Conjugate Gradient Algorithms Using Multiple Recursions *

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Abstract

Much is already known about when a conjugate gradient method can be implemented with short recursions for the direction vectors. The work done in 1984 by Faber and Manteuffel gave necessary and sufficient conditions on the iteration matrix A, in order for a conjugate gradient method to be implemented with a single recursion of a certain form. However, this form does not take into account all possible recursions. This became evident when Jagels and Reichel ([5],[6]) demonstrated that the class of matrices for which a practical conjugate gradient algorithm exists, can be extended to include unitary and shifted unitary matrices. The implementation uses short double recursions for the direction vectors. This motivates the study of multiple recursion algorithms. In this paper, we show that the conjugate gradient method for unitary and shifted unitary matrices can be implemented using a single short term recursion of a special type called an $(\ell,\, m)$ recursion with $\ell, m \leq 1$. We then examine the class of matrices for which a conjugate gradient method can be carried out using a general $(\ell,\, m)$ recursion.

1 Introduction

1.1 Motivation

A conjugate gradient (CG) method for the solution of an $N \times N$ linear system of equations

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

is defined with respect to a Hermitian positive definite (HPD) inner product matrix B, and the matrix A. We denote a conjugate gradient method by CG(B, A). These methods produce iterates that are uniquely defined as follows:

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

where

$$\mathcal{K}_{i+1}(\underline{r}_0, A) = \mathrm{sp}\{\underline{r}_0, A\underline{r}_0, ..., A^i\underline{r}_0\},$$

is the Krylov subspace of dimension $i+1$ generated by the initial residual $\underline{r}_0$, and the matrix A, the error at step $i+1$ is denoted by $\underline{e}_{i+1} = \underline{x} - \underline{x}_{i+1}$, and $\perp_B$ represents orthogonality in the B-inner product (c.f.[1]). CG(B, A) is implemented via the construction of a B-orthogonal basis $\{\underline{p}_j\}_{j=0}^{i}$ for $\mathcal{K}_{i+1}(\underline{r}_0, A)$. The $\underline{p}_j$'s are called direction vectors. There are

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many algorithms for implementing CG(B, A), for example: Orthodir, Orthomin, Orthores, and GMRES. A result from 1984 by Faber and Manteuffel states that the class of matrices for which a conjugate gradient method can be implemented via a single short s-term recursion of the form

$$\underline{p}_{i+1} = A\underline{p}_i - \sum_{j=i-s+2}^{i} \sigma_{i,j}\underline{p}_j, \tag{1}$$

for the direction vectors, is limited to matrices that are B-normal(s-2) (see Section 4.2), or to matrices with only a small number of distinct eigenvalues [3]. For these matrices, Orthodir and GMRES are two implementations of CG(B, A) that have recursions of the form given by (1). Joubert and Young [7] extended this result, showing that the Orthomin and Orthores implementations of CG(B, A) also yield short recursions for the direction vectors for B-normal(s-2) matrices.

The work done by Gragg [4] demonstrates that for a unitary matrix U, an orthonormal basis for $\mathcal{K}_{i+1}(\underline{r}_0, U)$ can be constructed using a pair or recurrence formulas. Shifted unitary matrices have the form

$$A = \rho U + \xi I, \tag{2}$$

where U is unitary, I is the identity matrix, and ρ and ξ are complex scalars. Jagels and Reichel ([5],[6]) observed that for matrices of this form, $\mathcal{K}_{i+1}(\underline{r}_0, A) = \mathcal{K}_{i+1}(\underline{r}_0, U)$, and from this they show how to use the Gragg algorithm (see Section 2.1) to construct an efficient minimal residual algorithm. This is an example of a class of matrices that is not B-normal(s-2), for small s, but for which a conjugate gradient method can be implemented using a pair of short recursions. Thus, by considering double recursions, the class of matrices for which a practical conjugate gradient algorithm exists can be extended to include unitary and shifted unitary matrices. In this paper, we will explore multiple recursions further.

Section 2 reviews the related work done by Gragg, Jagels and Reichel. In Section 3, we give an alternative minimal residual algorithm for shifted unitary matrices. Next, we will show that the pair of recurrence formulas used to construct an orthonormal basis for $\mathcal{K}_{i+1}(\underline{r}_0, A)$, when A is of the form (2), can be rewritten as a single recursion of the form

$$\underline{p}_{i+1} = \sum_{j=i-m}^{i} \beta_{i,j} A\underline{p}_j - \sum_{j=i-\ell}^{i} \sigma_{i,j}\underline{p}_j, \tag{3}$$

where $\ell = m = 1$. Section 4 considers general recursions of this form, where ℓ, m can be any integers ≥ 0. If a conjugate gradient method can be implemented with a short recursion of the form (3), we say $A \in \mathcal{CG}_B(\ell,\, m)$. Sufficient conditions on the matrix A are given for $A \in \mathcal{CG}_B(\ell,\, m)$. In [2] it is shown that for $\ell,\ m \leq 2$ these are also necessary conditions. Necessary conditions for $\ell,\ m > 2$ remain an open question. Section 5 summarizes these results. We conclude with a few remarks about work still in progress.

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.
$\mathrm{sp}\{\underline{x}_j\}$	–	The linear span of the vectors $\underline{x}_j$.
$\Sigma(A)$	–	Spectrum of A.
$\mathcal{K}_\ell(\underline{r}_0, A)$	–	$\mathrm{sp}\{\underline{r}_0, A\underline{r}_0, ..., A^{\ell-1}\underline{r}_0\}$ Krylov subspace of dimension ℓ.
$d(\underline{r}_0, A)$	–	Maximum dimension of Krylov subspace generated by $\underline{r}_0$ and A.
$d(A)$	–	Degree of the minimal polynomial of A.

2 Unitary and shifted unitary matrices

2.1 The Gragg algorithm for unitary matrices

It was shown by Gragg [4] that if U is an $N \times N$ unitary matrix, an orthonormal basis for $\mathcal{K}_\ell(\underline{v}_0, U)$ can be constructed with two short recursions. Suppose we let $\underline{v}_0 = \frac{\underline{r}_0}{\|\underline{r}_0\|}$, the normalized initial residual, and use a Gram-Schmidt process to construct an orthonormal basis $\{\underline{v}_j\}_{j=0}^{\ell-1}$ for $\mathcal{K}_\ell(\underline{r}_0, U)$. Denote the $N \times \ell$ matrix

$$V_\ell = \begin{bmatrix} | & | & & | \\ \underline{v}_0 & \underline{v}_1 & \cdots & \underline{v}_{\ell-1} \\ | & | & & | \end{bmatrix},$$

and suppose that $d(\underline{r}_0, U) = N$, where $d(\underline{r}_0, U)$ is the dimension of the maximum Krylov subspace generated by $\underline{r}_0$ and U. At step N the recursions for the $\underline{v}_j$'s may be written in matrix notation as

$$UV_N = V_N H_N, \tag{4}$$

where H_N is an $N \times N$ upper Hessenberg matrix. Since U is unitary, and by construction V_N is unitary, it follows from (4) that $V_N H_N$ is unitary and

$$(V_N H_N)^* V_N H_N = H_N^* H_N = I_N,$$

the $N \times N$ identity matrix. Therefore, H_N is a unitary, upper Hessenberg matrix. A QR factorization of H_N yields

$$H_N = Q_N R_N,$$

where Q_N is $N \times N$ unitary, and R_N is $N \times N$ upper triangular. Since $R_N = Q_N^* H_N$, it follows that R_N is also unitary. R_N being unitary and upper triangular implies that

$$R_N = \mathrm{diag}(\cdots e^{i\theta_j} \cdots),$$

for some $\theta_j,\ j = 1, \ldots, N$. Without loss of generality we may assume that $R_N = I_N$. The upper Hessenberg structure of H_N allows for the QR factorization to be computed efficiently using elementary unitary matrices

$$H_N = G_1 G_2 \cdots G_{N-1} R_N, \tag{5}$$

where

$$G_j = \begin{bmatrix} I_{j-1} & & & \\ & -\gamma_j & \sigma_j & \\ & \sigma_j & \bar{\gamma}_j & \\ & & & I_{N-j-1} \end{bmatrix},$$

and $\gamma_j \in \mathcal{C},\ |\gamma_j| \leq 1$, and $\sigma_j = (1 - |\gamma_j|^2)^{1/2}$. Since each G_j is a rank 2 correction of the identity matrix, it follows that the information content of H_N is of order N. By substituting (5) into (4) and equating columns we obtain:

$$\begin{aligned} U\underline{v}_0 &= -\gamma_1 \underline{v}_0 + \sigma_1 \underline{v}_1 \\ &\gamma_1 = -\langle U\underline{v}_0, \underline{v}_0 \rangle \\ &\sigma_1 = (1 - |\gamma_1|^2)^{1/2} \\ U\underline{v}_1 &= -\gamma_2(\sigma_1 \underline{v}_0 + \bar{\gamma}_1 \underline{v}_1) + \sigma_2 \underline{v}_2 \\ &\gamma_2 = -\langle U\underline{v}_1, \sigma_1 \underline{v}_0 + \bar{\gamma}_1 \underline{v}_1 \rangle \\ &\sigma_2 = (1 - |\underline{\gamma}_2|^2)^{1/2} \\ &\vdots \end{aligned}$$

Rearranging yields the Gragg algorithm:

$$\begin{aligned} \underline{v}_0 = \tilde{\underline{v}}_0 &= \frac{\underline{r}_0}{\|\underline{r}_0\|} \\ &\vdots \\ &\gamma_i = -\langle U\underline{v}_{i-1}, \tilde{\underline{v}}_{i-1} \rangle \\ &\sigma_i = (1 - |\gamma_i|^2)^{1/2} \\ \sigma_i \underline{v}_i &= U\underline{v}_{i-1} + \gamma_i \tilde{\underline{v}}_{i-1} \\ \tilde{\underline{v}}_i &= (\sigma_i \tilde{\underline{v}}_{i-1} + \bar{\gamma}_i \underline{v}_i) \\ &\vdots \end{aligned}$$

See ([4],[6]) for a more complete presentation. Another derivation of this double recursion for unitary matrices is given by Watkins [10].

2.2 A minimal residual algorithm for shifted unitary matrices

Jagels and Reichel [6] use the Gragg algorithm to construct an efficient minimal residual algorithm for the solution of the linear system, $A\underline{x} = \underline{b}$, where A is a shifted unitary matrix

(2). They observe that $\mathcal{K}_\ell(\underline{r}_0, A) = \mathcal{K}_\ell(\underline{r}_0, U)$. Thus, the Gragg algorithm can be used to construct an orthonormal basis for $\mathcal{K}_\ell(\underline{r}_0, A)$. This basis is then used to construct a minimal residual algorithm as follows:

At step ℓ of the Gram-Schmidt process, the recursions for the basis vectors, $\{\underline{v}_j\}_{j=0}^{\ell}$, can be written in matrix form as

$$UV_\ell = V_{\ell+1} H_{\ell+1,\ell}^{(U)}, \tag{6}$$

where $H_{\ell+1,\ell}^{(U)}$ is the $(\ell+1) \times \ell$ upper Hessenberg matrix,

$$H_{\ell+1,\ell}^{(U)} = G_1 G_2 \cdots G_{\ell-1} \tilde{G}_\ell,$$

and

$$G_j = \begin{bmatrix} I_{j-1} & & & \\ & -\gamma_j & \sigma_j & \\ & \sigma_j & \bar{\gamma}_j & \\ & & & I_{\ell-j-1} \end{bmatrix}, \qquad \tilde{G}_\ell = \begin{bmatrix} I_{\ell-1} & & \\ & \gamma_\ell & \\ & \sigma_\ell & \end{bmatrix}.$$

Using (2) and (6) we see that

$$AV_\ell = (\rho U + \xi I) V_\ell = V_{\ell+1}(\rho H_{\ell+1,\ell}^{(U)} + \xi \hat{I}_\ell) = V_{\ell+1} H_{\ell+1,\ell}^{(A)}, \tag{7}$$

where

$$\hat{I}_\ell = \begin{bmatrix} I_\ell \\ \underline{0}^T \end{bmatrix} \in \mathcal{C}^{(\ell+1)\times\ell}.$$

We remark here, that instead of deriving $H_{\ell+1,\ell}^{(A)}$ from $H_{\ell+1,\ell}^{(U)}$, one could obtain $H_{\ell+1,\ell}^{(A)}$ directly by substituting $U = \frac{1}{\rho}(A - \xi I)$ into the Gragg algorithm. Now, the standard argument for constructing a GMRES algorithm (c.f.[9]) is employed. Since $\|\underline{r}_0\|\underline{v}_0 = \underline{r}_0$, we have for some $\underline{y}_\ell \in \mathcal{C}^\ell$

$$\underline{r}_\ell = \underline{r}_0 - AV_\ell \underline{y}_\ell = V_{\ell+1}[\|\underline{r}_0\|\epsilon_1 - H_{\ell+1,\ell}^{(A)} \underline{y}_\ell],$$

where $\epsilon_1 = [1, 0, ..., 0]^T$. The objective is to choose $\underline{y}_\ell$ to minimize $\|\underline{r}_\ell\|$. Since $V_{\ell+1}$ has orthonormal columns, this may be accomplished by solving the $(\ell+1) \times \ell$ least squares problem

$$\|\underline{r}_0\|\epsilon_1 \approx H_{\ell+1,\ell}^{(A)} \underline{y}_\ell.$$

Since $(\rho H_{\ell+1,\ell}^{(U)} + \xi \hat{I}_\ell) = H_{\ell+1,\ell}^{(A)}$ is upper Hessenberg, a QR factorization of $H_{\ell+1,\ell}^{(A)}$ is accomplished by Givens matrices. The relationship between $H_{\ell+1,\ell}^{(A)}$ and $H_{\ell+1,\ell}^{(U)}$ allows the least squares problem to be solved using an algorithm that involves five short recursions. See ([6]) for details.

3 B-unitary and shifted B-unitary matrices

3.1 A new minimal residual algorithm for shifted unitary matrices

In this section, we present an alternative minimal residual algorithm for shifted unitary matrices. This reformulation will motivate the development in Section 4. First, let us restate the minimal residual method for the solution of the linear system, $A\underline{x} = \underline{b}$, as a conjugate gradient method whose iterates are uniquely defined by:

$$\begin{array}{lll} \underline{x}_{i+1} & = & \underline{x}_i + \alpha_i \underline{p}_i, \qquad \underline{p}_i \in \mathcal{K}_{i+1}(\underline{r}_0, A), \\ \underline{e}_{i+1} & \perp_{A^*A} & \mathcal{K}_{i+1}(\underline{r}_0, A). \end{array}$$

In this context, it is clear that the direction vectors, $\underline{p}_i$'s, must satisfy

$$\begin{array}{lll} \underline{p}_i & \in & \mathcal{K}_{i+1}(\underline{r}_0, A), \\ \underline{p}_i & \perp_{A^*A} & \mathcal{K}_i(\underline{r}_0, A). \end{array}$$

Suppose that $d(\underline{r}_0, A) = N$. We seek a basis, $\{\underline{p}_0, \underline{p}_1, ..., \underline{p}_{N-1}\}$, for $\mathcal{K}_N(\underline{r}_0, A)$, such that

$$\langle A^*A\underline{p}_i, \underline{p}_j \rangle = \begin{cases} 0 & i \neq j, \\ 1 & i = j. \end{cases}$$

Now, suppose that A is shifted unitary, i.e., $A = \rho U + \xi I$, where U is unitary and that $N = d(\underline{r}_0, U) = d(\underline{r}_0, A)$. Note that in this case $\mathcal{K}_\ell(\underline{r}_0, A) = \mathcal{K}_\ell(\underline{r}_0, U)$. Thus, it is sufficient to find an A^*A orthogonal basis for $\mathcal{K}_\ell(\underline{r}_0, U)$. Next, note that if U is unitary with respect to I, and $A = \rho U + \xi I$, then

$$A^*AU = UA^*A. \tag{8}$$

It follows that U is A^*A-unitary, or in other words, U is isometric with respect to the inner product $\langle A^*A\cdot, \cdot \rangle$,

$$\langle A^*AU\underline{x}, U\underline{y} \rangle = \langle UA^*A\underline{x}, U\underline{y} \rangle = \langle A^*A\underline{x}, \underline{y} \rangle, \quad \forall \underline{x},\ \underline{y} \in \mathcal{C}^N. \tag{9}$$

Gragg [4] gave a more general result than what we presented in Section 2.1. This result says that if a matrix U_B is isometric with respect to any inner product, $\langle B\cdot, \cdot \rangle$, then a B-orthonormal basis for $\mathcal{K}_\ell(\underline{r}_0, U_B)$ can be constructed with a short double recursion of the form given in Section 2.1. We show how this is done in the shifted unitary case, where U is isometric with respect to the inner product $\langle A^*A\cdot, \cdot \rangle$. Consider a Gram-Schmidt process to construct an A^*A-orthonormal basis for $\mathcal{K}_N(\underline{r}_0, U)$. At step N, the recursions can be written in matrix form as

$$UP_N = P_N H_N, \tag{10}$$

where H_N is a $N \times N$ upper Hessenberg matrix. Multiplying both sides of (10) by $P_N^* U^* A^* A$, we obtain

$$P_N^* U^* A^* AUP_N = P_N^* U^* A^* AP_N H_N.$$

Using (8) and (10) this becomes

$$P_N^* A^* AP_N = H_N^* P_N^* A^* AP_N H_N.$$

Since P_N is constructed so that $P_N^* A^* AP_N = I_N$, it follows that $I_N = H_N^* H_N$, and H_N is I-unitary. Therefore, H_N can be written as a product of Givens matrices. In fact, the iteration to produce an A^*A-orthonormal basis is exactly like the Gragg algorithm except that the standard inner product $\langle \cdot, \cdot \rangle$ is replaced by $\langle A^*A\cdot, \cdot \rangle$. The algorithm is:

$$\begin{array}{rcl} \underline{p}_0 = \tilde{\underline{p}}_0 & = & \underline{r}_0 / \|\underline{r}_0\|_{A^*A}, \\ & \vdots & \\ & & \gamma_i = -\langle AU\underline{p}_{i-1}, A\tilde{\underline{p}}_{i-1} \rangle, \\ & & \\ & & \sigma_i = (1 - |\gamma_i|^2)^{1/2}, \\ & & \\ \sigma_i \underline{p}_i & = & U\underline{p}_{i-1} + \gamma_i \tilde{\underline{p}}_{i-1} \\ & & \\ \tilde{\underline{p}}_i & = & (\sigma_i \tilde{\underline{p}}_{i-1} + \bar{\gamma}_i \underline{p}_i), \\ & \vdots & \end{array}$$

Given $\underline{x}_0$, the basis thus computed can be used to solve the linear system, $A\underline{x} = \underline{b}$, by adding at each step the recursions,

$$\begin{aligned} \underline{x}_{i+1} &= \underline{x}_i + \alpha_i \underline{p}_i, \quad \alpha_i = \frac{\langle A^* A\underline{e}_i, \underline{p}_i\rangle}{\langle A^* A\underline{p}_i, \underline{p}_i\rangle} = \langle \underline{r}_i, A\underline{p}_i\rangle, \\ \underline{r}_{i+1} &= \underline{r}_i - \alpha_i A\underline{p}_i. \end{aligned}$$

Note that the algorithm above requires multiplications by both U and A. To rearrange the algorithm to one requiring only multiplication by U, define the quantities

$$\underline{q}_i = A\underline{p}_i \quad \text{and} \quad \tilde{\underline{q}}_i = A\tilde{\underline{p}}_i.$$

Notice that for $A = \rho U + \xi I$, A and U commute, thus, multiplying the equations for $\underline{p}_i$, and $\tilde{\underline{p}}_i$ by A, we obtain

$$\sigma_i \underline{q}_i = U\underline{q}_{i-1} + \gamma_i \tilde{\underline{q}}_{i-1}, \quad \text{and} \quad \tilde{\underline{q}}_i = (\sigma_i \tilde{\underline{q}}_{i-1} + \bar{\gamma}_i \underline{q}_i).$$

Also, since $A\underline{p}_i = \rho U\underline{p}_i + \xi \underline{p}_i$, we can write

$$U\underline{p}_i = \frac{1}{\rho}(\underline{q}_i - \xi \underline{p}_i).$$

Using this information we rewrite the above minimal residual algorithm for shifted unitary matrices.

$$\begin{aligned} \underline{p}_0 &= \tilde{\underline{p}}_0 = \underline{r}_0 / \|\underline{r}_0\|_{A^*A}, \\ \underline{q}_0 &= \tilde{\underline{q}}_0 = A\underline{p}_0, \\ \underline{x}_1 &= \underline{x}_0 + \alpha_0 \underline{p}_0, \quad \alpha_0 = \langle \underline{r}_0, \underline{q}_0\rangle, \\ \underline{r}_1 &= \underline{r}_0 - \alpha_0 \underline{q}_0, \\ &\vdots \\ & \gamma_i = -\langle U\underline{q}_{i-1}, \tilde{\underline{q}}_{i-1}\rangle, \\ & \sigma_i = (1 - |\gamma_i|^2)^{1/2}, \\ \underline{q}_i &= \tfrac{1}{\sigma_i}(U\underline{q}_{i-1} + \gamma_i \tilde{\underline{q}}_{i-1}), \\ \underline{p}_i &= \tfrac{1}{\rho\sigma_i}(\underline{q}_{i-1} - \xi \underline{p}_{i-1}) + \tfrac{\gamma_i}{\sigma_i}\tilde{\underline{p}}_{i-1} \\ \tilde{\underline{q}}_i &= \sigma_i \tilde{\underline{q}}_{i-1} + \bar{\gamma}_i \underline{q}_i, \\ \tilde{\underline{p}}_i &= \sigma_i \tilde{\underline{p}}_{i-1} + \bar{\gamma}_i \underline{p}_i, \\ \underline{x}_{i+1} &= \underline{x}_i + \alpha_i \underline{p}_i, \quad \alpha_i = \langle \underline{r}_i, \underline{q}_i\rangle, \\ \underline{r}_{i+1} &= \underline{r}_i - \alpha_i \underline{q}_i, \\ &\vdots \end{aligned}$$

This algorithm requires the storage of 7 vectors:

$$\underline{x}_i,\ \underline{r}_i,\ \underline{p}_{i-1},\ \tilde{\underline{p}}_{i-1},\ \underline{q}_{i-1},\ \tilde{\underline{q}}_{i-1},\ U\underline{q}_{i-1}.$$

The approximate cost per iteration is:

1). 1 Matrix vector multiplication: $U\underline{q}_{i-1}$

2). 2 inner products: $\langle \underline{r}_i, \underline{q}_i \rangle$, $\langle U\underline{q}_{i-1}, \tilde{\underline{q}}_{i-1} \rangle$

3). 7 SAXPY.

The computational and storage requirements are comparable to the Jagels and Reichel algorithm, which requires approximately 1 matrix vector multiplication, 1 inner product, 6 SAXPY, and the storage of 6 vectors.

3.2 CG algorithms for general B-unitary and shifted B-unitary matrices

For shifted unitary matrices (2), U is isometric with respect to the inner product $\langle A^*A\cdot, \cdot \rangle$. Thus, an A^*A orthonormal basis for $\mathcal{K}_N(\underline{r}_0, A)$ can be generated with a pair of short recursions. Consequently, a minimal residual method, CG(B, A), with $B = A^*A$, can be implemented practically.

These results can be generalized to obtain practical conjugate gradient algorithms for any matrices that are isometric with respect to some inner product $\langle B\cdot, \cdot \rangle$ and for which $\langle B\underline{e}_i, \underline{p}_i \rangle$ is computable (see below). We refer to these matrices as B-unitary, and denote them by U_B. They satisfy

$$\langle BU_B\underline{x}, U_B\underline{y} \rangle = \langle B\underline{x}, \underline{y} \rangle, \quad \forall \underline{x},\ \underline{y} \in \mathcal{C}^N.$$

Matrix notation after step N of a Gram-Schmidt process to construct a B-orthonormal basis for $\mathcal{K}_N(\underline{r}_0, U_B)$ is given by

$$U_BP_N = P_NH_N, \tag{11}$$

where H_N is a $N \times N$ upper Hessenberg matrix. Multiplying through on the left by $P_N^*U_B^*B$ and then substituting in $P_N^*U_B^* = H_N^*P_N^*$ and $U_B^*BU_B = B$ in (11) yields

$$P_N^*BP_N = H_N^*P_N^*BP_NH_N.$$

Since $P_N^*BP_N = I_N$ by construction, it follows that H_N is I-unitary, thus it can be factored into a product of elementary unitary matrices. Analogous to the unitary case in Section 2, the substitution of this factorization for H_N into (11) and equating the columns yields the recursion formulas for the basis vectors.

A shifted B-unitary matrix A_B has the form

$$A_B = \rho U_B + \xi I.$$

Since $\mathcal{K}_N(\underline{r}_0, A_B) = \mathcal{K}_N(\underline{r}_0, U_B)$, the same B-orthonormal basis for $\mathcal{K}_N(\underline{r}_0, U_B)$ can be used for $\mathcal{K}_N(\underline{r}_0, A_B)$. Thus a conjugate gradient method for shifted B-unitary matrices can also be implemented with short recursions.

An algorithm for CG(B, A), where A is either B-unitary, or shifted B-unitary, can be obtained as follows: Construct a B-orthonormal basis for $\mathcal{K}_N(\underline{r}_0, A)$ using the Gragg algorithm generalized to the B-inner product. At each step i, perform the additional recursions,

$$\begin{aligned} \underline{x}_{i+1} &= \underline{x}_i + \alpha_i\underline{p}_i, \quad \alpha_i = \frac{\langle B\underline{e}_i, \underline{p}_i \rangle}{\langle B\underline{p}_i, \underline{p}_i \rangle} = \langle B\underline{e}_i, \underline{p}_i \rangle, \\ \underline{r}_{i+1} &= \underline{r}_i - \alpha_iA\underline{p}_i. \end{aligned}$$

Note that, since the computation of the α_i's involves the unknown quantity of the error, B must be chosen so that α_i is computable.

4 Single (ℓ, m) recursions

4.1 CG using single (ℓ, m) recursions

In Section 3, we saw that if A is a shifted B-unitary matrix, i.e., $A = A_B = \rho U_B + \xi I$, a double recursion,

$$\begin{aligned} \sigma_i \underline{p}_i &= U_B \underline{p}_{i-1} + \gamma_i \tilde{\underline{p}}_{i-1}, \\ \tilde{\underline{p}}_i &= \sigma_i \tilde{\underline{p}}_{i-1} + \bar{\gamma}_i \underline{p}_i, \end{aligned} \tag{12}$$

can be used to construct a B-orthonormal basis for $\mathcal{K}_N(\underline{r}_0, A)$, where $N = d(\underline{r}_0, A)$. At step $i+1$, form

$$\sigma_{i+1} \underline{p}_{i+1} = U_B \underline{p}_i + \gamma_{i+1} \tilde{\underline{p}}_i.$$

For $\tilde{\underline{p}}_i$, substitute the second equation in (12) to obtain

$$\sigma_{i+1} \underline{p}_{i+1} = U_B \underline{p}_i + \gamma_{i+1}(\sigma_i \tilde{\underline{p}}_{i-1} + \bar{\gamma}_i \underline{p}_i).$$

Solving the first equation in (12) for $\tilde{\underline{p}}_{i-1}$, and making this substitution into the above yields the recursion,

$$\underline{p}_{i+1} = \frac{1}{\sigma_{i+1}} U_B \underline{p}_i - \frac{\gamma_{i+1}\sigma_i}{\gamma_i \sigma_{i+1}} U_B \underline{p}_{i-1} + \left(\frac{\gamma_{i+1}\sigma_i^2}{\gamma_i \sigma_{i+1}} + \frac{\gamma_{i+1}\bar{\gamma}_i}{\sigma_{i+1}} \right) \underline{p}_i. \tag{13}$$

With the substitution of $U_B = \frac{1}{\rho}(A - \xi I)$, (13) becomes

$$\begin{aligned} \underline{p}_{i+1} &= \tfrac{1}{\rho\sigma_{i+1}} A\underline{p}_i - \tfrac{\gamma_{i+1}\sigma_i}{\rho\gamma_i\sigma_{i+1}} A\underline{p}_{i-1} \\ &+ \left(\tfrac{\gamma_{i+1}\sigma_i^2}{\gamma_i\sigma_{i+1}} - \tfrac{\xi}{\rho\sigma_{i+1}} + \tfrac{\gamma_{i+1}\bar{\gamma}_i}{\sigma_{i+1}} \right) \underline{p}_i + \tfrac{\gamma_{i+1}\sigma_i\xi}{\rho\gamma_i\sigma_{i+1}} \underline{p}_{i-1}. \end{aligned} \tag{14}$$

Thus, for shifted B-unitary matrices, the double recursion (12) can be rewritten as a single recursion (14), involving the two previous $A\underline{p}$'s and the two previous $\underline{p}$'s. (Notice that, if A is B-unitary, i.e., $A = U_B$, the double recursion (12) still yields a B-orthonormal basis for $\mathcal{K}_N(\underline{r}_0, A)$, and it can be rewritten as the single recursion given by (13).)

In this section, we will consider general recursions of the form

$$\underline{p}_{i+1} = \sum_{j=i-m}^{i} \beta_{i,j} A\underline{p}_j - \sum_{j=i-\ell}^{i} \sigma_{i,j} \underline{p}_j, \tag{15}$$

where ℓ and m can be any integers ≥ 0. If a recursion of this form yields a B-orthonormal basis for $\mathcal{K}_N(\underline{r}_0, A)$, for some integers $\ell,\ m \geq 0$, we say $A \in \mathcal{CG}_B(\ell, m)$. Note that, $\underline{p}_{i+1}$ can always be computed by a recursion of the form

$$\underline{p}_{i+1} = \sum_{j=i-m}^{i} \beta_{i,j} A\underline{p}_j - \sum_{j=0}^{i} \sigma_{i,j} \underline{p}_j,$$

because, given any $\{\beta_{i,j}\}_{j=i-m}^{i}$, there exists $\{\sigma_{i,j}\}_{j=0}^{i}$ given by

$$\sigma_{i,j} = \frac{\langle \sum_{j=i-m}^{i} \beta_{i,j} A\underline{p}_j, \underline{p}_j \rangle_B}{\langle \underline{p}_j, \underline{p}_j \rangle_B}, \qquad j = 0, ..., i.$$

However, we are interested in determining the class of matrices for which a B-orthonormal basis can be constructed using a short recursion of the form (15), that is, with both ℓ and m small. With this in mind, we make the following definition.

DEFINITION 4.1. *$A \in \mathcal{CG}_B(\ell,\, m)$ if for every $\underline{p}_0$ and every $0 \leq i \leq d(\underline{p}_0, A) - 1$, there exists coefficients $\{\beta_{i,j}\}_{j=i-m}^{i}$ such that*

$$\sigma_{i,k} = \frac{\langle \sum_{j=i-m}^{i} \beta_{i,j} A\underline{p}_j, \underline{p}_k \rangle_B}{\langle \underline{p}_k, \underline{p}_k \rangle_B} = 0, \qquad \text{for } k = 0, ..., i-\ell-1. \tag{16}$$

We note here, that the recursion (15) is of a more general form than that given by (1). By letting $m = 0$ and $\ell = s - 2$ in (15) we obtain the form (1). Also, the direction vectors for unitary and shifted unitary matrices can be constructed with a short (ℓ, m) recursion, whereas they cannot be obtained with a short recursion of the form (1). In a similar manner as in the unitary and shifted unitary cases, it can be shown that many short multiple recursions can be rewritten as single (ℓ, m) recursions, for some small $\ell,\ m$. These multiple recursions can be analyzed as single (ℓ, m) recursions.

4.2 Sufficient conditions for $A \in \mathcal{CG}_B(\ell,\, m)$

We first review some terminology on normal matrices. Recall that a conjugate gradient method is defined with respect to an HPD inner product matrix B, and the system matrix A. The B-adjoint of A is the unique matrix, $A^\dagger$, satisfying

$$\langle BA\underline{x}, \underline{y} \rangle = \langle B\underline{x}, A^\dagger \underline{y} \rangle, \qquad \forall \underline{x}, \underline{y} \in \mathcal{C}^N.$$

This yields, $A^\dagger = B^{-1}A^*B$. The matrix A is B-normal if it satisfies the following equivalent conditions:

i) $AA^\dagger = A^\dagger A$,

ii) $A, A^\dagger$ have the same complete set of B-orthogonal eigenvectors,

iii) $A^\dagger$ can be written as a polynomial of some degree η in the matrix A.

We say that A is B-normal(s) if it is B-normal, and s is the smallest degree for which $A^\dagger = P_\eta(A)$.

DEFINITION 4.2. *A is B-normal(ℓ, m) if A is B-normal and there exists polynomials $p_\ell(\lambda)$ and $q_m(\lambda)$, of degree ℓ and m respectively, such that*

$$A^\dagger q_m(A) = p_\ell(A). \tag{17}$$

Since $A^\dagger = \frac{p_\ell(A)}{q_m(A)}$, we say A is B-normal with rational degree ℓ/m.

Note that if $m = 0$, (17) becomes

$$A^\dagger = \hat{p}_\ell(A),$$

and A is B-normal(ℓ).

The following Lemma gives sufficient conditions on the matrix A for $A \in \mathcal{CG}_B(\ell,\, m)$.

LEMMA 4.1. *If A is B-normal(ℓ, m), then $A \in \mathcal{CG}_B(\ell,\, m)$.*

Proof. In order for $A \in \mathcal{CG}_B(\ell,\, m)$, (16) must be satisfied, or equivalently,

$$\sigma_{i,k} = \langle \sum_{j=i-m}^{i} \beta_{i,j}\underline{p}_j, A^\dagger \underline{p}_k\rangle_B = 0, \qquad k = 0, ..., i-\ell-1.$$

There are polynomials, ψ_k, $\tilde{\psi}_{k-m}$, and $r_{m-1}^{(k)}$ such that

$$\underline{p}_k = \psi_k(A)\underline{p}_0 = q_m(A)\tilde{\psi}_{k-m}(A)\underline{p}_0 + r_{m-1}^{(k)}(A)\underline{p}_0,$$

where the second equality follows upon division of $\psi_k(\lambda)$ by $q_m(\lambda)$. After multiplying by $A^\dagger$, since A is B-normal(ℓ, m), we can use (17) to yield

$$\begin{aligned} A^\dagger \underline{p}_k &= A^\dagger q_m(A)\tilde{\psi}_{k-m}(A)\underline{p}_0 + A^\dagger r_{m-1}^{(k)}(A)\underline{p}_0 \\ &= p_\ell(A)\tilde{\psi}_{k-m}(A)\underline{p}_0 + A^\dagger r_{m-1}^{(k)}(A)\underline{p}_0. \end{aligned}$$

For $k = 0, ..., i-\ell-1$,

$$\begin{aligned} p_\ell(A)\tilde{\psi}_{k-m}(A)\underline{p}_0 &\in \mathrm{sp}\{\underline{p}_0, \underline{p}_1, ..., \underline{p}_{i-m-1}\}, \\ &\text{and} \\ A^\dagger r_{m-1}^{(k)}(A)\underline{p}_0 &\in \mathrm{sp}\{A^\dagger\underline{p}_0, A^\dagger\underline{p}_1, ..., A^\dagger\underline{p}_{m-1}\}. \end{aligned}$$

Since $\mathrm{sp}\{\underline{p}_0, \underline{p}_1, ..., \underline{p}_{i-m-1}\}$ is B-orthogonal to $\mathrm{sp}\{\underline{p}_{i-m}, ..., \underline{p}_i\}$, we only need to choose $\{\beta_{i,j}\}_{j=i-m}^{i}$ so that

$$\langle \sum_{j=i-m}^{i} \beta_{i,j}\underline{p}_j, A^\dagger r_{m-1}^{(k)}(A)\underline{p}_0\rangle_B = 0, \qquad \text{for } k = 0, ..., i-\ell-1,$$

or equivalently, choose $\{\beta_{i,j}\}_{j=i-m}^{i}$ to satisfy

$$\text{(18)} \quad \begin{bmatrix} \langle \underline{p}_i, A^\dagger\underline{p}_0\rangle_B & \langle \underline{p}_{i-1}, A^\dagger\underline{p}_0\rangle_B & \cdots & \langle \underline{p}_{i-m}, A^\dagger\underline{p}_0\rangle_B \\ \langle \underline{p}_i, A^\dagger\underline{p}_1\rangle_B & \langle \underline{p}_{i-1}, A^\dagger\underline{p}_1\rangle_B & \cdots & \langle \underline{p}_{i-m}, A^\dagger\underline{p}_1\rangle_B \\ \vdots & \vdots & & \vdots \\ \langle \underline{p}_i, A^\dagger\underline{p}_{m-1}\rangle_B & \langle p_{i-1}, A^\dagger\underline{p}_{m-1}\rangle_B & \cdots & \langle \underline{p}_{i-m}, A^\dagger\underline{p}_{m-1}\rangle_B \end{bmatrix} \begin{pmatrix} \beta_{i,i} \\ \beta_{i,i-1} \\ \vdots \\ \beta_{i,i-m} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

This system can always be solved for the $\beta_{i,j}$'s. Therefore, if A is B-normal(ℓ, m), then $A \in \mathcal{CG}_B(\ell,\, m)$. ∎

REMARK 4.1. *While the system (18) always has a nontrivial solution, unless a solution exists for which $\beta_{i,i} \neq 0$, the desired result will not be achieved. If $\beta_{i,i} = 0$, equation (15) will yield $\underline{p}_{i+1} \in \mathcal{K}_{i-1}(\underline{p}_0,\, A)$ such that $\underline{p}_{i+1} \perp \mathcal{K}_{i-1}(\underline{p}_0,\, A)$, that is, $\underline{p}_{i+1} \equiv \underline{0}$. We call this condition breakdown of the algorithm. Using techniques similar to those in ([8]) it can be shown that breakdown occurrs for $\underline{p}_0$ in a set of measure zero. Moreover, there is a reorganization of the computations that avoids breakdown. Details will appear in [2].*

Next we characterize B-normal$(\ell,\, m)$ matrices. Recall that B-normal(ℓ, m) matrices satisfy

$$\text{(19)} \qquad A^\dagger = \frac{p_\ell(A)}{q_m(A)} = \frac{a_\ell A^\ell + \cdots + a_1 A + a_0 I}{b_m A^m + \cdots + b_1 A + b_0 I},$$

for some polynomials,

$$p_\ell(\mu) = a_\ell \mu^\ell + \cdots + a_1 \mu + a_0 \quad \text{and} \quad q_m(\mu) = b_m \mu^m + \cdots + b_1 + b_0,$$

of degree ℓ and m respectively. In the following Theorem which characterizes B-normal(ℓ, m) matrices, we will assume that ℓ and m are the smallest degrees for which (19) holds. This means that $a_\ell,\ b_m \neq 0$, and that $p_\ell(\mu)$ and $q_m(\mu)$ have no common roots, since otherwise, (19) would hold for some smaller degrees ℓ' and m'.

THEOREM 4.1. *Let A be B-normal(ℓ, m), where ℓ and m are the smallest degrees for which*

$$A^\dagger = \frac{p_\ell(A)}{q_m(A)}.$$

Let $d(A)$ be the degree of the minimal polynomial of A. Then,

1) If $\ell > m+1$, then $d(A) \leq \ell^2$,

2) if $\ell = m+1$, then $d(A) \leq \ell^2$ or A is B-normal$(1,0)$,

3) if $\ell < m$, and $b_0 \neq 0$, then $d(A) \leq m^2 + 1$,

4) if $\ell < m-1$ and $b_0 = 0$, then $d(A) \leq m^2$,

5) if $\ell = m-1$ and $b_0 = 0$, then $d(A) \leq m^2$, or A is B-normal$(0,1)$,

6) if $\ell = m$, then $d(A) \leq m^2 + 1$, or A is B-normal$(1,1)$,

Proof. From (19) it follows that the eigenvalues of a B-normal(ℓ, m) matrix can be written as:

$$\bar{\lambda}_i = \frac{p_\ell(\lambda_i)}{q_m(\lambda_i)}, \qquad \forall \lambda_i \in \Sigma(A). \tag{20}$$

We assume that $p_\ell(\lambda_i) \neq 0,\ \forall \lambda_i \in \Sigma(A)$, since otherwise, (20) would imply that $\lambda_i = 0$ and A is singular. We further assume that $q_m(\lambda_i) \neq 0,\ \forall \lambda_i \in \Sigma(A)$, since $q_m(\lambda_i) = 0$ and $p_\ell(\lambda_i) \neq 0$ for some $\lambda_i \in \Sigma(A)$ would imply that $\lambda_i = \infty$. Taking conjugates in (20) yields

$$\lambda_i = \frac{\bar{p}_\ell(\bar{\lambda}_i)}{\bar{q}_m(\bar{\lambda}_i)} = \frac{\bar{p}_\ell\left(\frac{p_\ell(\lambda_i)}{q_m(\lambda_i)}\right)}{\bar{q}_m\left(\frac{p_\ell(\lambda_i)}{q_m(\lambda_i)}\right)}, \qquad \forall \lambda_i \in \Sigma(A).$$

This can be expanded into

$$\begin{aligned}
\lambda_i &= \frac{\bar{a}_\ell\left(\frac{p_\ell(\lambda_i)}{q_m(\lambda_i)}\right)^\ell + \bar{a}_{\ell-1}\left(\frac{p_\ell(\lambda_i)}{q_m(\lambda_i)}\right)^{\ell-1} + \cdots + \bar{a}_0}{\bar{b}_m\left(\frac{p_\ell(\lambda_i)}{q_m(\lambda_i)}\right)^m + \bar{b}_{m-1}\left(\frac{p_\ell(\lambda_i)}{q_m(\lambda_i)}\right)^{m-1} + \cdots + \bar{b}_0} \\
&= \frac{(q_m(\lambda_i))^m}{(q_m(\lambda_i))^\ell} \; \frac{\bar{a}_\ell (p_\ell(\lambda_i))^\ell + \bar{a}_{\ell-1}(p_\ell(\lambda_i))^{\ell-1} q_m(\lambda_i) + \cdots + \bar{a}_0 (q_m(\lambda_i))^\ell}{b_m (p_\ell(\lambda_i))^m + b_{m-1}(p_\ell(\lambda_i))^{m-1} q_m(\lambda_i) + \cdots + b_0 (q_m(\lambda_i))^m},
\end{aligned}$$

$\forall \lambda_i \in \Sigma(A)$. Cross multiplication and collection of terms on one side yields

$$\begin{aligned}(21)\qquad &\lambda_i(q_m(\lambda_i))^\ell \left[\bar{b}_m(p_\ell(\lambda_i))^m + \bar{b}_{m-1}(p_\ell(\lambda_i))^{m-1}q_m(\lambda_i) + \cdots + \bar{b}_0(q_m(\lambda_i))^m\right] \\ &\quad -(q_m(\lambda_i))^m \left[\bar{a}_\ell(p_\ell(\lambda_i))^\ell + \bar{a}_{\ell-1}(p_\ell(\lambda_i))^{\ell-1}q_m(\lambda_i) + \cdots + \bar{a}_0(q_m(\lambda_i))^\ell\right] = 0,\end{aligned}$$

$\forall \lambda_i \in \Sigma(A)$.

First, consider the case when A is B-normal(ℓ, m) with $\ell > m$. Since $q_m(\lambda_i) \neq 0,\ \forall \lambda_i \in \Sigma(A)$, we can divide (21) by $(q_m(\lambda_i))^m$. It follows that the polynomial

$$\begin{aligned}(22)\qquad &\mu(q_m(\mu))^{\ell-m}\left[\bar{b}_m(p_\ell(\mu))^m + \bar{b}_{m-1}(p_\ell(\mu))^{m-1}q_m(\mu) + \cdots + \bar{b}_0(q_m(\mu))^m\right] \\ &\quad -\bar{a}_\ell(p_\ell(\mu))^\ell - \bar{a}_{\ell-1}(p_\ell(\mu))^{\ell-1}q_m(\mu) - \cdots - \bar{a}_0(q_m(\mu))^\ell = 0,\end{aligned}$$

whenever $\mu = \lambda_i$, and $\lambda_i \in \Sigma(A)$.

Proof of 1): If $\ell > m+1$ and $m = 0$, A is B-normal(ℓ). In [3] it was shown that these matrices have less that or equal to ℓ^2 distinct eigenvalues. Therefore, $d(A) \leq \ell^2$.

If $\ell > m+1$ and $m > 0$, the highest degree term of the polynomial in (22) is

$$-\bar{a}_\ell(a_\ell \mu^\ell)^\ell,$$

with degree ℓ^2. By hypothesis, $a_\ell \neq 0$, which implies (22) has at most ℓ^2 distinct roots. Thus, $d(A) \leq \ell^2$.

Proof of 2): If $\ell = m+1$ and $m = 0$, A is B-normal(1). It was shown in [3] that the eigenvalues of these matrices are collinear, that is, they lie on a straight line in the complex plane.

If $\ell = m+1$ and $m > 0$, the highest degree term of the polynomial in (22) is

$$\mu(b_m\mu^m)\bar{b}_m(a_\ell\mu^\ell)^m - \bar{a}_\ell(a_\ell\mu^\ell)^\ell,$$

with degree ℓ^2. Either the polynomial has at most ℓ^2 distinct roots, or (22) holds for all μ. In particular, (22) holds for the roots of $q_m(\mu)$, say μ_j, for $j = 1, ..., m$. Plugging μ_j into (22) yields

$$\bar{a}_\ell(p_\ell(\mu_j))^\ell = 0, \quad \text{for} \quad j = 1, ..., m.$$

This means that either $a_\ell = 0$ or $p_\ell(\mu_j) = 0$, for $j = 1, ..., m$, or both are zero. By hypothesis, $a_\ell \neq 0$ and $p_\ell(\mu)$ and $q_m(\mu)$ have no common roots, so it follows that (22) cannot hold for all μ, thus $d(A) \leq \ell^2$.

Next, consider the case when A is B-normal(ℓ, m), with $\ell \leq m$. Since $q_m(\lambda_i) \neq 0,\ \forall \lambda_i \in \Sigma(A)$, we can divide (21) by $(q_m(\lambda_i))^\ell$. We obtain the polynomial

$$\begin{aligned}(23)\qquad &\mu\left[\bar{b}_m(p_\ell(\mu))^m + \bar{b}_{m-1}(p_\ell(\mu))^{m-1}q_m(\mu) + \cdots + \bar{b}_0(q_m(\mu))^m\right] \\ &-(q_m(\mu))^{m-\ell}\left[\bar{a}_\ell(p_\ell(\mu))^\ell + \bar{a}_{\ell-1}(p_\ell(\mu))^{\ell-1}q_m(\mu) + \cdots + \bar{a}_0(q_m(\mu))^\ell\right] = 0,\end{aligned}$$

whenever $\mu = \lambda_i$, and $\lambda_i \in \Sigma(A)$. Since $p_\ell(\lambda)$ and $q_m(\lambda)$ are polynomials of degree ℓ and m respectively, a_ℓ and b_m are nonzero. However, it is possible that any of the other coefficients, $a_0, ..., a_{\ell-1}$ and $b_0, ..., b_{m-1}$, could be zero.

Proof of 3): If $\ell < m$ and $b_0 \neq 0$, the highest degree term of the polynomial in (23) is

$$\bar{b}_0\mu(b_m\mu^m)^m,$$

with degree m^2+1. By hypothesis, $b_0,\ b_m \neq 0$, and it follows that $d(A) \leq m^2+1$.

Proof of 4): Suppose that $\ell < m-1$ and $b_0 = 0$. We assume that $a_0 \neq 0$, for otherwise we could could factor μ out of both $p_\ell(\mu)$ and $q_m(\mu)$, showing that A is really B-normal$(\ell-1, m-1)$. The highest degree term of the polynomial in (23) is

$$\bar{a}_0(b_m\mu^m)^{m-1}(b_m\mu^m)^\ell = \bar{a}_0(b_m\mu^m)^m,$$

with degree m^2. Either the polynomial is zero for all μ, or $d(A) \leq m^2$. By hypothesis, $a_0,\ b_m \neq 0$, and it follows that (23) cannot be zero for all μ, thus, $d(A) \leq m^2$.

Proof of 5): Suppose that $\ell = m-1$ and $b_0 = 0$. We assume that $a_0 \neq 0$, since otherwise this would imply that A is B-normal$(\ell-1, m-1)$. There are 2 possibilities to consider, $\ell > 0$ and $\ell = 0$.

If $\ell > 0$, then $m > 1$ and it is possible for b_1 to be zero. If $b_1 = 0$, the highest degree term of the polynomial in (23) is

$$\bar{a}_0(b_m\mu^m)^{m-1}(b_m\mu^m)^\ell = \bar{a}_0(b_m\mu^m)^m,$$

with degree m^2. Either the polynomial has at most m^2 distinct roots, or it is zero everywhere. Since a_0 and b_m are nonzero by hypothesis, it follows that the polynomial has at most m^2 distinct roots, thus $d(A) \leq m^2$. If $b_1 \neq 0$, the highest degree term of the polynomial in (23) is

$$\bar{b}_1\mu(b_m\mu^m)^{m-1}(a_\ell\mu^\ell) - \bar{a}_0(b_m\mu^m)^m,$$

with degree m^2. Again, either $d(A) \leq m^2$, or (23) holds for all μ. In particular, it must hold for the roots of $p_\ell(\mu)$, say μ_j, for $j = 1, ..., \ell$. Plugging μ_j, for $j = 1, ..., \ell$ into (23) yields

$$\bar{a}_0(q_m(\mu_j))^m = 0, \qquad j = 1, ..., \ell.$$

To satisfy (23) for all μ, requires that either $a_0 = 0$, or $q_m(\mu_j) = 0$, for $j = 1, ..., \ell$, or both are zero. By hypothesis, $a_0 \neq 0$, and $p_\ell(\mu)$ and $q_m(\mu)$ have no common roots, thus, $d(A) \leq m^2$.

If $\ell = 0$, then $m = 1$, and it follows by hypothesis that $b_m = b_1 \neq 0,\ a_\ell = a_0 \neq 0$, and $b_0 = 0$. These matrices are B-normal$(0,1)$, where in addition, $b_0 = 0$. Therefore, $p_0(\mu) = a_0$ and $q_m(\mu) = b_1\mu$, and it follows that (20) becomes

$$\bar{\lambda}_i = \frac{a_0}{b_1\lambda_i}, \qquad \forall \lambda_i \in \Sigma(A),$$

or,

$$\bar{\lambda}_i\lambda_i = \frac{a_0}{b_1}, \qquad \forall \lambda_i \in \Sigma(A).$$

Therefore, $\frac{a_0}{b_1}$ must be positive and real. Matrices that are B-normal$(0,1)$, with $b_0 = 0$, have eigenvalues that lie on a circle of radius $\sqrt{\frac{a_0}{b_1}}$. That is, they are scaled unitary matrices.

Proof of 6): When A is B-normal(ℓ, m) with $\ell = m$, (19) becomes

$$A^\dagger = \frac{p_m(A)}{q_m(A)} = \frac{a_m}{b_m} + \frac{\tilde{p}_{m-1}(A)}{q_m(A)},$$

where the second equality follows upon division of $p_m(A)$ by $q_m(A)$. Denoting $\hat{A} = (A - \zeta I)$, where $\zeta = \frac{\bar{a}_m}{\bar{b}_m}$, the above can be rearranged yielding

$$\hat{A}^\dagger = \frac{\tilde{p}_{m-1}(A)}{q_m(A)} = \frac{\hat{p}_{m-1}(\hat{A})}{\hat{q}_m(\hat{A})}.$$

This shows that if A is B-normal(m,m), then there exists a constant ζ, such that $A-\zeta I$ is B-normal$(m-1,m)$. We apply the results from the $\ell < m$ case to the matrix $\hat{A}$. From this it follows that if A is B-normal(m,m), the only cases that yield more that m^2+1 distinct eigenvalues are B-normal$(1,1)$ matrices whose eigenvalues can be obtained by shifting the eigenvalues of a scaled unitary matrix by some constant ζ. These are the shifted unitary matrices described in Section 2. □

The next Theorem gives weaker sufficient conditions on the matrix A for $A \in \mathcal{CG}_B(\ell,\, m)$.

THEOREM 4.2. *$A \in \mathcal{CG}_B(\ell,\, m)$ if $d(A) \le \ell+m+2$, or if there exists polynomials, $p_{\ell'}(\lambda)$ and $q_{m'}(\lambda)$, of degree ℓ' and m' respectively, such that $\ell-\ell' \ge m-m' \ge 0$, and*

$$Q(A) = A^\dagger q_{m'}(A) - p_{\ell'}(A) \tag{24}$$

satisfies

$$\mathrm{Rank}(Q(A)) \le m-m'.$$

Proof. To show $A \in \mathcal{CG}_B(\ell,\, m)$, we need to show that there exists coefficients $\{\beta_{i,j}\}_{j=i-m}^{i}$ such that

$$\sigma_{i,k} = \langle \sum_{j=i-m}^{i} \beta_{i,j}\underline{p}_j, A^\dagger \underline{p}_k\rangle_B = 0, \qquad k=0,...,i-\ell-1.$$

There exits polynomials, ψ_k, $\tilde{\psi}_{k-m}$, and $r_{m-1}^{(k)}$ such that

$$\underline{p}_k = \psi_k(A)\underline{p}_0 = q_{m'}(A)\tilde{\psi}_{k-m'}(A)\underline{p}_0 + r_{m'-1}^{(k)}(A)\underline{p}_0,$$

where the second equality follows from dividing $\psi_k(A)$ by $q_{m'}(A)$. Multiplying through by $A^\dagger$ and then adding and subtracting $p_{\ell'}(A)\tilde{\psi}_{k-m'}(A)\underline{p}_0$ yields

$$A^\dagger\underline{p}_k = (A^\dagger q_{m'}(A) - p_{\ell'}(A))\tilde{\psi}_{k-m'}(A)\underline{p}_0 + p_{\ell'}(A)\tilde{\psi}_{k-m'}(A)\underline{p}_0 + A^\dagger r_{m'-1}^{(k)}(A)\underline{p}_0.$$

Now, since $\ell-\ell' \ge m-m' \ge 0$, we have for $k=0,...,i-\ell-1$ that

$$p_{\ell'}(A)\tilde{\psi}_{k-m'}(A)\underline{p}_0 \in \mathrm{sp}\{\underline{p}_0, \underline{p}_1, ..., \underline{p}_{i-m-1}\},$$

and thus

$$p_{\ell'}(A)\tilde{\psi}_{k-m'}(A)\underline{p}_0 \perp_B \sum_{j=i-m}^{i} \beta_{i,j}\underline{p}_j.$$

Also,

$$A^\dagger r_{m'-1}^{(k)}(A)\underline{p}_0 \in \mathrm{sp}\{A^\dagger\underline{p}_0, A^\dagger\underline{p}_1, ..., A^\dagger\underline{p}_{m'-1}\},$$

and by hypothesis,

$$(A^\dagger q_{m'}(A) - p_{\ell'}(A))\tilde{\psi}_{k-m'}(A)\underline{p}_0 \in \mathrm{Range}(Q(A)).$$

It follows that we only need to choose the $\beta_{i,j}$'s so that

$$(A^\dagger r_{m'-1}(A)\underline{p}_0 + Q(A)\tilde{\psi}_{k-m'}(A)\underline{p}_0) \perp_B \sum_{j=i-m}^{i} \beta_{i,j}\underline{p}_j.$$

Letting $\left\{\underline{\phi}_j\right\}_{j=1}^{t}$ be a basis for the Range$(Q(A))$, this is equivalent to solving the system

$$(25)\quad \begin{bmatrix} \langle \underline{p}_i, A^\dagger \underline{p}_0\rangle_B & \langle \underline{p}_{i-1}, A^\dagger \underline{p}_0\rangle_B & \cdots & \langle \underline{p}_{i-m}, A^\dagger \underline{p}_0\rangle_B \\ \vdots & \vdots & & \vdots \\ \langle \underline{p}_i, A^\dagger \underline{p}_{m'-1}\rangle_B & \langle \underline{p}_{i-1}, A^\dagger \underline{p}_{m'-1}\rangle_B & \cdots & \langle \underline{p}_{i-m}, A^\dagger \underline{p}_{m'-1}\rangle_B \\ \langle \underline{p}_i, \underline{\phi}_1\rangle_B & \langle \underline{p}_{i-1}, \underline{\phi}_1\rangle_B & \cdots & \langle \underline{p}_{i-m}, \underline{\phi}_1\rangle_B \\ \vdots & \vdots & & \vdots \\ \langle \underline{p}_i, \underline{\phi}_t\rangle_B & \langle \underline{p}_{i-1}, \underline{\phi}_t\rangle_B & \cdots & \langle \underline{p}_{i-m'}, \underline{\phi}_t\rangle_B \end{bmatrix} \begin{pmatrix} \beta_{i,i} \\ \vdots \\ \beta_{i,i-m'-1} \\ \beta_{i,i-m'} \\ \vdots \\ \beta_{i,i-s} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

The first m' rows correspond to making

$$A^\dagger r_{m'-1}(A)\underline{p}_0 \perp_B \sum_{j=i-m}^{i} \beta_{i,j}\underline{p}_j,$$

while the last t rows correspond to making

$$\text{Range}(Q(A)) \perp_B \sum_{j=i-m}^{i} \beta_{i,j}\underline{p}_j.$$

If $t = \dim(\text{Range}(Q(A))) \leq m - m'$, then the system can always be solved. Thus, $A \in \mathcal{CG}_B(\ell,\, m)$. □

REMARK 4.2. *As in Lemma 4.1, the system (25) will always have a nontrivial solution, but the algorithm will break down unless there is a solution with $\beta_{i,i} \neq 0$. We believe that, as in the case where A is B-normal(ℓ, m), breakdown occurrs for $\underline{p}_0$ in a set of measure zero and can be avoided by a reorganization of the computations. This is a current topic of exploration.*

5 Conclusion

To determine when a conjugate gradient method can be implemented economically, we must consider all possible forms of recursions for the direction vectors. The work by Jagels and Reichel ([5],[6]) demonstrates that the form of recursion given by (1) is not general enough to include all possibilities. In this paper, we have constructed a more general form of recursion called a single (ℓ, m) recursion. Since many multiple recursions can be written equivalently in this form, we began studying multiple recursion conjugate gradient algorithms by analyzing single (ℓ, m) recursions.

Sufficient conditions on the matrix A were determined, in order for a conjugate gradient method to be implemented with a single (ℓ, m) recursion. In the absence of breakdown, if A is B-normal(ℓ, m), or a low rank modification of a B-normal(ℓ, m) matrix, then a conjugate gradient algorithm can be carried out using an (ℓ, m) recursion. For B-normal(ℓ, m) matrices, breakdowns can be avoided by reorganizing the computations. We conjecture that this is also the case for the low rank modifications of B-normal(ℓ, m) matrices in Theorem 4.2. For $\ell,\ m \leq 2$, the conditions stated in Theorem 4.2 are also necessary. Details will be given in [2].

This work leaves many unanswered questions. For example: necessary conditions for $\ell,\ m > 2$, and the issue of breakdown in the (ℓ, m) recursion for low rank perturbations of B-normal(ℓ, m) matrices. To consider all possible recursions for the direction vectors,

those multiple recursions that cannot be written as single short (ℓ, m) recursions must be characterized. Further research is being done to address some of these issues.

References

[1] 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.

[2] T. Barth, Ph.D. thesis, in progress.

[3] 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, (1984) pp. 352-362.

[4] W. B. Gragg, *Positive definite Toeplitz matrices, the Arnoldi process for isometric operators, and Gaussian quadrature on the unit circle*, J. Comp. Appl. Math, 46 (1993), pp. 183-198.

[5] C. F. Jagels, and L. Reichel, *The isometric Arnoldi process and an application to iterative solution of large linear systems*, in Iterative Methods in Linear Algebra, eds. R. Beauwens and P. de Groen, Elsevier, Amsterdam, 1992, pp. 361-369.

[6] C. F. Jagels, and L. Reichel, *A Fast Minimal Residual Algorithm For Shifted Unitary Matrices*, Numer. Linear Algebra Appl., 1 (1994), pp. 555-570.

[7] W. D. Joubert, and D. M. Young, *Necessary and sufficient conditions for the simplification of generalized conjugate-gradient algorithms*, Linear Algebra Appl., 1988, pp. 449-485.

[8] W. D. Joubert, *Lanczos Methods for the Solution of Nonsymmetric Systems of Linear Equations*, SIAM J. on Matrix Analysis and Appl., vol. 13, no. 3, July 1992, pp. 926-943.

[9] Y. Saad, and M. H. Schultz, *GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems*, SIAM J. Sci. Statist. Comput., 1986, No. 7, pp. 856-869.

[10] D. S. Watkins, *Some Perspectives On The Eigenvalue Problem*, SIAM Reviews, Sept. 1993, Vol. 35, No. 3, pp. 430-471.