix. The convergence is measured in the relative residual norm, where QMR(0) is denoted by the solid line, QMR(1) the dashed line, and BCG(1) the dotted line. This behavior is typical of the examples we have run. BCG(1) demonstrates rather erratic convergence in the residual norm as compared to QMR(0) and QMR(1). All the examples we have run comparing QMR(0) and QMR(1) show very similar convergence plots measured in the residual norm.

The following identities may be derived from the Lanczos process and will be used in the theorems below. Recall from Section's 3.2 and 3.3, that the first column of $V_{(p)}$ is $\underline{r}_0/||\underline{r}_0||$, so that $\underline{r}_0 = ||\underline{r}_0|| V_{(p)} \underline{e}_1$, where $\underline{e}_1 = [1, 0, ..., 0]_N^T$. Multiplying from the left by $V_{(p)}^{-1}$ yields

$$V_{(p)}^{-1} \underline{r}_0 = ||\underline{r}_0|| \underline{e}_1. \tag{3.28}$$

From (3.21) we have that $(AV_{(p)})^{-1} = (V_{(p)} H_{(p)})^{-1}$ or

$$V_{(p)}^{-1} A^{-1} = H_{(p)}^{-1} V_{(p)}^{-1}. \tag{3.29}$$

By multiplying (3.21) from the left and again from the right by $V_{(p)}^{-1}$ we obtain

$$V_{(p)}^{-1} A = H_{(p)} V_{(p)}^{-1}, \tag{3.30}$$

and it follows that

$$V_{(p)}^{-1} p_n(A) = p_n(H_{(p)}) V_{(p)}^{-1}. \tag{3.31}$$

For any variable metric CG method, it follows from definition that

$$||\underline{e}_n||_B = \min_{p_n \in \mathcal{P}_n^\circ} ||p_n(A) \underline{e}_0||_B, \tag{3.32}$$

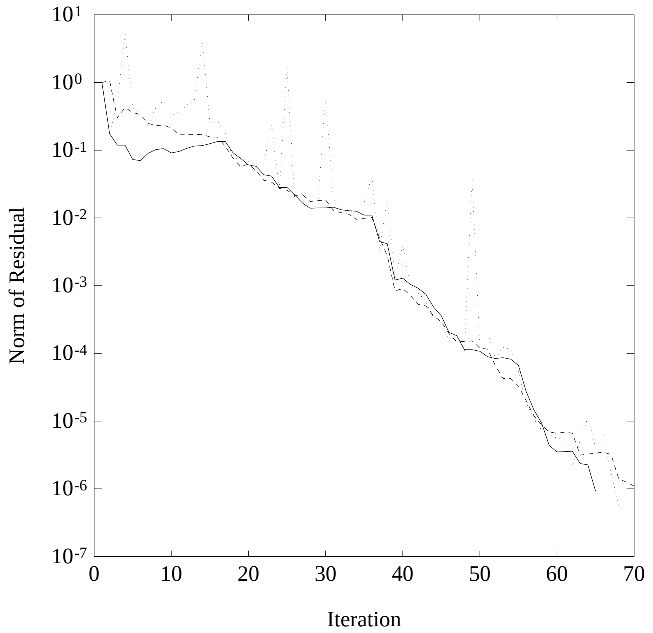

FIG. 3.1. *Convergence plots for QMR*(0) *(solid line), QMR*(1) *(dashed line), and BCG*(1) *(dotted line)*

where the HPD matrix, $B(\underline{x}_0)$, corresponds to the particular method. Recall that the matrix B is not unique. Any positive, diagonal matrix, Ω_N, in (3.27) for QMR(p), and (3.24) for BCG(p) will yield the same sequence of iterates. In the following convergence theorems for BCG(p) and QMR(p) we have set $\Omega_N = I_N$, the identity matrix. The reader should note that other choices for Ω_N will alter the bounds given in these theorems, and that it may be possible to choose Ω_N to yield smaller bounds for the relative residuals produced by these methods.

To be consistent with the presentation of BCG and QMR given earlier, we will assume these methods are implemented via the Lanczos process, without look-ahead strategies, and that there is no breakdown in this process. We also assume that $d(\underline{v}_0, A) = d(\underline{w}_0, A^*) = N$, and the Lanczos vectors are scaled to have unit length. A development with LAL is a straightforward generalization.

The next result is a generalization of the the bounds given in [FrNa91] for QMR(0).

THEOREM 3.1. *Let $H_{(p)}$ be the $N \times N$ matrix generated by N steps of the Lanczos iteration. For B given by*

$$B_{\mathrm{QMR}(p)} = A^* V_{(p)}^{-*} V_{(p)}^{-1} A, \tag{3.33}$$

the residual vectors generated by the QMR(p) methods satisfy:

$$\frac{||\underline{r}_n||}{||\underline{r}_0||} \le \sqrt{n+1} \min_{p_n \in \mathcal{P}_n^\circ} ||p_n(H_{(p)})\underline{\epsilon}_1||,$$

where $\underline{\epsilon}_1 = [1, 0, ..., 0]_N^T$. This bound can be computed from the first n columns of $H_{(p)}$.

Proof: For B given by (3.33), we can rewrite (3.32) as

$$\|V_{(p)}^{-1}A\underline{e}_n\| = \min_{p_n\in\mathcal{P}_n^\circ}\|V_{(p)}^{-1}Ap_n(A)\underline{e}_0\| = \min_{p_n\in\mathcal{P}_n^\circ}\|V_{(p)}^{-1}p_n(A)\underline{r}_0\|.$$

Using (3.28),(3.30), and (3.31), this becomes

$$\frac{\|V_{(p)}^{-1}\underline{r}_n\|}{\|\underline{r}_0\|} = \min_{p_n\in\mathcal{P}_n^\circ}\|p_n(H_{(p)})\underline{e}_1\|. \tag{3.34}$$

Since $\underline{r}_n \in \mathcal{K}_{n+1}(\underline{r}_0, A)$, we can write $\underline{r}_n = (V_{(p)})_{n+1}\underline{\xi}$, where $\underline{\xi}\in\mathcal{C}^{n+1}$ and $(V_{(p)})_{n+1}$ denotes the first $n+1$ columns of $V_{(p)}$. From this we see that

$$V_{(p)}^{-1}\underline{r}_n = \begin{pmatrix} \underline{\xi} \\ \underline{0} \end{pmatrix}_N = [\xi_0, \xi_1, ..., \xi_n, 0, ..., 0]_N^T,$$

and it follows that

$$\begin{aligned} \frac{\|\underline{r}_n\|}{\|\underline{r}_0\|} &= \frac{\|V_{(p)}V_{(p)}^{-1}\underline{r}_n\|}{\|\underline{r}_0\|} &= \frac{\|(V_{(p)})_{n+1}\underline{\xi}\|}{\|\underline{r}_0\|} \\ &\le \frac{\|(V_{(p)})_{n+1}\|\;\|\underline{\xi}\|}{\|\underline{r}_0\|} &= \|(V_{(p)})_{n+1}\|\,\frac{\|V_{(p)}^{-1}\underline{r}_n\|}{\|\underline{r}_0\|}. \end{aligned} \tag{3.35}$$

Since the columns of $V_{(p)}$ are unit vectors, it follows that $\|(V_{(p)})_{n+1}\| \le \sqrt{n+1}$ and, together with (3.34), we see a bound for the relative residuals is given by:

$$\frac{\|\underline{r}_n\|}{\|\underline{r}_0\|} \le \sqrt{n+1}\min_{p_n\in\mathcal{P}_n^\circ}\|p_n(H_{(p)})\underline{e}_1\|.$$

Since $p_n(H_{(p)})\underline{e}_1$ is just the first column of $p_n(H_{(p)})$, and $H_{(p)}$ is tridiagonal, it follows that this bound may be computed from the first n columns of $H_{(p)}$. $\square$

THEOREM 3.2. *Let $H_{(p)}$ be the $N\times N$ matrix generated by N steps of the Lanczos iteration. Denote by $(H_{(p)})^{n+1}$, the first $n+1$ rows of $H_{(p)}$. For B given by*

$$B_{\mathrm{BCG}(p)} = V_{(p)}^{-*}V_{(p)}^{-1}, \tag{3.36}$$

the residual vectors generated by the BCG(p) methods satisfy:

$$\frac{\|\underline{r}_n\|}{\|\underline{r}_0\|} \le \sqrt{n+1}\;\mathcal{C}((H_{(p)})^{n+1})\min_{p_n\in\mathcal{P}_n^\circ}\|p_n(H_{(p)})\underline{e}_1\|,$$

where $\underline{e}_1 = [1,0,...,0]_N^T$. This bound can be computed from the first $n+1$ rows of $H_{(p)}$.

Proof: For B given by (3.36), (3.32) becomes

$$\|V_{(p)}^{-1}\underline{e}_n\| = \min_{p_n\in\mathcal{P}_n^\circ}\|V_{(p)}^{-1}p_n(A)\underline{e}_0\|,$$

which can be rewritten as

$$\|V_{(p)}^{-1}A^{-1}\underline{r}_n\| = \min_{p_n\in\mathcal{P}_n^\circ}\|V_{(p)}^{-1}p_n(A)A^{-1}\underline{r}_0\|. \tag{3.37}$$

With (3.28)- (3.31), (3.37) becomes

$$\frac{\|H_{(p)}^{-1}V_{(p)}^{-1}\underline{r}_n\|}{\|\underline{r}_0\|} = \min_{p_n\in\mathcal{P}_n^o}\|H_{(p)}^{-1}p_n(H_{(p)})\underline{e}_1\|. \tag{3.38}$$

For simplification, we will use the notation:

$(M)_{n+1}$ to denote the first $n+1$ columns of the matrix, M, and

$(M)^{n+1}$ to denote the first $n+1$ rows.

Next, we write the residual vectors as

$$\underline{r}_n = V_{(p)}H_{(p)}H_{(p)}^{-1}V_{(p)}^{-1}\underline{r}_n. \tag{3.39}$$

Since $\underline{r}_n \in \mathcal{K}_{n+1}(\underline{r}_0, A)$ and the columns $(V_{(p)})_{n+1}$ span $\mathcal{K}_{n+1}(\underline{r}_0, A)$, it follows that $\underline{r}_n = (V_{(p)})_{n+1}\underline{\xi}$, where $\underline{\xi} \in \mathcal{C}^{n+1}$. From this we see that

$$V_{(p)}^{-1}\underline{r}_n = \begin{bmatrix} (V_{(p)}^{-1})^{n+1} \\ 0 \end{bmatrix}(V_{(p)})_{n+1}\underline{\xi} = \begin{pmatrix} \underline{\xi} \\ \underline{0} \end{pmatrix}_N = [\underline{\xi}_0, \underline{\xi}_1, ..., \underline{\xi}_n, 0, ..., 0]_N^T. \tag{3.40}$$

Using (3.40), we note that (3.39) may be rewritten as

$$\underline{r}_n = [(V_{(p)})_{n+1} : 0]\begin{bmatrix} (H_{(p)})^{n+1} \\ 0 \end{bmatrix}[(H_{(p)}^{-1})_{n+1} : 0]\begin{bmatrix} (V_{(p)}^{-1})^{n+1} \\ 0 \end{bmatrix}\underline{r}_n,$$

or

$$\underline{r}_n = (V_{(p)})_{n+1}(H_{(p)})^{n+1}(H_{(p)}^{-1})_{n+1}(V_{(p)}^{-1})^{n+1}\underline{r}_n. \tag{3.41}$$

Since the columns of $V_{(p)}$ are unit vectors, it follows that $\|(V_{(p)})_{n+1}\| \leq \sqrt{n+1}$. Taking norms in (3.41), dividing through by $\|\underline{r}_0\|$, and using (3.38) yields

$$\begin{aligned} \frac{\|\underline{r}_n\|}{\|\underline{r}_0\|} &\leq \sqrt{n+1}\ \|(H_{(p)})^{n+1}\|\ \frac{\|H_{(p)}^{-1}V_{(p)}^{-1}\underline{r}_n\|}{\|\underline{r}_0\|} \\ &= \sqrt{n+1}\ \|(H_{(p)})^{n+1}\|\ \min_{p_n\in\mathcal{P}_n^o}\|H_{(p)}^{-1}p_n(H_{(p)})\underline{e}_1\|. \end{aligned} \tag{3.42}$$

Since $H_{(p)}$ is tridiagonal and $p_n(H_{(p)})\underline{e}_1$ is the first column of $p_n(H_{(p)})$, it follows that $p_n(H_{(p)})\underline{e}_1$ can have nonzero entries only in the first $n+1$ rows. Therefore, $H_{(p)}^{-1}p_n(H_{(p)})\underline{e}_1 = (H_{(p)}^{-1})_{n+1}p_n(H_{(p)})\underline{e}_1$, and (3.42) becomes

$$\frac{\|\underline{r}_n\|}{\|\underline{r}_0\|} \leq \sqrt{n+1}\ \|(H_{(p)})^{n+1}\|\ \|(H_{(p)}^{-1})_{n+1}\|\ \min_{p_n\in\mathcal{P}_n^o}\|p_n(H_{(p)})\underline{e}_1\|.$$

Notice that $(H_{(p)})^{n+1}$ is the left inverse of $(H_{(p)}^{-1})_{n+1}$. Thus, $\|(H_{(p)})^{n+1}\|\ \|(H_{(p)}^{-1})_{n+1}\| = \mathcal{C}((H_{(p)})^{n+1})$, and it follows that a bound for the relative residuals produced by the BCG(p) methods is given by

$$\frac{\|\underline{r}_n\|}{\|\underline{r}_0\|} \leq \sqrt{n+1}\ \mathcal{C}((H_{(p)})^{n+1})\ \min_{p_n\in\mathcal{P}_n^o}\ \|p_n(H_{(p)})\underline{e}_1\|.$$

From the tridiagonal structure of $H_{(p)}$, it follows that both $\mathcal{C}((H_{(p)})^{n+1})$ and $p_n(H_{(p)})\underline{e}_1$ can be computed from the first $n+1$ rows of $H_{(p)}$. $\square$

4. Estimating the spectrum of A. For any fixed or variable metric conjugate gradient method, the error at each step is minimized with respect to an inner product norm, $\|\cdot\| = \langle B\cdot,\cdot\rangle^{1/2}$. Consequently, many of the results given in [MaOt92] for the CG iteration, apply to these methods. In particular, these methods produce direction vectors, $\underline{p}_n$'s, and residual vectors, $\underline{r}_n$'s, that satisfy

$$\underline{p}_n \perp_B \mathcal{K}_n(\underline{r}_0, A), \qquad A^{-1}\underline{r}_n \perp_B \mathcal{K}_n(\underline{r}_0, A).$$

Since $\underline{r}_n$, and $\underline{p}_n \in \mathcal{K}_{n+1}(\underline{r}_0, A)$, we can write

$$\underline{p}_n = \phi_n(A)\underline{r}_0, \qquad \underline{r}_n = \rho_n(A)\underline{r}_0,$$

for some polynomials $\phi_n(\lambda)$, $\rho_n(\lambda)$ of degree less than or equal to n. The polynomials $\phi_n(\lambda)$ and $\rho_n(\lambda)$ are called the B-orthogonal polynomials and the residual polynomials respectively.

The following theorems from [MaOt92] show how to find the roots of these polynomials.

THEOREM 4.1. *Suppose that* $\underline{p}_i = \phi_i(A)\underline{r}_0 \neq \underline{0}$ *with* $\phi_i(\lambda) = \prod_{j=1}^{b_i}(\lambda - \lambda_j)^{m_j}$ *and* $d_i \equiv \sum_{j=1}^{b_i} m_j = i$. *Suppose*

$$\underline{p}_i \perp_B \mathcal{K}_i(\underline{r}_0, A).$$

Let S_i *and* T_i *be any two* $N \times i$ *matrices whose columns span* $\mathcal{K}_i(\underline{r}_0, A)$. *Then the roots of*

$$\phi_i(\lambda) = 0$$

are the eigenvalues of the generalized eigenvalue problem

$$T_i^* BAS_i \underline{w} = \lambda T_i^* BS_i \underline{w}.$$

If $m_j > 1$, *then* $(T_i^* BS_i)^{-1}(T_i^* BAS_i)$ *has a Jordan block of size* m_j *associated with the eigenvalue* λ_j.

THEOREM 4.2. *Suppose that* $\underline{r}_i = \rho_i(A)\underline{r}_0 \neq 0$ *with* $\rho_i(\lambda) = \prod_{j=1}^{b_i}(1 - \frac{\lambda}{\lambda_j})^{m_j}$ *and* $d_i \equiv \sum_{j=1}^{b_i} m_j \leq i$. *Suppose*

$$A^{-1}\underline{r}_i \perp_B \mathcal{K}_i(\underline{r}_0, A).$$

Let S_i *and* T_i *be any two* $(N \times i)$ *matrices whose columns span* $\mathcal{K}_i(\underline{r}_0, A)$. *If* λ *is a root of*

$$\rho_i(\lambda) = 0$$

then $\frac{1}{\lambda}$ *is an eigenvalue of the generalized eigenvalue problem*

$$T_i^* BA^{-1} S_i \underline{w} = \frac{1}{\lambda} T_i^* BS_i \underline{w}.$$

If $m_j > 1$, *then* $(T_i^* BS_i)^{-1}(T_i^* BA^{-1} S_i)$ *has a Jordan block of size* m_j *associated with eigenvalue* $\frac{1}{\lambda_j}$. *If* $d_i < i$, *then* $(T_i^* BS_i)^{-1}(T_i^* BA^{-1} S_i)$ *has a nondiagonal Jordan block of size* i - d_i *associated with a zero eigenvalue.*

Details on the computation of these roots for the CG and the QMR iterations are given in [MaOt92] and [BaMa94], respectively. Next, we briefly review the results from [MaOt92] that show how these roots can be used to approximate the spectrum of A. First, we recall some definitions:

The B-field of values of A is defined as

$$\mathcal{F}_B(A) = \{\lambda : \lambda = \frac{\langle BA\underline{x}, \underline{x}\rangle}{\langle B\underline{x}, \underline{x}\rangle} \text{ for some } \underline{x} \neq \underline{0} \in \mathcal{C}^N\}. \tag{4.1}$$

The reciprocal B-field of values of A is the set

$$\mathcal{F}_B^{-1}(A^{-1}) = \{\lambda : \frac{1}{\lambda} \in \mathcal{F}_B(A^{-1})\}. \tag{4.2}$$

This technique for approximating the spectrum is based on two results:

(4.3) If λ is a root of an orthogonal polynomial, then $\lambda \in \mathcal{F}_B(A)$.

(4.4) If λ is a root of a residual polynomial, then $\dfrac{1}{\lambda} \in \mathcal{F}_B(A^{-1})$.

It follows from (4.2) and (4.4), that the roots of the residual polynomials are in $\mathcal{F}_B^{-1}(A^{-1})$. Notice that if $\mu_k \in \Sigma(A) \subseteq \mathcal{F}_B(A)$, then $\frac{1}{\mu_k} \in \Sigma(A^{-1}) \subseteq \mathcal{F}_B(A^{-1})$. From (4.2) we have that $\mu_k \in \mathcal{F}_B^{-1}(A^{-1})$. Therefore, we have both that $\Sigma(A) \subseteq \mathcal{F}_B(A)$ and $\Sigma(A) \subseteq \mathcal{F}_B^{-1}(A^{-1})$, thus

$$\Sigma(A) \subseteq \mathcal{G} \equiv \mathcal{F}_B(A) \cap \mathcal{F}_B^{-1}(A^{-1}).$$

It follows that the roots of the B-orthogonal polynomials and the roots of the residual polynomials can be used to construct regions that are in $\mathcal{F}_B(A)$ and $\mathcal{F}_B^{-1}(A^{-1})$, respectively. The intersection of these two regions can be used as an approximation of the spectrum. For details, the reader is referred to [MaOt92].

5. Conclusion. In this paper we have presented a framework for conjugate gradient-like methods. This structure provides tools for analyzing and comparing methods. Within this framework we defined a class of methods called variable metric conjugate gradient methods. Like the conjugate gradient method, these methods produce a sequence of iterates that satisfy a minimization property; that is, at each step the B norm of the error is minimized. For the CG method the matrix B is fixed for every initial guess. For a variable metric conjugate gradient method, B depends on the initial guess.

We have shown that the BCG and QMR methods can be classified as variable metric conjugate gradient methods. Generalizations of the BCG and QMR methods were defined by generalizing the underlying Lanczos process used in their implementation.

One consequence of this variable metric property is that these methods have associated B-orthogonal polynomials and residual polynomials. The roots of these polynomials can be used to approximate the spectrum of A. This variable metric property also provides an alternative approach to studying these methods. We can directly analyze and compare them by examining the metrics for which they are optimal.

Although convergence bounds for these methods are given by

$$\frac{||\underline{e}_n||}{||\underline{e}_0||} \le \mathcal{C}(B)^{1/2} \min_{p_n \in \mathcal{P}_n^o} \frac{||p_n(A)\underline{e}_0||}{||\underline{e}_0||},$$

the matrix B is dependent upon the initial guess, as well as the algorithm. For this bound to be useful, we need to bound $\mathcal{C}(B)^{1/2}$. A future direction of research might be the determination of classes of matrices for which uniform bounds on $\mathcal{C}(B(\underline{x}_0))$ can be established.

REFERENCES

[AMS90] S. F. Ashby, T. A. Manteuffel and P. E. Saylor, *A Taxonomy for Conjugate Gradient Methods*, SIAM J. Numer. Anal., 26 (1990), pp. 1542-1568.

[BaMa94] T. Barth and T. A. Manteuffel, *Estimating The Spectrum of A Using The Roots of the Polynomials Associated with the QMR Iteration*, submitted to SIAM J. Matrix Anal., March 1993.

[FaMa84] V. Faber and T. A. Manteuffel, *Necessary and Sufficient Conditions for the Existence of a Conjugate Gradient Method*, SIAM J. Numer. Analysis, Vol. 21, No. 2, pp. 352–362 (1984).

[FrGuNa91] R. W. Freund, M. H. Gutknecht, and N. M. Nachtigal, *An Implementation of the Look-Ahead Lanczos Algorithm for Non-Hermitian Matrices*, SIAM J. Sci. Comput., Vol. 14, No. 1, pp. 137-158, January 1993.

[FrNa91] R. W. Freund and N. M. Nachtigal, *QMR: a quasi-minimal residual method for non-Hermitian linear systems*, Numerische Mathematik 60 (1991), pp. 315-339.ddocument

[JoMa90] W. D. Joubert, and T. A. Manteuffel, *Iterative Methods for Nonsymmetric Linear Systems.*, "Iterative Methods for Large Linear Systems,", Academic Press, San Diego, 1990, pp. 149-171.

[MaOt92] T. A. Manteuffel, and J. S. Otto, *On The Roots of the Orthogonal Polynomials and Residual Polynomials Associated with a Conjugate Gradient Method*, to appear, Journal of Numerical Linear Algebra, 1993.

[Sa81] Y. Saad, *Krylov subspace methods for solving large unsymmetric linear systems*, J. Mathematics of Computation, Vol 37, pp. 105-126, (1981).

[Sa82] Y. Saad, *The Lanczos biorthogonalization algorithm and other oblique projection methods for solving large unsymmetric systems*, SIAM J. Numer. Anal., Vol 19, pp. 470-484, (1982).