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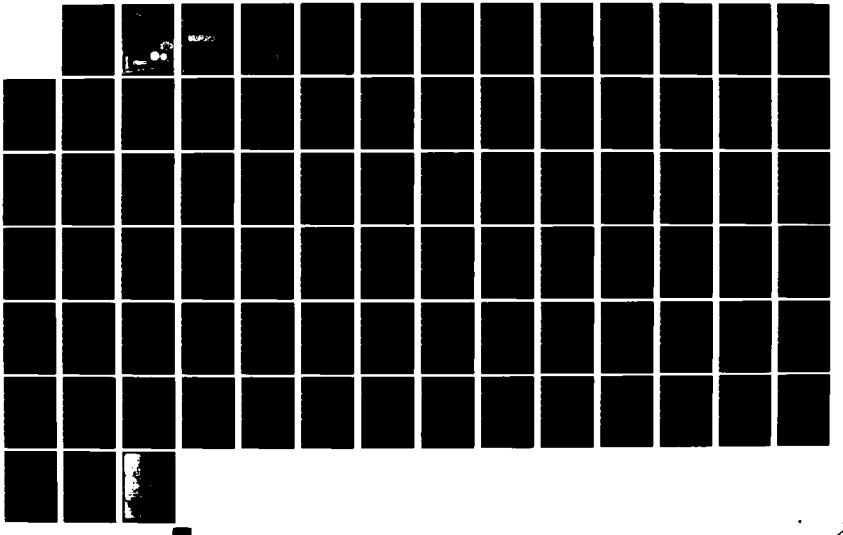

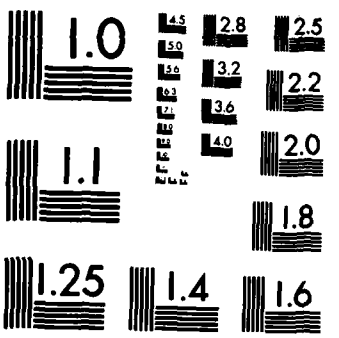

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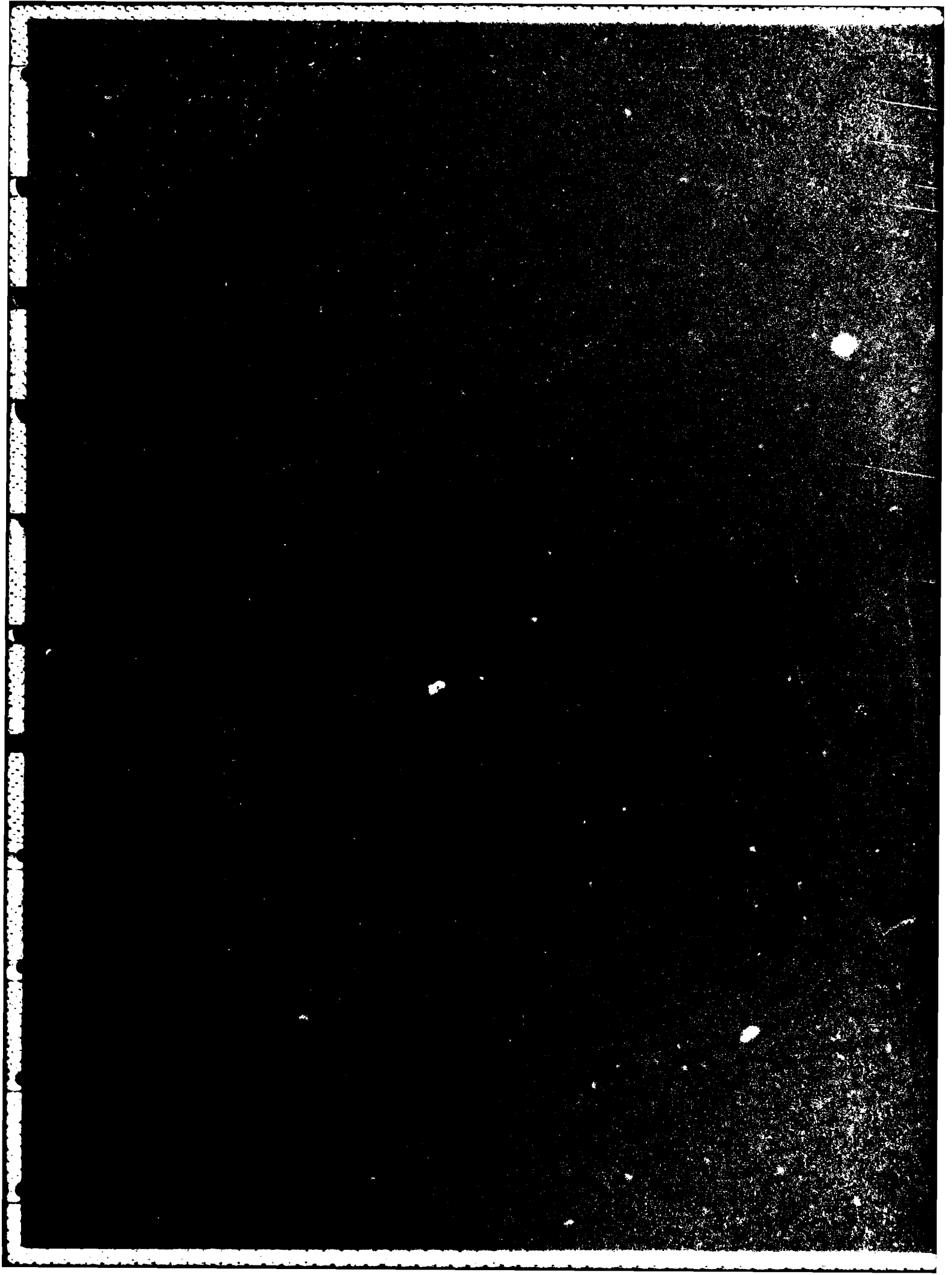

ANALYSIS OF THE LOOK AHEAD LANCZOS ALGORITHM*

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ABSTRACT

The two-sided Lanczos algorithm is known to suffer instability in the form of serious breakdown. This occurs when the associate moment matrix does not permit a triangular factorization. This work uses the notion of a generalized pivot to inexpensively circumvent the breakdown in most cases, with the 2×2 pivot examined in detail. The case where the generalized pivot is of no avail is analyzed, introducing a surprising characterization for that form of serious breakdown.

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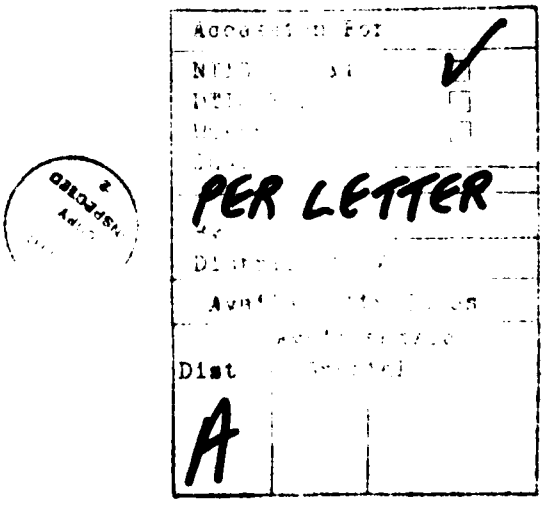

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Introduction

In 1950, Lanczos introduced his method for computing eigenvalues and eigenvectors of $n \times n$ matrices. His method soon came to be regarded as transforming a general matrix to tridiagonal form. Unfortunately, modifications involving considerable extra work were required to maintain accuracy. The Lanczos process lost favor when the more stable Givens (1954) and Householder (1958) methods were introduced.

As if to seal the fate of the Lanczos process for non-symmetric matrices (we call it the two-sided Lanczos algorithm), Wilkinson produced an example which demonstrates the instability of the algorithm even with infinite precision arithmetic (Wilkinson [1958]).

Recently the symmetric Lanczos has returned as a viable method for finding some eigenvalues and eigenvectors of large symmetric matrices. With the current interest in handling large problems, the non-symmetric Lanczos process is ripe for reconsideration.

Chapter I presents the classical two-sided Lanczos process. The material is not new, and is presented in an informal manner so as to provide a background and establish notation. Much of what could be presented as formal theorems is merely noted in passing and left without proof.

The key to our work, which Chapter I emphasizes, is the importance of certain underlying Krylov subspaces and the relative unimportance of the resulting tridiagonal matrix. The weakness of the two-sided Lanczos process lies in its inflexibility in specifying the bases vectors in the sequence of subspaces and our remedy relaxes the Lanczos requirements, but by as little as possible.

Chapter II introduces the general look-ahead algorithm from two aspects taken up in Chapter I, the two-sided Gram-Schmidt process and the LDU factorization of the moment matrix generated by $n \times n$ B and starting p^* and q. From these two perspectives we generalize the notion of pivot to make the Lanczos process more flexible without much extra work. There are many factors to consider in selecting the appropriate look-ahead and Chapter II explores two important points.

Chapter III continues the discussion of the look-ahead procedure, but restricts the generalization of the pivot to the 2×2 case alone. The relationships of classical factorizations to the look-ahead procedure are shown as well as those of some less obvious factorizations. Finally, though somewhat out of place, the Kahan, Parlett and Jiang (KPJ [1981]) residual bounds are generalized to handle the 2×2 case.

From Chapters II and III we become aware of two forms of what Wilkinson calls "serious breakdown". One form we call "curable", and it is for this case that the look-ahead Lanczos algorithm is designed.

The other form of serious breakdown we call "incurable". For this type of breakdown no simple procedure is available. However, in Chapter IV we exhibit a surprising characterization of incurable breakdown (the mismatch theorem) shows that this rare occurrence is only slightly less fortunate than encountering an invariant subspace.

Notation

Throughout this work we will use B to denote the real $n \times n$ matrix given to the algorithm, and suppose that each eigenvalue of B

is associated with only one Jordan block. In general, upper case Roman letters will denote matrices, and lower case Roman letters will denote vectors (though a and b will denote scalars and i, j, k, ℓ, m and n are reserved as integers). Upper case Greek letters are used for special matrices (usually diagonal), lower case Greek letters are scalars. Script letters are spaces.

Square brackets ([ ]) indicate a matrix so that $[q_1,\ldots,q_n]$ is a matrix with columns q_i. The matrix, I_k, is reserved as the $k \times k$ identity matrix. $N(A)$ denotes the column nullspace of the matrix A. The norms $\|\cdot\|$ and $\|\cdot\|_F$ are the Euclidean and Frobenius norms, respectively. Conjugate transpose is denoted by $*$ (eg. A^*) with $-*$ denoting conjugate transpose of the inverse.

I. The Two-Sided Lanczos Algorithm

1.1 Introduction

In this chapter we describe the Lanczos algorithm as applied to a nonsymmetric $n \times n$ matrix B. In fact, we shall describe it in three different ways: (i) the Gram-Schmidt process applied to Krylov sequences, (ii) the three term recurrence relation and (iii) the triangular factorization of the moment matrix. None of these viewpoints is new, but each is relevant to the modification of the Lanczos algorithm that is the focus of this work. Moreover, these sections establish our notation.

In the course of establishing the Lanczos algorithm in the context of exact arithmetic we want to bring out the underlying subspaces and those which reflect a particular basis in the space. We propose that the basic algorithm of this chapter be called the *two-sided Lanczos algorithm* to distinguish it from its better known--and stable--version for symmetric matrices. In the symmetric case the temptation to identify $\mathbf{R}^n$ with its dual $\mathbf{R}_*^n$ is too strong to resist and the algorithm simplifies significantly in exchange for identifying objects which are logically different.

The final sections of this chapter seem to be out of place being motivated by considerations such as avoidance of overflow or underflow in computer implementations. In exact arithmetic the particular scaling of the Lanczos vectors is of no consequence; in practice it does matter. We give a thorough discussion of the subject and recommend a novel, and slightly redundant formulation.

The material covered in this chapter is not new so that the presentation is less formal than might be expected. Also, the reader is assumed to be familiar with the Gram-Schmidt process for orthonormalizing a sequence of vectors.

1.2 Krylov subspaces and sequences

Given non-zero $q \in \mathbb{C}^n$, $p^* \in \mathbb{C}^n_*$, the *Krylov matrices* K_ℓ and $\tilde{K}_\ell$ are defined by

$$K_\ell = K_\ell(q,B) = [q,Bq,\ldots,B^{\ell-1}q]$$

$$\tilde{K}^*_\ell = \tilde{K}^*_\ell(p^*,B) = \begin{bmatrix} p^* \\ p^*B \\ \vdots \\ p^*B^{\ell-1} \end{bmatrix}$$

The columns of K_ℓ form the Krylov column sequence generated from q. Similarly, the rows of $\tilde{K}^*_\ell$ from the Krylov row sequence generated by p^*.

These column and row sequences are the *primary* vectors which determine the column and row Krylov subspaces defined by

$$\mathcal{K}^\ell = \mathcal{K}^\ell(q,B) = \text{span } K_\ell = K_\ell\mathbb{C}^\ell$$

$$\mathcal{K}^\ell_* = \mathcal{K}^\ell_*(p^*,B) = \text{span } \tilde{K}^*_\ell = \mathbb{C}^\ell_*\tilde{K}^*_\ell$$

These subspaces play the central role in the understanding of the Lanczos algorithm.

The fact that $B^\ell q$ converges to the dominant eigenvector of B as $\ell \to \infty$ is misleading in the context of Lanczos. There is no interest in letting ℓ exceed n (in the symmetric case, ℓ is

typically about $3\sqrt{n}$) and an important topic in approximation theory is derivation of expressions which measure the closeness of certain eigenvectors to K^ℓ and K_*^ℓ.

If $K^{\ell+1} = K^\ell$ then it is easily verified that K^ℓ is invariant under B. Such subspaces are what we want, and there is no loss in assuming that we have not achieved our goal, i.e. we may assume that

$$\dim(K^\ell) = \dim(K_*^\ell) = \ell \ .$$

For theoretical purposes the columns of K_ℓ (or the rows of $\tilde{K}_\ell^*$) form a satisfactory basis for K^ℓ (K_*^ℓ) and show the key role of polynomials.

LEMMA 1.1 *There is a one-to-one correspondence between* $K^\ell(q,B)$ *and* $P_{\ell-1} = \{\pi(t),\ \pi(t) = \sum_{i=0}^{\ell-1} \pi_i t^i\}$. *For each* $\pi \in P_{\ell-1}$ *there is a* $\pi(B)q = \sum_{i=0}^{\ell-1} (B^i q)\pi_i \in K^\ell$ *and vice-versa. Similarly,* $p^*\pi(B) \in K_*^\ell$.

1.3 Two-Sided Gram-Schmidt (TSGS)

In his original paper (Lanczos [1950]), Lanczos remarked how round off errors made the Krylov vectors useless for computation. He proposed better bases for K^ℓ and K_*^ℓ by applying the Gram-Schmidt process to the Krylov vectors. This produces a biorthonormal pair of bases $\{q_1,q_2,\ldots,q_\ell\}$ and $\{p_1^*,p_2^*,\ldots,p_\ell^*\}$ in each space. The nature of the Gram-Schmidt process forces q_j to be the component of $B^{j-1}q$ orthogonal to K_*^{j-1} and p_j^* the component of p^*B^{j-1} orthogonal to K^{j-1}. The algorithm then is as follows:

Select p^* and q so that $p^*q = 1$. Set $p_1 = p^*$, $q_1 = q$.

For $j = 1,\ldots,\ell-1$

$$\begin{aligned} \tilde{r}_{j+1} &= B^j q - \sum_{i=1}^{j} q_i (p_i^* B^j q) \\ \tilde{s}_{j+1}^* &= p^* B^j - \sum_{i=1}^{j} (p^* B^j q_i) p_i^* \\ q_{j+1} &= \tilde{r}_{j+1} / \beta^{(j+1)} \\ p_{j+1}^* &= \tilde{s}_{j+1}^* / \gamma^{(j+1)} \end{aligned} \tag{1.1}$$

where $\beta^{(j+1)}\gamma^{(j+1)} = \omega^{(j+1)} := \tilde{s}_{j+1}^* \tilde{r}_{j+1}$.

Note that q_{j+1} is the unique vector (to within scaling) in K^{j+1} orthogonal to K_*^j. Similarly, p_{j+1}^* is unique in K_*^{j+1} orthogonal to K^j. The specification of $\beta^{(j+1)}$ is postponed until later. For now, it is simply a non-zero scalar.

It is convenient to regard these *Lanczos vectors* as columns (or rows) of matrices,

$$Q_\ell = [q_1,\ldots,q_\ell] \qquad P_\ell^* = \begin{bmatrix} p_1^* \\ \vdots \\ p_\ell^* \end{bmatrix}$$

with $P_\ell^* Q_\ell = I_\ell$ by construction.

Note that the Krylov vector $B^{k-1}q$ is not needed until the k^{th} iteration in (1.1). *In fact, the Krylov vectors are not needed explicitly at all.* At step j in (1.1) $B^{j-1}q$ and p^*B^{j-1} can be replaced by Bq_{j-1} and $p_{j-1}B$, respectively. To see this we use the result of the previous section that $K^{j-1}(q,B) = \{\pi(B)q: \pi \in P_{j-2}\}$. In particular, $q_{j-1} = \phi(B)q$ where the degree of $\phi = j-2$ (otherwise, q_{j-1} would be in K^{j-2}).

$$\begin{aligned}\text{span}\{q_1,\ldots,q_{j-1},Bq_{j-1}\} &= \text{span}\{q_1,\ldots,q_{j-1},B\phi(B)q\}\\ &= \text{span}\{q_1,\ldots,q_{j-1},\phi_{j-2}B^{j-1}q+\tilde{\phi}(B)q\} \quad \tilde{\phi}\in P^{j-2}\\ &= \text{span}\{q_1,\ldots,q_{j-1},\phi_{j-2}B^{j-1}q\}\\ &= \text{span}\{q_1,\ldots,q_{j-1},B^{j-1}q\} = K^j(q,B)\end{aligned}$$

Similarly for p_{j-1}^*B and p^*B^{j-1}.

The algorithm (1.1) is then replaced by:

For $j = 1,2,\ldots,\ell-1$

$$\begin{aligned}r_{j+1} &= Bq_j - \sum_{i=1}^{j} q_i(p_i^*Bq_j)\\ s_{j+1}^* &= p_j^*B - \sum_{i=1}^{j}(p_j^*Bq_i)p_i^*\\ q_{j+1} &= r_{j+1}/\beta_{j+1}\\ p_{j+1}^* &= s_{j+1}^*/\gamma_{j+1}\end{aligned} \tag{1.2}$$

where $\beta_{j+1}\gamma_{j+1} = \omega_{j+1} := s_{j+1}^*r_{j+1}$.

The beauty of (1.2) is that the sums simplify to only two non-zero terms as shown in the following lemma.

LEMMA 1.2 $p_i^*Bq_j = p_j^*Bq_i = 0$ *for* $i < j-1$.

PROOF. We will only consider $p_j^*Bq_i$ since the argument is the same for both. Consider $q_i = \pi_i(B)q$, $\pi_i \in P^{i-1}$. Then $Bq_i = B\pi_i(B)q = \tilde{\pi}_i(B)q$, $\tilde{\pi}_i \in P^i$. Then from Lemma 1.1, $Bq_i \in K^{i+1}$. By construction, $p_j^* \perp K^\ell$, $\ell < j$. Therefore, $p_j^* \perp K^{i+1}$, $i+1 < j$. Thus, $p_j^*Bq_i = 0$, $i < j-1$. ∎

We isolate the non-zero coefficients by the following notation:

$$\beta_j = p_j^* B q_{j-1} \quad (= p_j^* r_j)$$
$$\gamma_j = p_{j-1}^* B q_j \quad (= s_j^* q_j)$$
$$\alpha_j = p_j^* B q_j$$

The familiar three term recurrence then is:

$$q_0 = p_0 = 0$$
$$q_1 = q/\beta_1 \ , \quad p_1^* = p^*/\gamma \ ; \quad \beta_1\gamma_1 = \omega_1 = p^*q \ .$$

For $j = 1,\ldots,\ell-1$ do

$$\begin{aligned} r_{j+1} &= Bq_j - q_j\alpha_j - q_{j-1}\gamma_{j-1} \\ s_{j+1}^* &= p_j^* B - \alpha_j p_j^* - \beta_j p_{j-1}^* \\ q_{j+1} &= r_{j+1}/\beta_{j+1} \\ p_{j+1}^* &= s_{j+1}^*/\gamma_{j+1} \end{aligned} \tag{1.3}$$

where $$\beta_{j+1}\gamma_{j+1} = \omega_{j+1} = s_{j+1}^* r_{j+1} \tag{1.4}$$

Clearly, if $\omega_{j+1} = 0$ the algorithm cannot continue. An analysis of, and a remedy for, this condition is the purpose of this work. For the moment, though, we will assume that $\omega_i \neq 0$ for $i = 1,\ldots,j+1$.

This ends the tranditional description of the (two-sided) Lanczos algorithm. The discussion of the problem of termination is postponed until our stabilizing algorithm is presented (Chapters II and III). We now illuminate various relationships which govern the coefficients α, β and γ, and the Lanczos vectors $\{p_i^*\}$ and $\{q_i\}$.

1.4 The Lanczos polynomial and the moment matrix

From the previous section we have $q_k = \pi(B)q$ where π is of degree k-1. It is convenient to specify π as follows

$$q_k = (\frac{1}{\beta^{(k)}})\chi_{k-1}(B)q \tag{1.5}$$

where $\chi_{k-1}(t)$ is a monic polynomial of degree k-1 and $\beta^{(k)}$ is defined in (1.1). The three term recurrence (1.3) for the q_i's yields a related recurrence for the *Lanczos polynomials* χ_i. Set $\chi_{-1}(t) = 0$, $\chi_0(t) = 1$. Then, by substituting (1.5) in (1.3) one obtains

$$\chi_k(t) = (t-\alpha_k)\chi_{k-1}(t) - \omega_k\chi_{k-2}(t) \tag{1.6}$$

where α_k and ω_k were defined in (1.4). Similarly,

$$p_k^* = (\frac{1}{\gamma^{(k)}})p^*\chi_{k-1}(B) \ .$$

Moreover, $\beta^{(k)} = \beta_1\cdot\beta_2\cdot\cdots\cdot\beta_k$ and $\gamma^{(k)} = \gamma_1\cdot\gamma_2\cdot\cdots\cdot\gamma_k$. Further, it is the product ω_k $(= \beta_k\gamma_k)$ which determines the Lanczos polynomials. The choice of β_k only affects the norms of q_k and p_k^*.

Next we relate the Lanczos polynomial to a certain triangular matrix. Recall

$$K_j = [q, Bq, \ldots, B^{j-1}q] \ , \quad \tilde{K}_j^* = \begin{bmatrix} p^* \\ p^*B \\ \vdots \\ p^*B^{j-1} \end{bmatrix} \ .$$

The two-sided Gram-Schmidt process dictates that

$$Q_j = [q_1, \ldots, q_j] = K_j L_j^{-*} \Delta_\beta^{-1} \tag{1.7a}$$

where L_j^{-*} is some $j \times j$ unit upper triangular matrix and $\Delta_\beta = \text{diag}\{\beta^{(1)},\ldots,\beta^{(j)}\}$, and, similarly,

$$P_j^* = \begin{bmatrix} p_1^* \\ \vdots \\ p_j^* \end{bmatrix} = \Delta_\gamma^{-1}\tilde{L}_j^{-1}\tilde{K}_j^* \tag{1.7b}$$

where $\Delta_\gamma = \text{diag}\{\gamma^{(1)},\ldots,\gamma^{(j)}\}$ and $\tilde{L}_j^{-1}$ is unit lower triangular.

Note that the inverse of a unit lower triangular matrix is also unit lower triangular. Thus, the i^{th} row of $\tilde{L}_j^{-1}$ contains the coefficients of the $(i-1)^{st}$ Lanczos polynomial χ_{i-1} since

$$\begin{aligned} p_i^* &= (\frac{1}{\gamma^{(i)}})p^*\chi_{i-1}(B) \\ &= (\frac{1}{\gamma^{(i)}})(\chi_0^{(i-1)},\chi_1^{(i-1)},\ldots,\chi_{i-2}^{(i-1)},1)\tilde{K}_i^* . \end{aligned}$$

Similarly the i^{th} column of L_j^{-*} contains the coefficients of the $(i-1)^{st}$ Lanczos polynomial, so that $L_j^{-1} = \tilde{L}_j^{-1}$.

Note, now, that

$$\tilde{K}_j^* K_j =: M_j(p^*,q,B) \tag{1.8}$$

the *moment matrix* whose $(i,k)^{th}$ element is $p^*B^{[(i-1)+(k-1)]}q$. Using (1.8), along with a rearrangement of (1.7a) and (1.7b) and $P_j^*Q_j = I_j$, we have

$$\begin{aligned} M_j &= \tilde{K}_j^* K_j \\ &= L_j\Delta_\gamma P_j^* Q_j \Delta_\beta L_j^* = L_j \Omega_j L_j^* \end{aligned} \tag{1.9}$$

where $\Omega_j = \Delta_\gamma\Delta_\beta = \text{diag}\{\omega_1,\omega_1\omega_2,\ldots,\omega_1\omega_2\cdots\omega_j\}$. That is, running the Lanczos algorithm for j steps is equivalent to the triangular factorization of the moment matrix M_j. In particular, a breakdown in the

Lanczos algorithm ($\omega_i = 0$) corresponds to failure in the triangular factorization and vice versa. We may, if it helps, consider the problem of stability in terms of the extensively studied triangular factorization.

As noted before, these relationships are not new (Lanczos himself used Gaussian elimination in his original algorithm), but neither are they widely comprehended.

1.5 Matrix formulation of the Lanczos Algorithm

The three term recurrence can be written compactly by the introduction of a tridiagonal matrix, J. Consider algorithm (1.3), and write $r_i = q_i\beta_i$ and $s_i^* = \gamma_i p_i^*$. Then

$$[r_2,\ldots,r_{k+1}] = [Bq_1-q_1\alpha_1, Bq_2-q_2\alpha_2-q_1\gamma_2,\ldots, Bq_k-q_k\alpha_k-q_{k-1}\gamma_k]$$

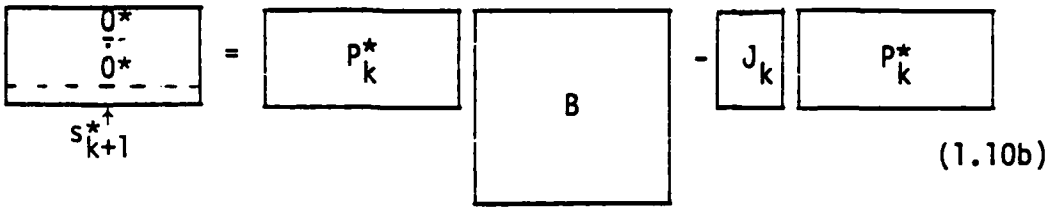
and

$$\begin{bmatrix} s_2^* \\ \vdots \\ s_{k+1}^* \end{bmatrix} = \begin{bmatrix} p_1^*B-\alpha_1 p_1^* \\ \vdots \\ p_k^*B-\alpha_k p_k^*-\beta_k p_{k-1}^* \end{bmatrix}$$

becomes

$$\left[\underline{0}..\underline{0} \mid r_{k+1}\right] = \left[B\right]\left[Q_k\right] - \left[Q_k\right]\left[J_k\right] \qquad (1.10a)$$

and



(1.10b)

where

$$J_k = \begin{bmatrix} \alpha_1 & \gamma_2 & & & \\ \beta_2 & \alpha_2 & \gamma_3 & & \\ & \beta_3 & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & & & \cdot & \cdot & \gamma_k \\ & & & & \beta_k & \alpha_k \end{bmatrix} = P_k^* B Q_k \, . \qquad (1.10c)$$

A simplified notation for the rank one matrices simplifies the matrix formulations (1.10a) and (1.10b) to

$$r_{k+1} e_k^* = BQ_k - Q_k J_k$$
$$e_k s_k^* = P_k^* B - J_k P_k^*$$

with the convention that the e_k is the last column of the $k \times k$ identity matrix, I_k, while the other vectors are of dimension n.

Finally, we relate J_k to the Lanczos polynomials by considering its characteristic polynomial, $\det(tI_k - J_k)$. Expanding by the bottom row, we find

$$\det(tI_k - J_k) = (t-\alpha_k)\det(tI_{k-1} - J_{k-1}) - (-\beta_k)(-\gamma_k)\det(tI_{k-2} - J_{k-2}) \, .$$

Further, $\det(tI_1 - J_1) = t - \alpha_1 = \chi_1(t)$. Recall that $\beta_k \gamma_k = \omega_k$ and compare with (1.6) to see that

χ_k is the characteristic polynomial of J_k .

Another approach to formulating some of these results comes from the theory of orthogonal polynomials with respect to an inner product, in our case the χ_k are orthogonal with respect to the inner product induced by the moment matrix $M(p^*,q,B)$ (see Brezinski [1980]). But we will not make explicit use of this viewpoint, since M is not guaranteed to be positive definite, and one's intuition may be misled by the improper inner product induced by it.

1.6 The moment matrix and the Lanczos polynomial

Up to this point, we have linked the moment matrix to the Lanczos algorithm but not to our goal of finding some eigenvalues of a nonsymmetric matrix. The dependence of approximate eigenvalue on only the moment matrix will be of importance in later chapters.

Let

$$M_{ij} = \begin{bmatrix} m_i & m_{i+1} & \cdots & m_j \\ \vdots & & & \\ m_j & m_{j+1} & \cdots & m_{2j-i+1} \end{bmatrix}$$

where $m_k = p^*B^kq$. Then

LEMMA 1.3 $\chi_k(t) = \det[tM_{0,k-1} - M_{1,k}]/(\omega^{(1)}\cdots\omega^{(k)})$, $\omega^{(i)} = \omega_1\cdots\omega_i$.

PROOF.
$$\begin{aligned} J_k &= P_k^*BQ_k \\ &= \Delta_\gamma^{-1}L_k^{-1}\tilde{K}_k^*BK_kL_k^{-*}\Delta_\beta^{-1} \quad \text{from (1.7a), (1.7b)} \\ &= \Delta_\gamma^{-1}L_k^{-1}M_{1,k}L_k^{-*}\Delta_\beta^{-1} \end{aligned}$$

and

$$\begin{aligned} I_k &= P_k^*Q_k \\ &= \Delta_\gamma^{-1}L_k^{-1}M_{0,k-1}L_k^{-*}\Delta_\beta^{-1} . \end{aligned}$$

Since L_k is unit lower triangular

$$\begin{aligned}\chi_k(t) &= \det(tI_k - J_k) \\ &= \det(\Delta_\gamma^{-1})\det(tM_{0,k-1} - M_{1,k})\det(\Delta_\beta^{-1}) \\ &= \det(tM_{0,k-1} - M_{1,k})/(\omega^{(1)}\cdots\omega^{(k)}) \ . \end{aligned}$$

■

The moment matrix $M_{i,j}$ is a special Hankel matrix (the $(k,\ell)^{th}$ element is a function of $(k+\ell)$) and this fact yields another determinental description of the Lanczos polynomial.

LEMMA 1.4

$$\chi_k(t) = \frac{1}{\omega^{(1)}\cdots\omega^{(k)}} \det \begin{bmatrix} m_0 & m_1 & \cdots & m_k \\ m_1 & m_2 & \cdots & m_{k+1} \\ \vdots & & & \vdots \\ m_{k-1} & m_k & \cdots & m_{2k-1} \\ 1 & t & \cdots & t^k \end{bmatrix} \tag{1.11}$$

PROOF. The $(k+1)\times(k+1)$ matrix on the right of (1.11) can be expressed as

$$\begin{bmatrix} M_{0,k-1} & m^{(k)} \\ (1\ t\cdots t^{k-1}) & t^k \end{bmatrix}$$

Observe that

$$\left[\begin{array}{ccc:c} & & & \\ & M_{0,k-1} & & m_1^{(k)} \\ & & & \\ \hdashline 1 & t\cdots & t^{k-1} & t^k \end{array}\right]\begin{bmatrix} t & 0 & \cdots & 0 \\ -1 & t & \ddots & \vdots \\ 0 & -1 & \ddots & 0 \\ \vdots & \ddots & \ddots & \\ 0 & \cdots & 0 & -1\ t \end{bmatrix} = \left[\begin{array}{ccc:c} & & & \\ & tM_{0,k-1} - M_{1,k} & & m^{(k)} \\ & & & \\ \hdashline 0 & \cdots & 0 & t^k \end{array}\right]$$

Take determinants, cancel t^k, and use Lemma 1.3 to obtain the formula.

■

1.7 Off-diagonal elements of J

Up to now, no mention of the selection of β_j (and thus γ_j) has been made. In exact arithmetic no consideration is necessary, since the directions of the p_j's and the q_j's are the determining factors. In finite precision, this is not the case.

Such practical considerations may appear out of place in our discussion of the two-sided Lanczos process, but are necessary and propert. The problems of stabilization must be attacked in the context that they are encountered, not in the ideal. Thus we assume that we are now working in finite arithmetic and must adjust accordingly.

We certainly wish to avoid extremes in the selection of β_j. Taking β_j to be the largest machine number, for example, is unreasonable. Not so obvious is the innocent choice of $\beta_j = 1$ as the following example shows.

EXAMPLE 1.1

$$B = \begin{bmatrix} \alpha_1 & 2^{-m} & & & \\ 2^{-m} & \alpha_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & 2^{-n} \\ & & & 2^{-m} & \alpha_n \end{bmatrix}, \quad p_1^* = e_1^*, \quad q_1 = e_1$$

where m is some small positive integer (say 4) and α_i is arbitrary.

It is easily verified that the Lanczos algorithm produces

$$p_\ell^* = 2^{(\ell-1)m} e_\ell^*$$

$$q_\ell = 2^{(1-\ell)m} e_\ell$$

$$J_\ell = \begin{bmatrix} \alpha_1 & 2^{-2m} & & & & \\ 1 & \alpha_2 & 2^{-2m} & & & \\ & 1 & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & 2^{-2m} \\ & & & & 1 & \alpha_n \end{bmatrix}$$

From this example we see that even for a symmetric matrix, the sacrifice of symmetry causes exponential growth in the elements of one set of vectors and exponential decline in the other.

If symmetry is such a desirable property, perhaps the selection of $\beta_j = |\gamma_j| = \sqrt{|\omega_j|}$ would be better. As it turns out, we gain nothing over $\beta_j = 1$ as the following example demonstrates.

EXAMPLE 1.2

$$B = \begin{bmatrix} \alpha_1 & 2^{m} & & & \\ 2^{-m} & \alpha_2 & 2^{m} & & \\ & 2^{-m} & \ddots & \ddots & \\ & & \ddots & \ddots & 2^{m} \\ & & & 2^{-m} & \alpha_n \end{bmatrix}, \quad p_1^*, q_1, m \text{ and } \alpha_i \text{ as before}$$

Here again $p_\ell^* = 2^{(\ell-1)m} e_\ell^*$ and $q_\ell = 2^{(1-\ell)m} e_\ell$ while

$$J_\ell = \begin{bmatrix} \alpha_1 & 1 & & \\ 1 & \alpha_2 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & \alpha_n \end{bmatrix}$$

So the entity of interest is again not the resulting matrix, but the bases with which we are dealing.

The risk of element growth (or decline) can be reduced by forcing the norms of the resulting vectors, p_ℓ^* and q_ℓ, to be equal. This criterion forces

$$\beta_\ell = (|\omega_\ell| \|r_\ell\| / \|s_\ell\|)^{1/2}$$
$$\gamma_\ell = \text{sign}(\omega_\ell)(|\omega_\ell| \|s_\ell\| / \|r_\ell\|)^{1/2}$$

Since $\omega_\ell = s_\ell^* r_\ell$

$$\|p_\ell^*\|^2 = \|q_\ell\|^2 = (|\omega_\ell| / (\|r_\ell\| \|s_\ell^*\|))^{-1}$$
$$= (\cos(\angle(s_\ell^*, r_\ell)))^{-1}$$
$$= \sec(\angle(s_\ell^*, r_\ell)) = \sec(\angle(p_\ell^*, q_\ell))$$

Therefore, the norms of each vector is not less than one and becomes large only as the vector pair (p_ℓ^*, q_ℓ) approach orthogonal. Further if B is symmetric, the process reduces (with $p_1 = q_1$) to the symmetric Lanczos algorithm.

1.8 The generalized problem

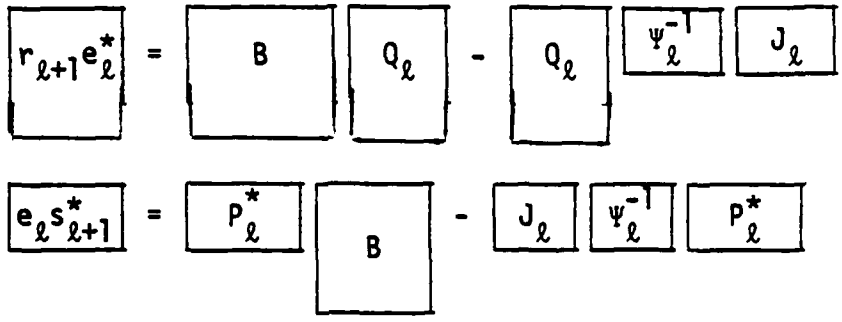
An alternative to allowing any growth in the elements of p_ℓ^* and q_ℓ is to force the norms of these vectors to be unity. We then have that $p_\ell^* q_\ell = \cos(\angle(p_\ell^*, q_\ell))$. In terms of the ultimate goal of our work, we have generalized the problem to finding eigenvalues for the matrix pencil $J_\ell - \lambda \Psi_\ell$ where

$$J_\ell = P_\ell^* B Q_\ell$$

and

$$\Psi_\ell = \text{diag}\{\psi_1, \psi_2, \ldots, \psi_\ell\} = P_\ell^* Q_\ell \ .$$

Pictorially, (1.10a) and (1.10b) become



The three term recurrences (1.3) then are

$$\begin{aligned} r_{\ell+1} &= Bq_\ell - q_\ell(\alpha_\ell/\psi_\ell) - q_{\ell-1}(\gamma_\ell/\psi_{\ell-1}) \\ s^*_{\ell+1} &= p^*_\ell B - (\alpha_\ell/\psi_\ell)p^*_\ell - (\beta_\ell/\psi_{\ell-1})p^*_{\ell-1} \\ \omega_{\ell+1} &= s^*_{\ell+1} r_{\ell+1} \end{aligned} \tag{1.12a}$$

and

$$\begin{aligned} q_{\ell+1} &= r_{\ell+1}/\|r_{\ell+1}\|, \quad p^*_{\ell+1} = s^*_{\ell+1}/\|s^*_{\ell+1}\| \\ \beta_{\ell+1} &= p^*_{\ell+1} B q_\ell = \omega_{\ell+1}/\|s^*_{\ell+1}\| \\ \gamma_{\ell+1} &= p^*_\ell B q_{\ell+1} = \omega_{\ell+1}/\|r_{\ell+1}\| \\ \psi_{\ell+1} &= p^*_{\ell+1} q_{\ell+1} = \cos(\angle(p^*_{\ell+1}, q_{\ell+1})) = \omega_{\ell+1}/(\|s^*_{\ell+1}\|\|r_{\ell+1}\|) \end{aligned} \tag{1.12b}$$

1.9 Summary

The insight that comes from relating the Lanczos algorithm to the moment matrix is this: once p^* and q are chosen the success or failure of the process is determined. If any of the moment matrices M_j is singular then the algorithm will halt at step j-1 with $\omega_j = 0$. If either $r_j = 0$ or $s^*_j = 0^*$ then an invariant subspace, our goal, has been captured; otherwise (i.e. $\omega_j = 0$, $s^*_j \neq 0$ and $r_j \neq 0$), the

choice of p^* and q was unfortunate. It could happen that no eigenvalue of J_j is close to an eigenvalue of B and in such a case, the effort seems wasted. This is called serious breakdown.

EXAMPLE 1.3 (Wilkinson, [1958])

$$B = \begin{bmatrix} 5 & 1 & -1 \\ -5 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}, \quad p^* = [.6 \ .3 \ -.1], \quad q = \begin{bmatrix} .6 \\ -1.4 \\ .3 \end{bmatrix}$$

$$p_2^* = p^*B - \alpha p^* = [.6 \ .2 \ -.267]$$

$$q_2 = Bq - q\alpha = \begin{bmatrix} .5 \\ -.833 \\ .5 \end{bmatrix}$$

where $\alpha = p_1^* B q_1 / p_1^* q_1 = 4/3$,

$$p_2^* q_2 = 0 \quad \text{serious breakdown!}$$

The foregoing analysis shows that the Lanczos scheme is too rigid to be stable. The great practical advantage is that the projection of B onto K^ℓ and K_*^ℓ is tridiagonal. If these spaces contain good approximations to the desired eigenvectors, then the computation of these approximations requires the calculation of certain eigenpairs of an $\ell \times \ell$ tridiagonal matrix, a relatively easy task.

II. The Look-Ahead Lanczos Algorithm

2.1 Introduction

The ideas presented in Chapter I not only establish the Lanczos algorithm from a general mathematical perspective, but lay the foundation for the modifications that give it more flexibility. That the subspaces, and not the particular bases, are important, allows a modification of the Lanczos process which furnishes a potentially powerful tool.

The "look-ahead" Lanczos algorithm presented below is a way to relax the two-sided Lanczos algorithm. As in Chapter I, the two-sided Gram-Schmidt process and the factorization of moment matrices play important roles in the understanding of our new algorithm.

We will assume here that $K^n = \mathbb{R}^n$ and $K_*^n = \mathbb{R}_*^n$. This is not necessary for the study but simplifies the presentation. In those places where $K^n = \mathbb{R}^n$ is assumed, we might just as easily assume a sufficiently large invariant subspace, but such conditions add nothing to the presentation and conceal key ideas.

2.2 Breakdown and the Two-Sided Gram-Schmidt

To understand breakdown in Lanczos and our remedy for it, it is necessary to focus on the generation of two inter-related sets of vectors. The sets, related by biorthogonality, form bases for the row and column spaces K_*^n and K^n, respectively.

First, though, let us consider the general case. Let $F^k = \text{span}\{f_1,\ldots,f_k\}$, $G_*^k = \text{span}\{g_1,\ldots,g_k\}$ with $F^n = \mathbb{R}^n$ and $G_*^n = \mathbb{R}^n$. Define the matrices

$$F_k = [f_1,\ldots,f_k] \qquad G_k^* = \begin{bmatrix} g_1^* \\ \vdots \\ g_k^* \end{bmatrix}$$

where the columns of F_k form the *primary vectors* of F^k and the rows of G_k^* form the primary vectors of G_*^k. Note that $\text{rank}(F_k) = \text{rank}(G_k^*) = k$.

Applying the two-sided Gram-Schmidt process to F^{k-1} and G_*^{k-1}, we get

$$\hat{F}^{k-1} = \text{span}\{\hat{f}_1,\ldots,\hat{f}_k\} = F^{k-1}$$
$$\hat{G}_*^{k-1} = \text{span}\{\hat{g}_1,\ldots,\hat{g}_k\} = G_*^{k-1}$$

where $\hat{f}_i \in F^i$, $\hat{g}_i^* \in G_*^i$, $\|\hat{f}_i\| = \|\hat{g}_i\| = 1$, and $\hat{g}_i^*\hat{f}_j = \delta_{ij}\,\psi_i$ with $\psi_i = \cos \angle(\hat{g}_i^*,\hat{f}_i)$. Next we apply TSGS to F^i and G_*^i by forming

$$\begin{aligned} \tilde{f}_k &= (f_k - \sum_{i=1}^{k-1} \hat{f}_i(\hat{g}_i^* f_k/\psi_i) \\ \tilde{g}_k^* &= (g_k^* - \sum_{i=1}^{k-1} (g_k^*\hat{f}_i/\psi_i)\hat{g}_i^* \end{aligned} \tag{2.1}$$

and then normalize to obtain

$$\begin{aligned} \hat{f}_k &= \tilde{f}_k/\|\tilde{f}_k\| \ , \\ \hat{g}_k^* &= \tilde{g}_k^*/\|\tilde{g}_k^*\| \ , \\ \psi_k &= \hat{g}_k^*\hat{f}_k \ . \end{aligned}$$

Note that neither $\tilde{f}_k$ nor $\tilde{g}_k$ is zero since the f's and g's form bases for $\mathbf{R}^n$ and $\mathbf{R}_*^n$ (this point will be elaborated below).

Let us assume that $\tilde{g}_k^*\tilde{f}_k = 0$ and thus $\psi_k = \hat{g}_k^*\hat{f}_k = 0$. We cannot continue the Gram-Schmidt process since that would involve division by zero in (2.1). A different pair of sets may be selected to replace

$\{f_1,\ldots,f_n\}$ and $\{g_1,\ldots,g_n\}$ since the latter pair proved unsatisfactory. Unfortunately, we have no more guarantee of success with a new pair of sets than we did with the original pair.

EXAMPLE 2.1: $n = 3$

$$F_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad G_3^* = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

$$\hat{f}_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad \hat{g}_1^* = [.5,0,.5]$$

$$\tilde{f}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} - 0.* \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\tilde{g}_2^* = [0,0,1] - 0^*[.5,0,.5] = [0,0,1]$$

and $$\tilde{g}_2^*\tilde{f}_2 = 0 \ .$$

2.3 Look-ahead in Two-Sided Gram-Schmidt

The defect with the standard TSGS does not lie with the primary vectors $\{f_1,\ldots,f_n\}$ and $\{g_1^*,\ldots,g_n^*\}$ since these form bases for $\mathbf{R}^n$ and $\mathbf{R}_*^n$. Rather, one (or both) sequences of vectors was used in an unfortunate order. For each $\tilde{f}_j$ there must be some $m \geq j$ such that $g_m^* f_j \neq 0$. We formalize this concept in the following lemma.

LEMMA 2.1. *Let* $F^k = \text{span}\{f_1,\ldots,f_k\}$ *and* $G_*^k = \text{span}\{g_1^*,\ldots,g_k^*\}$ *with* $F^n = \mathbf{R}^n$ *and* $G_*^n = \mathbf{R}_*^n$. *Let* $\hat{f}_i$ *be defined by* $\|\hat{f}_i\| = 1$, $\hat{f}_i \in F^i$, $\hat{f}_i \perp G_*^{i-1}$, *and let* $\hat{g}_i^*$ *be defined by* $\|\hat{g}_i^*\| = 1$, $\hat{g}_i^* \in G_*^i$, $\hat{g}_i^* \perp F^{i-1}$. *Further, for* $i < k$, *let* $\psi_i = \hat{g}_i^*\hat{f}_i \neq 0$. *Then there is an* $m \geq k$ *such that*

$$\bar{g}_m^* \hat{f}_k \neq 0$$

where $\bar{g}_m^* \in G_*^m$, $\bar{g}_m^* \perp F^{k-1}$.

PROOF. First, since $F_k = [f_1,\ldots,f_k]$ has rank k and $\hat{f}_k$ has a non-zero component in the direction f_k (from (2.1)), $f_k = F_k v \neq 0$. Now, $G_n^* = \begin{bmatrix} g_1^* \\ \vdots \\ g_n^* \end{bmatrix}$ has full rank, so $G_n^* f_k \neq 0$. Thus there is some m such that $g_m^* \hat{f}_k \neq 0$. By construction, $g_\ell^* \hat{f}_k = 0$ for $\ell < k$, so $m \geq k$. Let $\bar{g}_m^* = g_m^* - \sum_{i=1}^{k-1} (g_m^* \hat{f}_i / \psi_i) \hat{g}_i^*$. By noting that $\bar{g}_m^* \hat{f}_k = g_m^* \hat{f}_k \neq 0$, the result follows. ∎

Thus, on breakdown, we can switch g_m^* and g_k^* and continue the process.

2.4 The look-ahead scheme and subspaces

What effect does the switching of primary vectors have on the subspaces? The exchange of g_m^* with g_k^* can be considered a reselection of subspaces of G_*^n. Thus, for $i = k,\ldots,m-1$

$$G_*^i \text{ becomes } \tilde{G}_*^i = \text{span}\{g_1^*,\ldots,g_{k-1}^*,g_m^*,g_{k+1}^*,\ldots,g_i^*\} .$$

For all other i, G_*^i remains unchanged.

This dynamic interpretation may not preserve all properties of the original subspaces (such as $BK^i \subset K^{i+1}$ in the case of Krylov subspaces). We, therefore, present the following interpretation.

When $\tilde{g}_k^* \tilde{f}_k = 0$, we find the first g_m^* such that $g_m^* \tilde{f}_k \neq 0$, generate $\bar{g}_k^* = g_m^* - \sum_{i=1}^{k-1} (g_m^* \hat{f}_i / \psi_i) \hat{g}_i^*$, and normalize $\tilde{f}_k$ and $\bar{g}_k^*$ to form $\hat{f}_k$ and $\hat{g}_k^*$. Now, in place of $\hat{g}_k^* \in G_*^k$, we have $\hat{g}_k^* \in G_*^m$.

Further, for $i = k+1,\ldots,m$ (from 2.1),

$$\tilde{g}_i^* = g_i^* - \sum_{j=1}^{i-1} (g_i^* \hat{f}_j / \psi_j) \hat{g}_j^* \in G_*^m$$

since $\hat{g}_k^*$ is included in the sum. In other words, instead of generating one row basis vector from each $G_*^k,\ldots,G_*^m$, we are generating $(m-k+1)$ row basis vectors from G_*^m.

The set of vectors we finally generate is, in fact, a basis for the subspace $G_*^m \backslash G_*^{k-1} \subset G_*^m$ (i.e., $G_*^m \backslash G_*^{k-1}$ is the subspace of G_*^m orthogonal to F^{k-1}). Thus, a solution to serious breakdown in TSGS consists of selecting a basis from a larger subspace.

2.5 The look-ahead scheme and matrices

We do not need to restrict ourselves to only changing the row subspaces. We can, in fact, "look-ahead" in both row and column subspaces and select bases from $G_*^m \backslash G_*^{k-1}$ and $F^m \backslash F^{k-1}$.

If we let $H^* = \begin{bmatrix} h_1^* \\ \vdots \\ h_\ell^* \end{bmatrix}$ and $C = [c_1,\ldots,c_\ell]$, $\ell = m-k+1$, with

$$h_i^* = g_{k-i+1}^* - \sum_{j=1}^{k-1} (g_{k-i+1}^* \hat{f}_j / \psi_j) \hat{g}_j^*$$

$$c_i = f_{k-i+1} - \sum_{j=1}^{k-1} (\hat{g}_j^* f_{k-i+1} / \psi_j) \hat{f}_j$$

then any bases we choose have the matrix representation

V^*H^* for row vectors

CU for column vectors

for some invertible, $\ell \times \ell$ matrices U and V^*.

Further, if we let $N = H^*C$, the "connection" matrix of inner products, and $\tilde{h}_i^* = e_i^* V^* H^*$ and $\tilde{c}_i = CUe_i$, then

$$N = V^{-*}\tilde{\Psi}U^{-1}$$

where $\tilde{\Psi} = \text{diag}\{\tilde{h}_1^*\tilde{c}_1, \ldots, \tilde{h}_\ell^*\tilde{c}_\ell\}$ (assuming biorthogonality of the $\tilde{h}_i^*$'s and $\tilde{c}_i$'s). Thus, to each selection of bases vectors corresponds a particular factorization of the inner product matrix N.

2.6 Two-Sided Gram-Schmidt and LDU factorization

We have related the "look-ahead" scheme to some factorization for a matrix. We wish now to weld this concept onto our LDU factorization of the moment matrix. Again, we will discuss general spaces and will return to our actual objective, Krylov subspaces, in the next section.

Consider the modified two-sided Gram-Schmidt process, i.e. at step k,

$$f_\ell \leftarrow f_\ell - \sum_{i=1}^{k-1} \hat{f}_i (\hat{g}_i^* f_\ell / \psi_i) = f_\ell - \hat{f}_{k-1}(\hat{g}_{k-1}^* f_\ell / \psi_{k-1}) \qquad \ell \geq k$$

$$g_\ell^* \leftarrow g_\ell^* - \sum_{i=1}^{k-1} (g_\ell^* \hat{f}_i / \psi_i)\hat{g}_i^* = g_\ell^* - (g_\ell^* \hat{f}_{k-1}/\psi_{k-1})\hat{g}_{k-1}^* \qquad \ell \geq k$$

$$\hat{f}_k \leftarrow f_k / \|f_k\|, \quad \hat{g}_k^* \leftarrow g_k^* / \|g_k^*\|, \quad \psi_k \leftarrow \hat{g}_k^* \hat{f}_k .$$

So, by construction $g_\ell^* \hat{f}_j = \hat{g}_j^* f_\ell = 0$ for $j < k$, $\ell \geq k$ (here g_i^* and f_i denote vectors updated at each step).

In matrix notation this becomes

$$\Gamma_k^{-1}\left[\begin{array}{c|c} L_k^{-1} & \\ \hline E_k & I_{n-k} \end{array}\right] G_n^* = \begin{bmatrix} g_1^* \\ \vdots \\ g_k^* \\ g_{k+1}^* \\ \vdots \\ g_n^* \end{bmatrix} = \hat{G}_k^*$$

and

$$F_n\left[\begin{array}{c|c} U_k^{-1} & Z_k \\ \hline & I_{n-k} \end{array}\right] \Phi_k^{-1} = [\hat{f}_1,\ldots,\hat{f}_k,f_{k+1},\ldots,f_n] = \hat{F}_k$$

where $\Gamma_k = \text{diag}\{\|g_1^*\|,\ldots,\|g_k^*\|,1,\ldots,1\}$

and $\Phi_k = \text{diag}\{\|f_1\|,\ldots,\|f_k\|,1,\ldots,1\}$.

Then

$$\hat{G}_k^*\hat{F}_k = \left[\begin{array}{c|c} \psi_1 \cdots \psi_k & 0 \\ \hline 0 & C^{(k)} \end{array}\right] = \Gamma_k^{-1}\left[\begin{array}{cc} L_k^{-1} & \\ E_k & I_{n-k} \end{array}\right] C^{(1)} \left[\begin{array}{cc} U_k^{-1} & Z_k \\ & I_{n-k} \end{array}\right] \Phi_k^{-1}$$

where

$$C^{(j)} = \begin{bmatrix} g_j^*\hat{f}_j & g_j^*f_{j+1} & \cdots & g_j^*f_n \\ g_{j+1}^*\hat{f}_j & g_{j+1}^*f_{j+1} & \cdots & g_{j+1}^*f_n \\ \vdots & \vdots & & \vdots \\ g_n^*\hat{f}_j & g_n^*f_{j+1} & \cdots & g_n^*f_n \end{bmatrix}$$

is the matrix of inner products at step k.

Here we have just reiterated the correspondence between TSGS and the LDU factorization of $C^{(1)}$. Now, to what does the look-ahead scheme correspond?

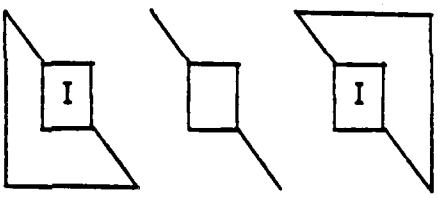
As shown in the previous section, the extraction of biorthogonal basis vectors from $G_*^{\ell+1} \backslash G^k$ and $F^{\ell+k} \backslash F^k$ corresponds to the factorization of an $\ell \times \ell$ inner product matrix. This $\ell \times \ell$ matrix is the ℓ^{th} principle submatrix of $C^{(k)}$.

The matrix interpretation of the look-ahead scheme is as follows:

> We perform Gaussian elimination for k-1 steps and then encounter a zero pivot. We do not wish to use either partial or complete pivoting for various reasons (e.g. not all elements are readily available). Following Kahan (Parlett and Bunch [1971]) we prefer to generalize the notion of a pivot, from a scalar quantity to a matrix. We then search for a suitably well-conditioned principle submatrix, and using an appropriate factorization, use that as our pivot.

Pictorially, the final factorization is then

$C^{(1)} =$



2.7 Lanczos and look-ahead

We now have a method to remedy the breakdown of the two-sided Gram-Schmidt process. To interpret this for Lanczos we replace F^k with K^k and G_*^k with K_*^k.

As we have seen, the selection of bases vectors corresponds to the factorization of a particular matrix. In the Lanczos process, it is convenient not to use the principle submatrix of the moment matrix (matrix of inner products) but to use a scaled version. This will become clear as we present the look-ahead.

Let

$$\tilde{S} = \begin{bmatrix} \tilde{s}_1^* \\ \vdots \\ \tilde{s}_k^* \\ \tilde{s}_{k+1}^* \\ \vdots \\ \tilde{s}_n^* \end{bmatrix} = \begin{bmatrix} L_k & \\ \tilde{Z}_k & I_{n-k+1} \end{bmatrix}^{-1} \begin{bmatrix} p^* \\ p^*B \\ \vdots \\ p^*B^{n-1} \end{bmatrix}$$

and

$$\tilde{R} = [\tilde{r}_1,\ldots,\tilde{r}_k,\tilde{r}_{k+1},\ldots,\tilde{r}_n] = [q,Bq,\ldots,B^{n-1}q] \begin{bmatrix} L_k^* & \tilde{Z}_k^* \\ & I_{n-k+1} \end{bmatrix}^{-1}$$

where $\tilde{Z}_k$ is such that $\tilde{s}_j^*$ is orthogonal to K^{k-1} (and, by symmetry, $\tilde{r}_j$ is orthogonal to K_*^{k-1}) for $j \geq k$. Then

$$M_n = K_n^* K_n = \begin{bmatrix} L_k & \\ \tilde{Z}_k & I_{n-k+1} \end{bmatrix} \begin{bmatrix} \tilde{\Omega}_{k-1} & 0 \\ 0 & \tilde{M}_{n-k+1} \end{bmatrix} \begin{bmatrix} L_k^* & \tilde{Z}_k^* \\ & I_{n-k+1} \end{bmatrix}$$

$$= \begin{bmatrix} \hat{L}_k & \\ \hat{Z}_k & \gamma^{(k)} I_{n-k+1} \end{bmatrix} \begin{bmatrix} I_{k-1} & 0 \\ 0 & \hat{M}_{n-k+1} \end{bmatrix} \begin{bmatrix} \bar{L}_k^* & \bar{Z}_k^* \\ & \beta^{(k)} I_{n-k+1} \end{bmatrix}$$

with $\tilde{\Omega}_{k-1} = \text{diag}\{\omega_1,\omega_1\omega_2,\ldots,\omega_1\cdots\omega_{k-1}\}$, and $\hat{L}_k$ and $\bar{L}_k^*$ no longer with unit diagonals. In Lanczos, it is the principle submatrices of $\hat{M}_{n-k+1}$ rather than those of $\tilde{M}_{n-k+1}$ with which we have interest.

We thus consider the 1×1 principle submatrix of $\hat{M}_{n-k+1}$, ω_k. If $\omega_k = 0$, we try the 2×2 principle submatrix of $\hat{M}_{n-k+1}$ and so on until we have a suitable pivot.

2.8 Effects of the look-ahead scheme on the J matrix

We must pay a price for stepping outside the strict sequence of Krylov subspaces.

For this section we need to adjust our notation. Let i denote the i^{th} step of the "look-ahead" algorithm whether the pivot is 1×1, 2×2, or larger. Let ℓ denote the actual vector index and let

$$P_i^* = \begin{bmatrix} p_\ell^* \\ \vdots \\ p_{\ell+k-1}^* \end{bmatrix} \quad \text{and} \quad Q_i = [q_\ell,\ldots,q_{\ell+k-1}]$$

whenever a $k\times k$ pivot is used. Then

$$J_m = \begin{bmatrix} P_1^* \\ \vdots \\ P_m^* \end{bmatrix} B[Q_1,\ldots,Q_m]$$

$$= \begin{bmatrix} P_1^*BQ_1 & \cdots & P_1^*BQ_m \\ \vdots & & \vdots \\ P_m^*BQ_1 & \cdots & P_m^*BQ_m \end{bmatrix}$$

The P's and Q's enjoy the same orthogonality properties that the p's and q's did in the two-sided Lanczos algorithm. That is

$$P_i^*Q_j = 0 \ , \quad i \neq j \ .$$

Thus, J_m reduces to *block* tridiagonal

$$J_m = \begin{bmatrix} A_1 & \Gamma_2 & & \\ B_2 & A_2 & \ddots & \\ & \ddots & \ddots & \Gamma_n \\ & & B_n & A_n \end{bmatrix}$$

(B_j here denotes upper case β); the dimensions of the blocks being

determined by the dimensions of the P's and Q's.

2.9 Subspaces for look-ahead Lanczos

Recall that factorization of the pivot matrix corresponds to selection of a pair of bases. The factorization used needs to hold some advantage over the infinite number of other choices; an advantage that must be reflected in the selection of the associated basis vectors.

Before continuing, it is necessary to indicate precisely what the subspaces are and how they are produced. These spaces correspond to $G_*^n \backslash G_*^{k-1}$ and $F^m \backslash F^k$ of section 2.6.

Let $k-1$ be the number of successful steps of the two-sided Lanczos process, that is, we have successfully found bases for K^{k-1} and K_*^{k-1}. Let us now assume that breakdown has occurred. We need to find m such that $K^m \backslash K^{k-1}$ and $K_*^m \backslash K_*^{k-1}$ have $m-k+1$ dimensional biorthogonal bases. How do we find them?

First we need a set of primary vectors spanning the appropriate subspaces. Recall from Chapter I that $Bq_{j-1} \in K^j$. Similarly, $Br_k \in K^{k+1}$ since $r_* \in K^k$, $r_k \notin K^{k-1}$. Further, $B^2 r_k \in K^{k+2}$, $B^3 r_k \in K^{k+3}$ and so on. So, with r_k at hand, the representative vectors for K^{k-1} through K^m are obtained by matrix products with B. To obtain vectors in $K^m \backslash K^{k-1}$ we need only orthogonalize each $B^i r_k$ to K_*^{k-1}. Such orthogonalizations require that bases vectors for (perhaps all) K^{k-1} and K_*^{k-1} be available.

We can avoid keeping these bases around by following the two-sided Lanczos algorithm. Let $\tilde{r}_k$ be the current residual, and generate the rest of the primary vectors for $K^m \backslash K^{k-1}$ as follows.

For $j = k,\ldots,m-1$

$$\tilde{r}_{j+1} = B\tilde{r}_j - q_{k-1}(p_{k-1}^* B\tilde{r}_j/\psi_{k-1}) \qquad (2.2a)$$

LEMMA 2.2. $\tilde{r}_\ell \perp K_*^{k-1}$

PROOF. $\tilde{r}_k \perp K_*^{k-1}$ by construction so $B\tilde{r}_* \perp K_*^{k-2}$. Since $q_{k-1} \perp K_*^{k-2}$, $\tilde{r}_{k+1} \perp K_*^{k-2}$. Now $p_{k-1}^* r_{k+1} = p_{k-1}^* Br_k - \psi_{k-1}(p_{k-1}^* Br_k/\psi_{k-1}) = 0$; thus $\tilde{r}_{k+1} \perp K_*^{k-1}$. The result follows by induction. ∎

Similarly, we may generate $K_*^m \backslash K_*^{k-1}$ by the following: Let $\tilde{s}_k$ be the current residual.

For $j = k,\ldots,m-1$

$$\tilde{s}_{j+1}^* = s_j^* B - (\tilde{s}_j Bq_{k-1}/\psi_{k-1})p_{k-1}^* \,. \qquad (2.2b)$$

2.10 Choosing orthogonal bases

We now have row and column vectors spanning the subspaces of consequence. From these vectors we will generate bases to continue our process. But how shall we decide between different bases?

Assume that Q is $n \times \ell$ ($\ell = m-k+1$) matrix whose column space is $K^m \backslash K^{k-1}$ and P^* is such that P^*Q is diagonal and the row space of P^* is $K_*^m \backslash K_*^{k-1}$. There is no loss in generality in forcing all bases vectors to have Euclidean norm of unity. It follows that

$$1 \le \|P^*\| \le \sqrt{\ell}\,, \quad 1 \le \|Q\| \le \sqrt{\ell}\,.$$

A prevalent measure of the linear independence of P^*'s rows is

$$\mathrm{cond}(P^*) = \|P^*\|\|P^+\| = \sigma_1(P^*)/\sigma_\ell(P^*)$$

where P^+ denotes the pseudo-inverse of P^*,

$\sigma_1(P^*) \geq \sigma_2(P^*) \geq \cdots \geq \sigma_\ell(P^*) > 0$ are the singular values of P^*. Our normalization ensures that $\sqrt{\ell} \geq \sigma_1(P^*)$ and so our interest focuses on $\sigma_\ell(P^*)$. Note further that

$$\sigma_\ell(P^*) \leq (\sigma_1(P^*)\cdots\sigma_\ell(P^*))^{1/\ell} = \det(P^*P)^{1/2} .$$

There seems to be little prospect of estimating $\sigma_\ell(P^*)$ or $\sigma_\ell(Q)$ directly.

We try another approach. Let $\ell = n$ and suppose that $P^*Q = \Omega_n = \text{diag}\{\sigma_1,\ldots,\sigma_n\}$ with $1 \geq \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n > 0$. In this case

$$\begin{aligned} P^* &= Q\Omega_n^{-1} \\ \text{cond}(P^*) &= \|P^*\|\|P^*\| \\ &= \|P\|\|Q\Omega_n^{-1}\| \\ &\leq \sqrt{n}\,\sqrt{n}\,\sigma_n^{-1} = n/\sigma_n \end{aligned}$$

This suggests that among biorthogonal bases we should prefer those which maximize

$$\min_i |p_i^* q_i| . \tag{2.3}$$

The assumption $\ell = n$ was for simplicity only. In general, for $\ell < n$, $P^+ = Q\Omega_\ell^{-1}$ and so

$$\text{cond}(P^*) = \|P^*\|\|Q\Omega_\ell^{-1}\| \leq \|P^*\|\|Q\|\|\Omega_\ell^{-1}\| \leq \ell/\sigma_\ell .$$

To return to the look-ahead Lanczos, we wish to select bases which maximize (2.3) over $k \leq i \leq m$. This is a non-trivial problem. We will discuss the 2×2 pivot in Chapter III but leave the general case as beyond the scope of this work.

2.11 Practical side of pivot selection

In the previous section we discussed the selection of bases for a particular pair of subspaces $K^m \backslash K^{k-1}$ and $K_*^m \backslash K_*^{k-1}$. In particular we must not only select bases within subspaces, but between subspaces themselves. If say $\cos \angle(r_k, s_k^*)$ were very small but non-zero, exact arithmetic would allow the Lanczos process to continue, whereas finite precision would cause the Lanczos process to behave erroneously.

To employ the cosines of angles between the different possible bases, we must first decide which angles are important and which are not. We do not wish, for example, to only compare all possible bases in $K^m \backslash K^{k-1}$ and $K_*^m \backslash K_*^{k-1}$. By ignoring the bases of smaller subspaces, we may miss a smaller subspace coupled with a subspace beyond consideration at step k which would yield a superior pair of bases.

Instead we assume that to each pivot block corresponds one "optimal" pair of bases and we then

$$\underset{j=1,\ldots,\ell}{\text{maximize}} \quad \underset{i=1,\ldots,j}{\text{minimum}} \; |p_i^* q_j| \; . \tag{2.4}$$

This criterion gives a way to determine the "best" pivot at each step.

Of practical consideration is fast memory limitations. We need to reduce memory requirements as much as possible. Further, the block tridiagonal form is not immediately amenable to eigenvalue analysis. Thus some restrictions on the form of the J matrix are in order.

Recall that the blocks of the J matrix are of the form $P_i^* B Q_j$ where $|i-j| \leq 1$. If P_i^* is $k \times n$ and Q_j is $n \times m$, $P_i B Q_j$ is $k \times m$. Thus, with a maximum pivot size of ℓ, the bandwidth of J may be as large as 3ℓ.

We can reduce the maximum bandwidth to $2\ell+1$ by preserving the order of one Krylov sequence. For example, if $q_i \in K^i$ for all i, $p_j^* B q_i = 0$, $|i-j| < 1$, and the J matrix retains the Hessenberg form.

2.12 Summary

We now have a method for stabilizing the two-sided Lanczos process. This stabilization preserves as much as possible of the Krylov space structure. The cost of our remedy may seem expensive, several extra matrix-vector products, but will be absorbed in use, as seen in Chapter III.

Further, (2.4) gives a clear measure of the superiority of one pair of bases over another and one pivot size over another. The differences in dimension of the competing subspaces is unimportant. That is, if, at step i, we use a $k \times k$ pivot instead of an $\ell \times \ell$ pivot, $k < \ell$, the problem of selecting bases vectors at step i+1 is independent of the selection at step i, in spite of the overlap of subspaces.

Finally, we can not ignore the fact that there is available only a limited amount of storage. The vectors we can retain in memory and the size of the J matrix are limited. The storage crunch is reduced by forcing one Krylov sequence to remain intact. Further, by limiting pivot size we can limit the bandwidth of J and the number of vectors that must be kept in fast storage.

In other words, the look-ahead mechanism allows us to balance the competing demands for well-conditioned bases and limited fast storage. It turns out that the simple extension to allow 2×2 pivots eliminates many instances of bad bases without a significant increase in storage requirements.

III. 2 × 2 Pivot

3.1 Introduction

In this chapter we complete our discussion of the generalized pivot. The analysis is non-trivial so we confine ourselves to the 2×2 case and leave the general case to subsequent work.

The relationship between the pivot factorization and the bases is exhibited for some familiar factoring schemes. Further, the angles between the subspaces, à la Davis and Kahan, is presented. This approach gives bases independent of the primary vectors and presents us with a tool for finding the best bases in the sense of Chapter II (section 2.11).

To complete the discussion of the look-ahead algorithm, we need a criterion for judging approximate eigenvalues. Alas, none exists. However, Kahan, Parlett and Jiang have produced residual bounds on approximate eigensystems and we generalize their discussion of residual bounds for Lanczos to encompass the look-ahead Lanczos.

Much of the discussion refers to quantities defined in Chapter II. As a brief review, recall s_j^* and r_j denote the row and columns residual vectors at step j with $s_j^* \perp K^{j-1}$ and $r_j \perp K_*^{j-1}$. Further, the look-ahead procedure determines biorthogonal bases vectors in $K^m \backslash K^{j-1}$ (all vectors in K^m orthogonal to K_*^{j-1}) and $K_*^m \backslash K_*^{j-1}$.

The pivot matrix will be defined explicitly for the two dimensional case. The explicit relationship between the pivot factorization and the bases determined by that factorization (section 2.6) will be used without being rederived.

3.2 Subspace considerations

As in Chapter II, assume that the two-sided Lanczos has proceeded for j-1 steps without serious breakdown. That is the bases vectors $\{q_1,\ldots,q_{j-1}\}$ and $\{p_1^*,\ldots,p_{j-1}^*\}$ are such that $q_i \in K^i$ and $p_i^* \in K_*^i$. We now assume that the current residuals r_j and s_j^* are too nearly orthogonal to proceed with the Lanczos process.

Following section 2.9, we generate the primary vectors which determine the subspaces of interest, $K^{j+1}\backslash K^{j-1}$ and $K_*^{j+1}\backslash K_*^{j-1}$. With r_j and s_j^* already present, the remaining primary vectors are defined from (2.2a) and (2.2b) by

$$\begin{aligned} \tilde{r}_{j+1} &= Br_j - q_{j-1}(\omega/\psi_{j-1}) \\ \tilde{s}_{j+1}^* &= s_j^*B - (\omega/\psi_{j-1})p_{j-1}^* \end{aligned} \tag{3.1}$$

where $\omega = s_j^*r_j$ and $\psi_{j-1} = p_{j-1}^*q_{j-1}$.

Let $R = K^{j+1}\backslash K^{j-1}$ and $S_* = K^{j+1}\backslash K^{j-1}$ be the planes for which we wish to generate biorthogonal bases. Then

$$\begin{aligned} R &= \text{span}\{r_j,\tilde{r}_{j+1}\} \subset \mathbf{R}^n \\ S_* &= \text{span}\{s_j^*,\tilde{s}_{j+1}^*\} \subset \mathbf{R}_*^n . \end{aligned}$$

Let $R = [r_j,\tilde{r}_{j+1}]$, $S^* = \begin{bmatrix} s_j^* \\ \tilde{s}_{j+1}^* \end{bmatrix}$, then the pivot matrix W is defined by

$$W = S^*R = \begin{bmatrix} \omega & \theta \\ \theta & \hat{\omega} \end{bmatrix} .$$

(See section 2.7, Chapter II.) For this chapter, W is assumed to be non-singular.

Note that for any selection of biorthogonal bases $\hat{R} = [\hat{r},\hat{r}_+]$ and $\hat{S}^* = [\hat{s},\hat{s}_+]$ in R and S_*, respectively, there exist invertible

2×2 matrices U and V^* such that

$$\begin{aligned} \hat{R} &= RU \\ \hat{S}^* &= V^*S \ . \end{aligned} \tag{3.2}$$

Further, from Chapter II

$$W = V^{-*}\hat{\Psi}U \tag{3.3}$$

where $\hat{\Psi} = \hat{S}^*\hat{R} = \text{diag}\{\hat{\psi}_1, \hat{\psi}_2\}$.

Assume that $\hat{R}$, $\hat{S}^*$ is the pair of bases which is produced by the look-ahead procedure. Recall that to compare this choice with the biorthogonal pair of vectors produced by the two-sided Lanczos process ((2.4) with $\ell = 2$), we must calculate the cosines between the possible bases vectors.

This appears to be extra work, since it seems to require the generation of $\hat{R}$ and $\hat{S}^*$. However, by utilizing (3.2) and (3.3) the cost becomes minimal (see the algorithm in the appendix for details). The labor involves the primary vectors for the subspaces but does not require $\hat{R}$ and $\hat{S}^*$ explicitly. Further, if the two-sided Lanczos is used instead of the 2×2 pivot scheme, the matrix-vector products in (3.1) are not wasted (again, details accompany the algorithm in the appendix).

3.3 Pivot factorization

When discussing factorizations of matrices, some obvious candidates come to mind. These factorizations are exhibited below in terms of their correspondence to bases vectors in the underlying subspaces R and S^*, and their effect on the J-matrix. Here, we are only

concerned with the directions of the bases vectors, and ignore the effects of scaling.

1. LU Factorization

$$W = \begin{bmatrix} 1 & 0 \\ \theta/\omega & 1 \end{bmatrix} \begin{bmatrix} \omega & \theta \\ & \omega - \theta^2/\omega \end{bmatrix}$$

Here both the row and column Krylov sequences are preserved. Thus, locally, the J-matrix is both upper and lower Hessenberg.

This factorization corresponds to two successive steps of the two-sided Lanczos process.

2. UL Factorization

$$W = \begin{bmatrix} 1 & \theta/\hat{\omega} \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \omega - \theta^2/\hat{\omega} & 0 \\ \theta & \hat{\omega} \end{bmatrix}$$

Here both $\tilde{r}_{j+1}$ and $\tilde{s}^*_{j+1}$ are preserved but r_j and s^*_j are modified. This is equivalent to exchanging $\tilde{s}^*_{j+1}$ and s^*_j and $\tilde{r}_{j+1}$ with r_j in the Krylov sequences. We can preserve a mixed symmetry in J ($|j_{k,\ell}| = |j_{\ell,k}|$) with appropriate scaling, but the Hessenberg form is lost.

3. QR Factorization

$$W = \tau^{-1} \begin{bmatrix} \omega & -\theta \\ \theta & \omega \end{bmatrix} \begin{bmatrix} \tau^2 & \theta(\omega+\hat{\omega}) \\ 0 & \omega\hat{\omega} - \theta^2 \end{bmatrix} \tau^{-1}$$

$$\tau^2 = \theta^2 + \omega^2$$

Here the Hessenberg form of J is again preserved. The row space bases vectors, though, are both in K^{j+1}_* so that a definite bump above the super-diagonal is created.

4. LU with Interchange

$$W = \begin{bmatrix} \omega/\theta & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \theta & \hat{\omega} \\ 0 & \theta - \omega\hat{\omega}/\theta \end{bmatrix}$$

The factorization corresponds to partial pivoting in the LU factorization of W. In terms of the residual vectors the column Krylov sequence $(q_j \in K^j,\ q_{j+1} \in K^{j+1})$ is preserved (thus the Hessenberg form of J) but in the row Krylov sequence s_j^* and $\tilde{s}_{j+1}^*$ are exchanged (thus a definite bump above the super-diagonal of J).

5. Spectral Decomposition

$$\begin{aligned} W &= U^* \Psi U \\ U^*U &= I\ , \quad \Psi = \mathrm{diag}\{\psi_1, \psi_2\} \\ \psi_1 &= \tfrac{1}{2}(\omega + \hat{\omega} + ((\omega - \tilde{\omega})^2 + 4\theta^2)^{1/2}) \\ \psi_2 &= \tfrac{1}{2}(\omega + \hat{\omega} - ((\omega - \hat{\omega})^2 + 4\theta^2)^{1/2}) \end{aligned}$$

Here the row vectors both come from K_*^{j+1} and the column vectors come from K^{j+1}. Thus the J-matrix bulges on both sides of the off-diagonal as in the UL factorization. Also, with appropriate scaling mixed symmetry is preserved.

3.4 The angles between q_i and p_i^*

We digress slightly to lay the foundations for a useful analytic tool. Recall (from section 3.2) that R and S (not S_*) are subspaces of $\mathbb{R}^n$.

In [Davis & Kahan, 1970] it is shown to be proper to speak of the (two) angles between R and S. In addition to the well known minimum angle between a vector in R and a vector in S, there is another

well defined angle which has to be included in a full assessment of the relationship between R and S. These angles depend only on R and S but, nevertheless, there is a distinguished pair of bases associated with them. This "angle basis" will be useful in our analysis.

We denote this basis by columns of $\hat{Q} = [\hat{q},\hat{q}_+]$ for R and the columns of $\hat{P} = [\hat{p},\hat{p}_+]$ for S. (For this section only we "transpose" S_* and P^* in order to consider R and S subspaces of the same $\mathbb{R}^n$.)

The matrices $\hat{Q}$ and $\hat{P}$ are distinguished by four properties:

(i) $\hat{P}^*\hat{Q} = I_2$

(ii) $\hat{P}^*\hat{P} = I_2$

(iii) $\hat{Q}^*\hat{Q} = I_2$

(iv) $\angle(\hat{q},\hat{p}) = \min \angle(r,s)$ over $r \in R$ and $s \in S$

When $\angle(\hat{q},\hat{p}) < \angle(\hat{q}_+,\hat{p}_+)$ then $\hat{P}$ and $\hat{Q}$ are unique to within $\pm$. For reasons given below this pair of bases is not preferred in the Look-Ahead Lanczos algorithm.

We note in passing that properties (i) and (iv) together determine $\hat{p}_+$ and $\hat{q}_+$ (provided that $\hat{p}$ and $\hat{q}$ are unique).

PROOF. The vector $\hat{q}_+$ is in the one dimensional subspace of R orthogonal to $\hat{p}$. Similarly $\hat{p}_+$ is in the one dimensional subspace of S orthogonal to $\hat{q}$.

3.5 The angle basis and the SVD of P^*Q

Kahan and Davis show how to find $\hat{Q}$ and $\hat{P}$ from any pair of orthogonal bases of R and S. Let P^* and Q be orthonormal bases for S^* and R. Then

$$P^* = V^*S^*$$
$$Q = RU \tag{3.4}$$

where V^* and U are invertible 2×2 matrices.

The bases $\hat{P}^*$ and $\hat{Q}$ are then found as follows:

$$\hat{P}^* = \hat{V}^*P^*$$
$$\hat{Q} = Q\hat{U} \tag{3.5}$$

where $P^*Q = \hat{V}\Sigma\hat{U}^*$ is the singular value decomposition (SVD) of P^*Q and $\Sigma = \text{diag}\{\sigma_1,\sigma_2\}$ is the matrix of the cosines of the angles between R and S^*.

Of practical interest is the fact that σ_1 and σ_2 can be obtained from R and S^* without forming any intermediate vectors. This follows from rearranging (3.4) and substituting in (3.5) to get

$$\hat{V}\Sigma\hat{U}^* = V^{-*}WU^{-1} .$$

So the angle basis comes from an unobvious factorization of W.

3.6 Maximizing bases

We now wish to find a pair of bases which is the best in the sense of (2.11), that is, the bases $\{p^*,p_+^*\}$ and $\{q,q_+\}$ such that

$$\underset{p,q}{\text{maximum minimum}} \{|p^*q|,|p_+^*q_+|\}$$

is attained. The maximum can be determined as the following theorem shows.

THEOREM 3.1. *Let* $\psi(P^*,Q) = \text{minimum}\{|p^*q|, |p_+^*q_+|\}$ *where* $P^* = \{p^*, p_+^*\}$ *and* $Q = \{q, q_+\}$ *are any pair of biorthogonal bases for* S^* *and* R, *respectively, with* $\|p^*\| = \|p_+^*\| = 1$ *and* $\|q\| = \|q_+\| = 1$. *Then*

$$\underset{P,Q}{\text{maximum}}\ \psi(P,Q) = \frac{2\sigma_1\sigma_2}{\sigma_1+\sigma_2} \quad (\equiv \textit{harmonic mean of } \sigma_1 \textit{ and } \sigma_2)$$

where $\sigma_1 \geq \sigma_2 \geq 0$ *are the cosines of the angles between* S^* *and* R. *Further,*

$$\sigma_2 \leq \underset{P,Q;\ p^*p_+=0}{\text{maximum}}\ \psi(P,Q) \leq \sigma_1 .$$

PROOF. Let $\hat{P}^*$ and $\hat{Q}$ denote the angle bases of section 3.4. Let

$$\tilde{P}^* = \begin{bmatrix} \tilde{p}^* \\ \tilde{p}_+^* \end{bmatrix} \quad \text{and} \quad \tilde{Q} = [\tilde{q}, \tilde{q}_+]$$

be any other biorthogonal bases with $\|\tilde{p}^*\| = \|\tilde{p}_+^*\| = 1$ and $\|\tilde{q}\| = \|\tilde{q}_+\| = 1$. Thus, if we let V be such that

$$\tilde{P}^* = V^*\hat{P}^*$$

then $V^* = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\psi & \cos\psi \end{bmatrix}$ for some pair of angles θ and ψ. Further, to preserve biorthogonality, if

$$\tilde{Q} = \hat{Q}U$$

then U has the form

$$U = \begin{bmatrix} \tau_1^{-1}\sigma_2\cos\psi & -\tau_2^{-1}\sigma_2\sin\theta \\ -\tau_1^{-1}\sigma_1\sin\psi & \tau_2^{-1}\sigma_1\cos\theta \end{bmatrix}$$

where $\tau_1^2 = \sigma_1^2\sin^2\psi + \sigma_2^2\cos^2\psi$ and $\tau_2^2 = \sigma_1^2\cos^2\theta + \sigma_2^2\sin^2\theta$. Then

$\tilde{P}^*\tilde{Q} = \text{diag}\{\tilde{\sigma}_1,\tilde{\sigma}_2\}$ with

$$\tilde{\sigma}_1 = \tau_1^{-1}\sigma_1\sigma_2\cos(\theta+\psi) , \quad \tilde{\sigma}_2 = \tau_2^{-1}\sigma_1\sigma_2\cos(\theta+\psi) .$$

Define $\zeta_1(\theta,\psi)$ and $\zeta_2(\theta,\psi)$ by

$$\zeta_1(\theta,\psi) = \sigma_1\sigma_2\cos(\theta+\psi)/\tau_1(\psi)$$
$$\zeta_2(\theta,\psi) = \sigma_1\sigma_2\cos(\theta+\psi)/\tau_2(\theta)$$

where

$$(\tau_1(\psi))^2 = \sigma_1^2\sin^2\psi + \sigma_2^2\cos^2\psi$$
$$(\tau_2(\theta))^2 = \sigma_1^2\cos^2\theta + \sigma_2^2\sin^2\theta .$$

Then

$$\psi(P,Q) = \text{minimum}\{\zeta_1(\theta,\psi),\zeta_2(\theta,\psi)\}$$

for appropriate θ, ψ. Our problem thus becomes finding $\max_{\theta,\psi} \text{minimum}\{\zeta_1(\theta,\psi),\zeta_2(\theta,\psi)\}$. We do this with the help of two lemmas. The first isolates stationary points on level curves.

LEMMA 3.1. *For fixed* ψ, $\zeta_1(\theta,\psi)$ *has a relative maximum at* $\theta = -\psi$ *and* $\zeta_2(\theta,\psi)$ *has a relative maximum at* $\theta = \arctan(-\frac{\sigma_1^2}{\sigma_2^2}\tan\psi)$. *Further* $V^*\hat{P}^*$ *is orthonormal at* $\theta = -\psi$ *and* $\hat{Q}U$ *is orthonormal at* $\theta = \arctan(-\frac{\sigma_1^2}{\sigma_2^2}\tan\psi)$.

PROOF. $\frac{\partial}{\partial\theta}\zeta_1(\theta,\psi) = -\frac{\sigma_1\sigma_2\sin(\theta+\psi)}{\tau_1(\psi)} = 0$ when $\theta = -\psi$

$$\frac{\partial^2}{\partial\theta^2}\zeta_1(\theta,\psi)\Big|_{\theta=-\psi} = -\sigma_1\sigma_2/\tau_1(\psi) \le 0$$

$$\frac{\partial}{\partial\theta}\zeta_2(\theta,\psi) = -\sigma_1\sigma_2(\sigma_2^2\sin\theta\cos\psi + \sigma_1^2\cos\theta\sin\psi)/(\tau_2(\theta))^3$$
$$= 0 \text{ when } \tan\theta = -\sigma_1^2/\sigma_2^2\tan\psi$$

$$\frac{\partial^2}{\partial\theta^2}\zeta_2(\theta,\psi) = -\sigma_1\sigma_2[(\sigma_2\cos\theta\cos\psi - \sigma_1^2\sin\theta\sin\psi)/(\tau_2(\theta))^3$$
$$+ (\sigma_2^2\sin\theta\cos\psi + \sigma_1^2\cos\theta\sin\psi)\cdot\frac{\partial}{\partial\theta}[(\tau_2(\theta))^{-3}]]$$
$$= -\sigma_1\sigma_2(\sigma_1\sigma_2\cos^2\theta/\tau_2(\theta) + \sigma_1\sigma_2\sin^2\theta/\tau_2(\theta))/(\tau_2(\theta))^3$$
$$\text{when} \quad \tan\theta = (-\sigma_1^2/\sigma_2^2)\tan\psi$$
$$= -(\sigma_1\sigma_2)^2/(\tau_2(\theta))^4 \le 0$$

When $\theta = -\psi$

$$V^* = \begin{bmatrix}\cos\psi & -\sin\psi \\ \sin\psi & \cos\psi\end{bmatrix}.$$

Now let $\frac{\sigma_2}{\sigma_1}\tan\theta = -\frac{\sigma_1}{\sigma_2}\tan\psi = \tan\alpha$ for some α. Then

$$\sin\alpha = \sigma_2(\sin\theta)/\tau_2(\theta) = -\sigma_1(\sin\psi)/\tau_1(\psi)$$
$$\cos\alpha = \sigma_1(\cos\theta)/\tau_2(\theta) = \sigma_2(\cos\psi)/\tau_1(\psi)$$

so that

$$U = \begin{bmatrix}\cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha\end{bmatrix}. \qquad \blacksquare$$

The second lemma establishes the point where ψ changes from $\zeta_1(\theta,\psi)$ to $\zeta_2(\theta,\psi)$.

LEMMA 3.2. $\zeta_1(\theta,\psi) = \zeta_2(\theta,\psi) = \sigma_1\sigma_2\sin(2\psi)/\sqrt{\sigma_1^2\sin^2\psi + \sigma_2^2\cos^2\psi}$ (3.6)

when $\theta = \psi - \frac{\pi}{2}$.

PROOF. $\zeta_1(\theta,\psi) = \zeta_2(\theta,\psi)$ when $\tau_1(\psi) = \tau_2(\theta)$, i.e.

$$\sigma_1^2\sin^2\psi + \sigma_2^2\cos^2\psi = \sigma_1^2\cos^2\theta + \sigma_2^2\sin^2\theta$$

or $$\tfrac{1}{2}((\sigma_1^2+\sigma_2^2) - (\sigma_1^2-\sigma_2^2)\cos 2\psi) = \tfrac{1}{2}((\sigma_1^2+\sigma_2^2) + (\sigma_1^2-\sigma_2^2)\cos 2\theta)$$

which reduces to

$$\cos 2\psi = -\cos 2\theta$$

which occurs when

$$2\psi = 2\theta + \pi$$

$$\text{or} \qquad \psi = \theta + \frac{\pi}{2} : \tag{3.7}$$

Substituting (3.7) into $\zeta_1(\theta,\psi)$ and $\zeta_2(\theta,\psi)$ gives the result. ∎

We now have two lemmas which seem unrelated to the problem. However, for a fixed ψ, $\max(\Psi)$ must occur either at a relative maxima or when $\zeta_1 = \zeta_2$. That is, for fixed ψ, either

$$\Psi = \zeta_2 \quad \text{for all} \quad \theta$$

$$\text{or} \qquad \Psi = \begin{cases} \zeta_2 & \text{when} \quad \tau_1(\psi) < \tau_2(\theta) \\ \zeta_1 & \text{when} \quad \tau_1(\psi) \geq \tau_2(\theta) \end{cases}$$

The symmetry of the properties of the two planes R and $S_\star$ means that for orthogonal bases, only $\zeta_2(\theta,\psi)$ with $\theta = -\psi$ need be maximized along with maximizing (3.6).

When $\theta = -\psi$

$$\sigma_2 \leq \zeta_2(-\psi,\psi) = \sigma_1\sigma_2/\sqrt{\sigma_1^2\cos^2\psi + \sigma_2^2\sin^2\psi} \leq \sigma_1 \tag{3.8}$$

However, when $\zeta_2(-\psi,\psi) > \zeta_1(-\psi,\psi)$, $\Psi = \zeta_1(-\psi,\psi)$, so that the cross-over point from ζ_2 to ζ_1 is of interest. Thus, we are again concerned with maximizing (3.6). (Note that (3.8) constitutes the second part of the theorem.)

From (3.6) we have

$$\Psi(\psi) = \zeta_1(\psi-\tfrac{\pi}{2},\psi) = \zeta_2(\psi-\tfrac{\pi}{2},\psi) = \sigma_1\sigma_2\sin 2\psi/\sqrt{\sigma_1^2\sin^2\psi + \sigma_2^2\cos^2\psi}$$

$$= \sigma_1\sigma_2\sin\psi/\sqrt{(\sigma_1^2/\sigma_2^2)\tan^2\psi + 1}\ .$$

$$\frac{d}{d\psi}(\Psi(\psi)) = 2\sigma_1 \cos\psi / \sqrt{((\sigma_1/\sigma_2)\tan\psi)^2 + 1}$$

$$- 2\sigma_1 \sin\psi \left(\frac{\sigma_1^2}{\sigma_2^2}\tan\psi \sec^2\psi\right) / \left(\left(\frac{\sigma_1}{\sigma_2}\tan\psi\right)^2 + 1\right)^{3/2}$$

$$= \frac{2\sigma_1}{\left(\left(\frac{\sigma_1}{\sigma_2}\tan\psi\right)^2 + 1\right)^{3/2}} \left\{ \cos\psi \left(\left(\frac{\sigma_1}{\sigma_2}\right)^2 \tan^2\psi + 1\right) - \frac{\sigma_1^2}{\sigma_2^2}\sin\psi\tan\psi\sec^2\psi \right\}$$

$$= \frac{2\sigma_1}{\left(\left(\frac{\sigma_1}{\sigma_2}\tan\psi\right)^2+1\right)^{3/2}} \left(\frac{1}{\sigma_2^2\cos^3\psi}\right)$$

$$\cdot \left(\sigma_1^2\cos^2\psi\sin^2\psi + \sigma_2^2\cos^4\psi - \sigma_1^2\sin^2\psi\right)$$

$$= c(-\sigma_1^2\sin^4\psi + \sigma_2^2\cos^4\psi)$$

$$= 0 \quad \text{when} \quad \tan^4\psi = \left(\frac{\sigma_1}{\sigma_2}\right)^2, \quad \text{i.e. when} \quad \psi = \arctan\sqrt{\sigma_1/\sigma_2}$$

$$\Psi(\arctan\sqrt{\tfrac{\sigma_1}{\sigma_2}}) = 2\sigma_1 \frac{\sqrt{\sigma_1}}{\sqrt{\sigma_1+\sigma_2}} / \sqrt{\frac{\sigma_1^2}{\sigma_2^2}\frac{\sigma_2}{\sigma_1} + 1}$$

$$= 2\sigma_1\sigma_2/(\sigma_1+\sigma_2) \; . \qquad \blacksquare$$

3.7 Practical 2 × 2 pivot

The column basis vectors for which Ψ attains its maximum, in general, will have non-zero components of $B^j q$. Similarly, the row basis vectors maximizing Ψ will have non-zero components in the direction $p^* B^j$. Therefore, the J-matrix is not Hessenberg, and to preserve Hessenberg form the optimum basis must be sacrificed.

This is not a great sacrifice. Recall that the max min cosine is the harmonic mean of the cosines of the angles between R and S_*, $\frac{2\sigma_1\sigma_2}{\sigma_1+\sigma_2}$. But

$$\sigma_2 \le 2\sigma_1\sigma_2/(\sigma_1+\sigma_2) \le 2\sigma_2$$

with the upper bound achieved only when $\sigma_2 \to 0$. Further, from Theorem 3.1, for P^* orthonormal

$$\sigma_2 \leq |p^*q|, |p_+^*q_+| \leq \sigma_1$$

Thus, by forcing P^* to be orthonormal, Ψ will never be less than half its maximum possible value. Further,

CLAIM. *For fixed* $q \in R$, $S^*q \neq 0$, *there are* p^* *and* $p_+^* \in S_*$ *and* $q_+ \in R$, *such that*

$$P^*Q \text{ is diagonal}$$

and

$$P^*P = I \ .$$

PROOF. Let $q \in R$. Let $\text{span}\{p_1, p_2\} = S^*$ with $\|p_1^*\| = \|p_2^*\| = 1$, $p_1^*q \neq 0$. Let

$$\tilde{p}_+^* = p_2^* - (p_2^*q/p_1^*q)p_1^* \ .$$

Then

$$p_+^* = \tilde{p}_+^*/\|\tilde{p}_+^*\|$$

$$p^* = (p_1^* - (p_1^*p_+)p_+^*)/(1 - (p_1^*p_+)^2)^{1/2}$$

Let $\tilde{q} \in R$, $\tilde{q} \neq q$, then

$$q_+ = \tilde{q} - (p^*\tilde{q}/p^*q)q \ .$$

If q is set as $r_j/\|r_j\|$ and P^* is orthogonal, the J-matrix remains Hessenberg while the cosine of the maximum angle is no worse than half the optimum.

3.8 Residual bounds

For symmetric matrices, the Rayleigh-Ritz procedure gives the best approximation to eigenvalues when approximate eigenvectors are known, and this theory has been exploited in the symmetric Lanczos process (Parlett [1980]). Kahan, Parlett and Jiang ([1981]) approached the non-symmetric case and produced residual bounds to measure convergence in the sense of backwards error analysis.

We summarize the results below and extend them to handle the look-ahead procedure. The terminology established for the symmetric case, though not precisely correct in the non-symmetric case, is used. Thus "*Ritz value*" denotes an eigenvalue of the J-matrix, and "*Ritz vector*" corresponds to a particular approximation to an eigenvector of B.

It is important to note that for scalar θ and vectors x and y^* we are not producing a bound on $|\lambda(B)-\theta|$ as can be done in the symmetric case, but a lower bound on $\|B-\tilde{B}\|$ where $n \times n$ $\tilde{B}$ has (θ,x,y^*) as an eigentriple [(α,z,w^*) is called an *eigentriple* of C if $Cz = z\alpha$ and $w^*C = \alpha w^*$]. Thus we assess the convergence of (θ,x,y^*) to eigentriples of B in terms of the deformation needed to make them exact.

The main results of the Kahan, Parlett and Jiang paper (KPJ) will be presented without proof, beginning with the main theorem of their work.

THEOREM 3.2 (Kahan, Parlett and Jiang). *Let* $n \times n$ B *and* $n \times m$ *orthonormal* P *and* Q *be given. For any* $m \times m$ D *let*

$$R = BQ - QC$$

$$S^* = P^*B - DP^*$$

$$C = (P^*Q)^{-1}D(P^*Q)$$

and $$Z_{11} = P^*(PQ-QC) = (P^*B-DP^*)Q \ .$$

Then there exist solutions E *of*

$$(B-E)Q = QC \quad \textit{and} \quad P^*(B-E) = DP^*$$

with minimal norms; some with

$$\|E\| = \min_E \|E\| = \max\{\|R\|,\|S^*\|\}$$

and others with

$$\|E\|_F = \min \|E\|_F = (\|R\|_F^2 + \|S^*\|_F^2 - \|Z_{11}\|_F^2)^{1/2} \ .$$

Let (θ,z,w^*) be an eigentriple of J_j, the J-matrix from the j^{th} step of the look-ahead procedure. Let $Q_j = [q_1,\ldots,q_j]$ and $P_j^* = \begin{bmatrix} p_1^* \\ \vdots \\ p_j^* \end{bmatrix}$, then the "Ritz vectors" x and y^* are defined by

$$x = Q_j z$$
$$y^* = w^* P_j^*$$

Assume that $w^*z = 1$ and $P_j^*Q_j = I_j$ so that $y^*x = 1$. Then

COROLLARY 3.1 (KPJ). *The closest matrix to* B *with* (θ,x,y^*) *as an eigentriple, is* B-E *for* E *satisfying*

$$\|E\| = \max\left\{\frac{|\beta_{j+1}\zeta_j|\,\|q_{j+1}\|}{\|x\|}, \frac{|\gamma_{j+1}\omega_j|\,\|p_{j+1}^*\|}{\|y^*\|}\right\}$$

where

$$BQ_j - Q_jJ_j = [0,\ldots,0,q_{j+1}\beta_{j+1}]$$
$$P_j^*B - J_jP_j^* = [0,\ldots,0,p_{j+1}\bar{\gamma}_{j+1}]$$

ζ_j *is the last element of* z

ω_j *the last element of* w *and* $\beta_{j+1}\gamma_{j+1} = s^*_{j+1}r_{j+1}$

and

COROLLARY 3.2 (KPJ). *Let* (θ,z,w^*) *be an eigentriple of* J_j *with* $w^*z = 1$. *Then for all* $k > j$, $(\theta,\tilde{z},\tilde{w}^*)$ *is an eigentriple of* $J_k - G_k$ *and with* e_i *the* i^{th} *column of* I_j

$$G_k = \left(\frac{\beta_{j+1}\zeta_j}{\|z\|}\right)e_{j+1}\tilde{z}^* + \left(\frac{\gamma_{j+1}\omega_j}{\|w^*\|}\right)\tilde{w}e^*_{j+1} .$$

Moreover,

$$\|G_k\| = \max\left\{\frac{|\beta_{j+1}\zeta_j|}{\|z\|}, \frac{|\gamma_{j+1}\omega_j|}{\|w^*\|}\right\}$$

$$\|G_k\|_F^2 = \frac{|\beta_{j+1}\zeta|^2}{\|z\|^2} + \frac{|\gamma_{j+1}\omega_j|^2}{\|w^*\|^2}$$

and both norms are independent of k.

The proof of the above corollary does not require strict use of the Lanczos process, but requires that the j^{th} step be done using a 1×1 pivot. Further, we can modify the proofs to handle the 2×2 pivot.

3.9 Residual bounds with 2×2 pivots

The key to generalizing Corollaries 3.1 and 3.2 is to remember the block tridiagonal structure of the J-matrix (section 2.8) so that

$$J_j = \begin{bmatrix} A_1 & \Gamma_2 & & \\ B_2 & A_2 & \ddots & \\ & \ddots & \ddots & \Gamma_\ell \\ & & B_\ell & A_\ell \end{bmatrix}$$

(recall that the i in A_j refers to the step count and is independent of the pivot size used). Let $B_{\ell+1} = [\zeta_{j+1}, \beta_{j+1}]$, $\Gamma_{\ell+1} = [\bar{\delta}_{j+1}, \bar{\gamma}_{j+1}]^*$ be the additions to the J-matrix for a 1×1 pivot. Then by putting $B_{\ell+1}$ in place of β_{j+1} and $\Gamma_{\ell+1}$ in place of $\gamma_{\ell+1}$ in Corollary 3.1, we get

COROLLARY 3.3. *The closest matrix to* B *with* (θ, x, y^*) *as an eigentriple is* B-E *satisfying*

$$\|E\| = \max\left\{\left(\frac{|\beta_{j+1}\zeta_j + \rho_{j+1}\zeta_{j-1}|}{\|x\|}\right)\|q_{j+1}\|, \left(\frac{|\gamma_{j+1}\omega_j + \delta_{j+1}\omega_{j-1}|}{\|y^*\|}\right)\|p^*_{j+1}\|\right\}$$

where

$$BQ_j - Q_j J_j = q_{j+1}(0, \ldots, 0, \zeta_{j+1}, \beta_{j+1}) \tag{3.9a}$$

$$P^*_j B - J_j P^*_j = (p_{j+1}(0, \ldots, \bar{\delta}_{j+1}, \bar{\gamma}_{j+1}))^* \tag{3.9b}$$

$$w^* = (\omega_1, \ldots, \omega_j), \quad z = (\zeta_1, \ldots, \zeta_j)^*$$

and

$$x = Q_j z \ , \quad y^* = w^* P^*_j \ .$$

PROOF. The equations (3.9a) and (3.9b) drop out of the Look-Ahead Lanczos algorithm. We may post multiply (3.9a) by any vector in $\mathbf{R}^j$. The most useful choice is the eigenvector z associated with the Ritz value θ, so that

$$\begin{aligned} Bx - x\theta &= BQ_j z - Q_j z\theta \\ &= BQ_j z - Q_j J_j z = q_j(0, \ldots, 0, \zeta_{j+1}, \beta_{j+1})z \end{aligned}$$

Similarly

$$y^*B - \theta y^* = w^*P_j^*B - \theta w^*P_j^*$$
$$= w^*P_j^*B - W^*J_jP_j^*$$
$$= w^*\begin{bmatrix} 0 \\ \vdots \\ \delta_{j+1} \\ \gamma_{j+1} \end{bmatrix} P_{j+1}^*$$

By applying Theorem 3.2 with $m = 1$, the result follows. ∎

The trick of replacing β_{j+1} by $B_{\ell+1}$ and γ_{j+1} by Γ_ℓ in the KPJ proof, Corollary 3.1 goes over to Corollary 3.3 in a straightforward way. Similarly, Corollary 3.2 generalizes to

COROLLARY 3.4. *Let* (θ,z,w^*) *be an eigentriple of* J_j *with* $w^*z = 1$. *Then for all* $k > j$, $(\theta,\tilde{z},\tilde{w}^*)$ *is an eigentriple of* $J_k - G_k$ *and (with* e_i *the* i^{th} *column of* I_j*)*

$$G_k = \left(\frac{\beta_{j+1}\zeta_j + \rho_{j+1}\zeta_{j-1}}{\|z\|}\right)e_{j+1}\tilde{z} + \left(\frac{\gamma_{j+1}\omega_j + \delta_{j+1}\omega_{j-1}}{\|w^*\|}\right)\tilde{w}e_{j+1}^* .$$

Moreover,

$$\|G_k\| = \max\left\{\frac{|\beta_{j+1}\zeta_j + \rho_{j+1}\zeta_{j-1}|}{\|z\|}, \frac{|\gamma_{j+1}\omega_j + \delta_{j+1}\omega_{j-1}|}{\|w^*\|}\right\}$$
$$\|G_k\|_F^2 = \frac{|\beta_{j+1}\zeta_j + \rho_{j+1}\zeta_{j-1}|^2}{\|z\|^2} + \frac{|\gamma_{j+1}\omega_j + \delta_{j+1}\omega_{j-1}|^2}{\|w^*\|^2}$$

and the norms are independent of k.

Though at present we have restricted ourselves to the 2×2 case, the generalization holds for any pivot size. The replacement of β_{j+1} and γ_{j+1} by B_{j+1} and Γ_{j+1}, respectively, is independent of the

length of B_{j+1} and Γ_{j+1}. Note that the residuals remain of rank one.

So now we can, in principle, test all the Ritz values, θ_i, at each step and determine which are acceptable in the sense of being eigenvalues of matrices close to B.

3.10 Summary

We now have an understanding of the effects of various factorizations of the 2×2 pivot, just as we saw the effects of various factorizations of the 1×1 pivot in Chapter I. Further, we have seen that the natural bases, the angle bases, are not the most desirable either for keeping J sparse or to keep $\angle(q_i, p_i^*)$ minimal.

Moreover, we determined just how much can be gained from any factorization and how to weigh this against a more convenient structure for the J-matrix. The increase of maximum $\min\{|p^*q|, |p_+^*q_+|\}$ by a factor of 2 may be the difference between continuing the Look-Ahead Lanczos process and admitting failure. However, without a convenient method for solving the eigenvalue problem for non-Hessenberg J, what was gained with the optimum basis is lost converting J to Hessenberg form.

Finally, the assessment of convergence of eigenelements of J to eigenelements of B has also been discussed. Though seemingly out of place in this chapter, this presentation completes the material necessary for producing a working (though not necessarily efficient) procedure. As noted, the residual bound calculations may be performed for every Ritz value at each step, and convergence of appropriate eigenelements can be determined.

IV. Serious Breakdown

4.1 Introduction

We have presented Lanczos without serious breakdown, and the Look-Ahead Lanczos for some cases of serious breakdown. However, there are cases where the Look-Ahead Lanczos process cannot succeed, no matter how large the pivot we use. This form of breakdown we call "incurable".

Incurable breakdown at first glance seems a disaster. We are in possession of non-zero residuals which are mutually orthogonal, for which there is no foreward looking remedy. We will show, however, that incurable breakdown is a blessing peculiarly related to the encountering of a zero residual.

To complete the discussion of the Look-Ahead Lanczos algorithm, we present a characterization motivated by the foregoing analysis of breakdown for which the look-ahead algorithm is successful. This characterization rounds out the analysis of the look-ahead.

4.2 Invariant subspaces

Suppose by some special relation of the starting vectors, that the Krylov subspaces become invariant before the n^{th} step. Say, let $K^k(q,B)$ and $K_*^\ell(p^*,B)$ be invariant subspaces with $k, \ell < n$. Note that in the discussion of incurable breakdown, we may disregard the case of $k = n$ or of $\ell = n$, since Chapter II shows that such breakdown is impossible.

Define the row and column generalized eigenvectors of B, w_i^* and z_j, respectively, so that $w_i^* z_j = \delta_{ij}$. Then it follows from the Jordan form of B that for some $i_1,\ldots,i_k$ and $j_1,\ldots,j_k$ that

$$K^k = \text{span}\{z_{i_1},\ldots,z_{i_k}\}$$
$$K^\ell = \text{span}\{w^*_{j_1},\ldots,w^*_{j_\ell}\}$$

We may assume that

$$q = \sum_{m=1}^{k} a_m z_{i_m} \qquad a_m \neq 0, \quad m = 1,\ldots,k \tag{4.1a}$$

and

$$p = \sum_{m=1}^{\ell} b_m w^*_{j_m} \qquad b_m \neq 0, \quad m = 1,\ldots,\ell \tag{4.1b}$$

since such vectors exist in K^k and $K^{(\ell)}_*$, respectively, and may be used to generate the Krylov subspaces.

Let s^*_m and r_m be the row and column residual vectors, respectively, at step m. Then incurable breakdown at step m is defined by

$$s^*_m \neq 0^*$$
$$r_m \neq 0$$
and
$$s^*_m B^j r_m = 0 , \quad j \geq 0 .$$

Thus incurable breakdown occurs when $s^*_m \perp K^k$ (or equivalently $r_m \perp K^\ell_*$). Note that incurable breakdown must occur at step $m < \min\{\ell,k\}$, since at step $j = \min\{\ell,k\}$ one residual is zero, which is not breakdown.

4.3 The moment matrix and incurable breakdown

Eventually we will link incurable breakdown to the eigenexpansions (4.1a) and (4.1b). We will accomplish this in steps, the first relating incurable breakdown to the rank of the moment matrix.

LEMMA 4.1. *Let* M_n *be the* $n \times n$ *moment matrix generated by* p^*, q *and* B. *Let* $\tilde{K}_n^*$ *be the row Krylov matrix and* K_n *the column Krylov matrix. Then incurable breakdown occurs if and only if*

$$\begin{aligned} \operatorname{rank}(M_n) &< \min\{\operatorname{rank}(\tilde{K}_n^*), \operatorname{rank}(K_n)\} \\ &= \min\{\dim(K_*^n), \dim(K^n)\} \end{aligned}$$

PROOF. *Sufficiency*: Assume that the Look-Ahead Lanczos algorithm suffers incurable breakdown at step m. Since the look-ahead algorithm is a modified two-sided Gram-Schmidt process, it is equivalent to making elementary matrix operations on $\tilde{K}_n^*$ and K_n. Let U and V^* be the matrices which perform these operations so that

$$e_j^* V^* \tilde{K}_n^* = \begin{cases} p_j^* & j < m \\ s_m^* B^{j-m} & j \geq m \end{cases}, \quad K_n U e_j = \begin{cases} q_j & j < m \\ B^{j-m} r_m & j \geq m \end{cases}$$

where e_j is the j^{th} column of I_n.

Recall that incurable breakdown means $s_m^* B^i r_m = 0$ for $i \geq 0$. Hence,

$$V^* K_n^* K_n U = V^* M_n U = \left[\begin{array}{c|c} I_{m-1} & 0^* \\ \hline 0 & M_{n-m+1}(s_m^*, r_m, B) \end{array}\right],$$

$$= \left[\begin{array}{c|c} I_{m-1} & 0^* \\ \hline 0 & 0 \end{array}\right]$$

Since U and V^* are invertible

$$\operatorname{Rank}(M_n) = \operatorname{rank}(V^* M_n U) = m - 1 .$$

To complete this part of the proof, note that

$$r_m \neq 0 \quad \text{implies} \quad \dim(\mathcal{K}^n) = \operatorname{rank}(K_n) = \operatorname{rank}(K_n U) \geq m$$

and $$s_m^* \neq 0 \quad \text{implies} \quad \dim(\mathcal{K}_*^n) = \operatorname{rank}(\tilde{K}_n^*) = \operatorname{rank}(V^* \tilde{K}_n^*) \geq m$$

Necessity: Let $m-1 = \operatorname{rank}(M_n) = \operatorname{rank}(K_n) \leq \operatorname{rank}(\tilde{K}_n^*)$ (say). Let U and V^* be as above. We need only show $r_m = 0$ to complete the proof. Let $Q_{m-1} = [q_1, \ldots, q_{m-1}]$, $P_{m-1}^* = \begin{bmatrix} p_1^* \\ \vdots \\ p_{m-1}^* \end{bmatrix}$. There is no loss in generality in assuming $P_{m-1}^* Q_{m-1} = I_{m-1}$. $\operatorname{Rank}(K_n) = m-1$ implies $r_m = Q_{m-1} c$ for some vector c. Now

$$0 = P_{m-1} r_m = P_{m-1}^* Q_{m-1} c = c \,. \qquad \blacksquare$$

EXAMPLE 4.1 (Incurable breakdown). Let

$$B = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad q = \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad p^* = [1,1,0,0] \,.$$

Then

$$K_4 = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \quad \text{and} \quad \tilde{K}_4^* = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix},$$

so that

$$M_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}.$$

Note that $p_1^* q_1 = p^* q = 1$. From (1.3)

$$r_2 = Bq - q\alpha = \begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \end{bmatrix} \quad \text{and} \quad s_2^* = p^*B - \alpha p^* = [0,-1,0,1] .$$

Further, $s_2^* B^j r_2 = 0$, $j \geq 0$, so we have incurable breakdown. Also note

$$\text{rank}(M_4) = 1 , \quad \text{rank}(K_4) = 2 , \quad \text{rank}(K_4^*) = 3 .$$

4.4 The mismatch theorem

The previous lemma characterizes incurable breakdown in terms of the rank of the moment matrix. Here we give a more illuminating explanation.

THEOREM 4.1 (Mismatch Theorem). *Let* p, q *and* B *be given. Let* $K^k = \text{span}\{q,Bq,\ldots,B^{k-1}q\}$ *and* $K_*^\ell = \text{span}\{p^*,p^*B,\ldots,p^*B^{\ell-1}\}$ *be invariant subspaces of dimension* k *and* ℓ, *respectively. Then incurable breakdown occurs at step* i *if and only if there are generalized row eigenvectors* $\{w_1^*,\ldots,w_i^*,w_{i+1}^*,\ldots,w_\ell^*\}$ *and generalized column eigenvectors* $\{z_1,\ldots,z_i,z_{\ell+1},\ldots,z_{k+\ell-i}\}$ *with*

$$w_{j_1}^* z_{j_2} = \delta_{j_1 j_2} \tag{4.2}$$

such that

$$K^k = \text{span}\{z_1,\ldots,z_i,z_{\ell+1},\ldots,z_{k+\ell-i}\}$$

and

$$K_*^\ell = \text{span}\{w_1^*,\ldots,w_i^*,w_{i+1}^*,\ldots,w_\ell^*\}$$

Condition (4.2) departs from the ordering which produces the Jordan canonical form for Jordan blocks, i.e.

$$Bz_j = z_j\lambda + z_{j+1}$$
$$w_j^*B = \lambda w_j^* + w_{j-1}^* \ .$$

There is no loss in generality in assuming (4.2) and reduces the complications in subscripts.

PROOF OF THEOREM. *Sufficiency:* Consider K_n and $\tilde{K}_n^*$. Since $\mathcal{K}^k$ is invariant

$$\text{rank}(K_n) = \dim(\mathcal{K}^n) = \dim(\mathcal{K}^k) = k$$

Similarly

$$\text{rank}(\tilde{K}_n^*) = \dim(\mathcal{K}_*^n) = \dim(\mathcal{K}_*^\ell) = \ell \ .$$

Thus using the invariance of $\mathcal{K}^k$ and $\mathcal{K}_*^\ell$, there are invertible X and Y such that

$$K_nX = [z_1,\ldots,z_i,z_{\ell+1},\ldots,z_{k+\ell-i},0,\ldots,0]$$
$$= [\tilde{z},\hat{z},\underline{0}] \ , \quad \tilde{z} = z_1,\ldots,z_i; \quad \hat{z} = z_{\ell+1},\ldots,z_{k+\ell-i}$$

and

$$Y\tilde{K}^* = \begin{bmatrix} w_1^* \\ \vdots \\ w_i^* \\ w_{i+1}^* \\ \vdots \\ w_\ell^* \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} \tilde{w}^* \\ \hat{w}^* \\ \underline{0}^* \end{bmatrix} \qquad \begin{aligned} \tilde{w} &= w_1,\ldots,w_i; \\ \hat{w} &= w_{i+1},\ldots,w_\ell \end{aligned}$$

Thus,
$$Y^*\tilde{K}_n^*K_nX = \begin{bmatrix} \tilde{w}^*\tilde{z} & \tilde{w}^*\hat{z} & \underline{0} \\ \hat{w}^*\tilde{z} & \hat{w}^*\hat{z} & \underline{0} \\ \underline{0} & \underline{0} & \underline{0} \end{bmatrix}$$
$$= \begin{bmatrix} I_i & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \text{ by (4.2)}$$

So, $\operatorname{rank}(M_n) = \operatorname{rank}(\tilde{K}_n^*K_n) = \operatorname{rank}(Y^*\tilde{K}_n^*K_nX) = i < k,\ell$. Thus, by Lemma 4.1, we have incurable breakdown.

Necessity: Assume that there is no mismatch, $i = k = \min(k,\ell)$ (say). Then

$$K^i = \operatorname{span}\{z_1,\ldots,z_i\}$$

and
$$\operatorname{rank}(K_n) = \dim(K^n) = \dim(K^i) = i = \operatorname{rank}(M_n) .$$

Thus by Lemma 4.2, there is no incurable breakdown. ∎

EXAMPLE 4.2. Let B, p^* and q be as in Example 4.1. The matrix B is normal so $w_j^* = z_j$ with eigenvalues i^j, $j = 1,\ldots,4$, $i = \sqrt{-1}$ and eigenvectors

$$z_1 = \begin{bmatrix} .5i \\ .5 \\ -.5i \\ -.5 \end{bmatrix} \quad z_2 = \begin{bmatrix} .5 \\ -.5 \\ .5 \\ -.5 \end{bmatrix} \quad z_3 = \begin{bmatrix} .5i \\ -.5 \\ -.5i \\ .5 \end{bmatrix} \quad z_4 = \begin{bmatrix} .5 \\ .5 \\ .5 \\ .5 \end{bmatrix}$$

In this case

$$p^* = z_1^* + z_3^* + z_4^* \qquad q = z_2 + z_4$$
$$K_*^4 = \operatorname{span}\{z_1^*,z_3^*,z_4^*\} \quad K^4 = \operatorname{span}\{z_2,z_4\}$$

4.5 Ritz values and incurable breakdown

For discussion of the Ritz values of the matrix J_i, let us assume, temporarily, that B has simple roots, so that $w_i^*B = \lambda_i w_i^*$ and $Bz_j = z_j\lambda_j$ for all i and j. The case of defective matrices, though not unlike the non-defective case, is somewhat more complicated and its discussion is postponed until the next section.

What the Mismatch Theorem has given us is that in the case of incurable breakdown

$$\begin{aligned} p^* &= \tilde{p}^* + \sum_{j=i+1}^{\ell} b_j w_j^* \\ q &= \tilde{q} + \sum_{j=\ell+1}^{k+\ell-i} a_j z_j \end{aligned} \tag{4.3}$$

where

$$\begin{aligned} \tilde{p}^* &= \sum_{j=1}^{i} b_j w_j^* \\ \tilde{q} &= \sum_{j=1}^{i} a_j z_j \end{aligned}$$

with $a_j \neq 0$, $j = 1,\ldots,i,\ell+1,k+\ell-i$; $b_m \neq 0$, $m = 1,\ldots,\ell$.

Then any element of the moment matrix $M_n(p,q,B)$ has the form

$$\begin{aligned} p^*Bq &= (\tilde{p}^* + \sum_{j=i+1}^{\ell} b_j w_j^*)B^m(\tilde{q} + \sum_{j=\ell+1}^{k+\ell-i} a_j z_j) \\ &= \tilde{p}^*B^m\tilde{q} + \tilde{p}^*(\sum_{j=\ell+1}^{k+\ell-i} a_j B^m z_j) + (\sum_{j=i+1}^{\ell} b_j w_j^* B^m)\tilde{q} \\ &\quad + (\sum_{j=i+1}^{\ell} b_j w_j^*)(\sum_{j=\ell+1}^{k+\ell-i} a_j B^m z_j) \\ &= \tilde{p}^*B^m\tilde{q} + \tilde{p}^*\sum_{j=\ell+1}^{k+\ell-i} \lambda_j^m a_j z_j + (\sum_{j=i+1}^{\ell} \lambda_j^m b_j w_j^*)\tilde{q} \\ &\quad + (\sum_{j=i+1}^{\ell} b_j w_j^*)(\sum_{j=\ell+1}^{k+\ell-i} \lambda_j^m a_j z_j) \end{aligned}$$

$$= \tilde{p}^* B^m \tilde{q} + \sum_{j=\ell+1}^{k+\ell-i} \lambda_j^m a_j \tilde{p}^* z_j + \sum_{j=i+1}^{\ell} \lambda_j^m b_j w_j^* \tilde{q}$$

$$+ \sum_{j_1=\ell+1}^{\ell+k-i} \sum_{j_2=\ell+1}^{\ell} b_{j_2} \lambda_{j_1}^m a_{j_1} w_{j_2}^* z_{j_1}$$

$$= \tilde{p}^* B^m \tilde{q}$$

Thus we get the following lemma:

LEMMA 4.2. *Let* p^*, $\tilde{p}^*$, q *and* $\tilde{q}$ *be defined by (4.3), then*

$$M_n(p^*,q,B) = M_n(\tilde{p}^*,\tilde{q},B) .$$

We can now show that incurable breakdown is not a misfortune as the following surprising result shows.

THEOREM 4.2. *Let* B *have distinct eigenvalues and let* J_i *be the block tridiagonal J-matrix produced by the Look-Ahead Lanczos process at step* i, *with* p^* *and* q *starting vectors. If incurable breakdown occurs at step* $i+1$ *then each Ritz value of* J_i *is an eigenvalue of* B.

PROOF. By the Mismatch Theorem p^* and q have the form (4.3). Consider now the Look-Ahead Lanczos with the $\tilde{p}^*$ and $\tilde{q}$ defined by (4.3). The subspaces $K_*^i(\tilde{p}^*,B)$ and $K^i(\tilde{q},B)$ are invariant, so that each Ritz value of the J-matrix generated using $\tilde{p}^*$ and $\tilde{q}$ is an eigenvalue of B. By using Lemma 4.2 and Lemma 1.4 (Chapter I) the result follows. ∎

EXAMPLE 4.4. Let p^*, q and B be as in Examples 4.1 and 4.2. Then

$$J_1 = \lambda(J_1) = \alpha_1 = p^* B q = 1 = \lambda_4(B) .$$

4.6 Defective matrices

By their biorthogonality, the generalized eigenvectors of the expansions in (4.3) influence only those components associated with its Jordan block, thus, the interaction within a single Jordan block to generalize Theorem 4.2.

Therefore, let B be a Jordan block of grade n, that is $n \times n$ B has the form

$$B = \begin{bmatrix} \lambda & 1 & & & \\ & \lambda & 1 & & \\ & & \lambda & \ddots & \\ & & & \ddots & 1 \\ & & & & \lambda \end{bmatrix}.$$

Then

LEMMA 4.3. *Let* $p^* = \sum_{i=1}^{k+\ell} b_i e_i^*$ *and* $q = \sum_{i=k+1}^{n} a_i e_i$ *where* e_i *is the* i^{th} *column of* I_n *and* $a_i \neq 0$ *and* $b_i \neq 0$. *Then the J-matrix generated by* p^*, q *and* B *is similar to a Jordan block of degree* ℓ.

For simplicity we make the following notational convention. Let

$$C = [c_{ij}] = \begin{bmatrix} c_{11} & c_{12} & \cdots & c_{1n} \\ \vdots & \vdots & & \vdots \\ c_{n1} & c_{n2} & \cdots & c_{nn} \end{bmatrix}$$

and define

$$C_{(i,j)} = \begin{bmatrix} c_{ii} & c_{ii+1} & \cdots & c_{ij} \\ \vdots & \vdots & & \vdots \\ c_{ji} & c_{ji+1} & \cdots & c_{jj} \end{bmatrix}$$

The proof of Lemma 4.3 is simplified by the following technical lemma.

LEMMA 4.4 $(B)_{(i,j)} = N_{i+j+1}$ *where* N_k *is the* $k \times k$ *Jordan block. Further,*

$$(B^m)_{(i,j)} = (N_{i+j+1})^m .$$

PROOF. The $(k,\ell)^{th}$ element of $B^m = \begin{cases} 0 & k > \ell \\ \binom{m}{\ell-k}\lambda^{m+\ell-k} & k \leq \ell \end{cases}$

Similarly the $(\hat{k},\hat{\ell})^{th}$ element of $N^m_{i+j+1} = \begin{cases} 0 & \hat{k} > \hat{\ell} \\ \binom{m}{\hat{m}}\lambda^{m+\hat{m}} & \hat{k} = \hat{\ell}+\hat{m},\ \hat{m} \geq 0 \end{cases}$ ■

PROOF OF LEMMA 4.3. Let $\tilde{p} = \sum_{i=k+1}^{k+\ell} b_i e_i^*$ and $\tilde{q} = \sum_{i=k+1}^{k+\ell} a_i e_i$ so that $p^* = \sum_{i=1}^{k} b_i e_i^* + \tilde{p}^*$ and $q = \tilde{q} + \sum_{i=k+\ell+1}^{n} a_i e_i^*$. Consider any element of the moment matrix

$$p^* B^j q = (\tilde{p}^* + \sum_{i=1}^{k} b_i e_i^*) B^j (\tilde{q} + \sum_{i=k+\ell+1}^{n} a_i e_i) .$$

Using an argument similar to that of the proof of Lemma 4.2 we have

$$\begin{aligned} p^* B^m q &= \tilde{p}^* B^j \tilde{q} \\ &= (\sum_{i=k+1}^{k+\ell} b_i e_i^*) B^j (\sum_{i=k+1}^{k+\ell} a_i e_i) \\ &= (\sum_{i=1}^{\ell} b_{i+k} \hat{e}_i^*)(B^j)_{(k+1,k+\ell)} (\sum_{i=1}^{\ell} a_{i+k} \hat{e}_i) = \hat{p}^* N_\ell^j \hat{q} \end{aligned}$$

where $\hat{e}_i$ is the i^{th} column of I_ℓ. Thus the moment matrix generated by p^*, q and B is the same as that generated by $\hat{p}^*$, $\hat{q}$ and N_ℓ with $\tilde{K}^\ell_*(\hat{p}^*, N_\ell) = R^\ell_*$ and $K^\ell(\hat{q}, N_\ell) = R^\ell$. Thus, the J-matrix generated by p^*, q and B is the same as that generated by $\hat{p}^*$, $\hat{q}$ and N_ℓ, the latter J-matrix being similar to N_ℓ. ■

Thus we have the following extension of Theorem 4.2.

THEOREM 4.3. *Let* B *be non-derogatory (i.e. each eigenvalue of* B *is associated with only one Jordan block) and let* J_i *be the* J*-matrix generated at step* i *of the Look-Ahead Lanczos. If incurable breakdown occurs at step* i+1*, then each Ritz value of* J_i *is an eigenvalue of* B.

4.7 Curable breakdown

We now have a characterization of incurable breakdown in terms of the row and column eigenvector expansions of the starting vectors. Such a characterization is also possible with curable breakdown (breakdown which the Look-Ahead algorithm with a suitable pivot circumvent). We start by defining curable breakdown of degree ℓ.

Let diagonalizable B and vectors p^* and q be given. Let s^*_{k+1} and r_{k+1} be the residual vectors after the k^{th} step of the Look-Ahead Lanczos. Then we say the look-ahead process suffers *curable breakdown of degree* ℓ *at step* k *if*

$$s^*_{k+1} B^m r_{k+1} = 0 \quad m = 0,\ldots,\ell-1 \tag{4.4a}$$

$$s^*_{k+1} B^\ell r_{k+1} \neq 0 \tag{4.4b}$$

With this breakdown, the $(\ell\times 1)\times(\ell\times 1)$ pivot matrix, X, is Hankel matrix of the form

$$X = \begin{bmatrix} 0 & \cdots & 0 & \xi \\ \vdots & & & * \\ & & & \vdots \\ 0 & & & \vdots \\ \xi & * & \cdots & * \end{bmatrix}$$

where $\xi = s_{k+1}^* B^{\ell} r_{k+1} \neq 0$ and $*$ denotes a possibly zero element. The point here is that X^{-1} exists so that the look-ahead process can continue.

Let

$$p^* = \sum_{i=1}^{n} b_i w_i^* \quad \text{and} \quad q = \sum_{i=1}^{n} a_i z_i \tag{4.5}$$

where each (λ_i, w_i^*, z_i) is an eigentriple of B. Then using (1.5), (4.4a) becomes

$$\begin{aligned} 0 = s_{k+1}^* B^m r_{k+1} &= (\gamma^{(k)})^{-1} p^* \chi_k(B) B^m \chi_k(B) q (\beta^{(k)})^{-1} \\ &= (\omega^{(k)})^{-1} \sum_{i=1}^{m} \sum_{j=1}^{n} b_i w_i^* B^m (\chi_k(B))^2 a_j z_j \\ &= \Big(\sum_{i=1}^{n} \lambda_i^m (\chi_k(\lambda_i))^2 \sum_{j=1}^{n} a_j b_i w_i^* z_j \Big) / \omega^{(k)} \\ &= \Big(\sum_{i=1}^{n} (\chi_k(\lambda_i))^2 \lambda_i^m a_i b_i \Big) / \omega^{(k)} \end{aligned}$$

where $\beta^{(k)}$, $\gamma^{(k)}$ and $\omega^{(k)}$ are as in Chapter I. If we let

$$x = (x_1, \ldots, x_n) \text{ with } x_i = a_i b_i \tag{4.6}$$

then

$$\begin{aligned} s_{k+1}^* B^m r_k &= \sum_{i=1}^{n} \lambda_i^m (\chi_k(\lambda_i))^2 x_i \\ &= (\lambda_1^m, \ldots, \lambda_n^m) \Delta_k x \,, \quad m = 0, \ldots, \ell-1 \end{aligned} \tag{4.7}$$

where $\Delta_k = \operatorname{diag}\{(\chi_k(\lambda_1))^2, \ldots, (\chi_k(\lambda_n))^2\}$. So (4.4a) in matrix form becomes

$$V_{\ell} \Delta_k x = 0$$

with V_{ℓ} the $\ell \times n$ Vandermonde matrix

$$V_\ell = \begin{bmatrix} 1 & \cdots & 1 \\ \lambda_1 & \cdots & \lambda_n \\ \vdots & & \vdots \\ \lambda_1^{\ell-1} & \cdots & \lambda_n^{\ell-1} \end{bmatrix} \tag{4.8}$$

Further (4.4b) is

$$s_k^* B^\ell r_{k+1} = (\lambda_1^\ell, \ldots, \lambda_n^\ell)\Delta_k x \neq 0 .$$

So

THEOREM 4.4. *Let* p^* *and* q *be as in (4.5) and non-defective* B *be given. Then curable breakdown of degree* ℓ *occurs at step* k *if and only if*

$$\Delta_k x \in N(V_\ell) \quad \textit{(the nullspace of } V_\ell\textit{)}$$

but

$$\Delta_k x \notin N(V_{\ell+1})$$

where $x = (x_1, \ldots, x_n)$ *as defined in (4.6),* $\Delta_k = \text{diag}\{(\chi_k(\lambda_1))^2, \ldots, (\chi_k(\lambda_n))^2\}$, V_m *is the* $m \times n$ *Vandermonde matrix for* $m = \ell, \ell+1$.

The above characterization is not entirely satisfying. We cannot escape the dependence of Δ_k on x and V_k. But we can see that the likelihood of selecting p^* and q generating such an x decreases with the increase in the degree of curable breakdown.

EXAMPLE 4.3. Consider

$$B = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad p^* = [1,0,0,0], \quad q = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} .$$

Then $$r_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad \text{and} \quad s_2^* = [0,0,0,1] ,$$

$$s_2^* B r_2 = [0,0,1,0] \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = 0 ,$$

and $$s_2^* B r_2 = [0,1,0,0] \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = 1 .$$

Here $$p^* = \sum_{i=1}^{4} w_i^* , \quad q = \sum_{i=1}^{4} z_i , \quad x = [.25,.25,.25,.25] ,$$

$$V_3 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & i & -i \\ 1 & 1 & -1 & -1 \end{bmatrix} \quad (i = \sqrt{-1}), \quad \Delta_1 x = \begin{bmatrix} .25 \\ .25 \\ -.25 \\ -.25 \end{bmatrix}$$

and $$V_2 \Delta_1 x = 0 , \quad V_3 \Delta_1 x = 1 .$$

4.8 Curable breakdown and defective matrices

To handle the case of defective matrices (a matrix is defective if it has at least one Jordan block of grade > 1), we may again confine ourselves to a single Jordan block. So let $n \times n$ B be of the form

$$B = \begin{bmatrix} \lambda & 1 & & \\ & \lambda & 1 & \\ & & \ddots & \ddots \\ & & & \ddots 1 \\ & & & \lambda \end{bmatrix} \tag{4.9}$$

Let p^* and q be as in (4.5). Let $s^*_{k+1} = \sum_{i=1}^{n} \hat{b}_i w_i^*$ and $r_{k+1} = \sum_{i=1}^{n} \hat{a}_i z_i$ so that

$$\hat{b}_i = \sum_{j=i}^{\min(k+i-1,n)} b_i \left(\frac{d^{j-i}}{dt^{j-i}} \chi_k(t)\right)\Big|_{t=\lambda}$$
$$\hat{a}_i = \sum_{j=\max(1,k-i+1)}^{i} a_i \left(\frac{d^{i-j}}{dt^{j-i}} \chi_k(t)\right)\Big|_{t=\lambda} \tag{4.10}$$

Consider from (4.4a)

$$\begin{aligned} 0 &= s^*_{k+1} B^m r_{k+1} \\ &= \left(\sum_{i=1}^{n} \hat{b}_i w_i^*\right) B^m \left(\sum_{i=1}^{n} \hat{a}_i z_i\right) \\ &= \left(\sum_{i=1}^{n} \hat{b}_i w_i^*\right)\left(\sum_{i=1}^{n} z_i \sum_{j=\max(1,m-i+1)}^{i} \binom{m}{j} a_j \lambda^{m-j}\right) \end{aligned}$$

Rearranging we get

$$\begin{aligned} 0 &= \left(\sum_{i=1}^{n} \hat{b}_i w_i^*\right)\left(\sum_{j=0}^{m} \binom{m}{j} \lambda^{m-j} \sum_{i=1}^{n-j} \hat{a}_{j+1} z_i\right) \\ &= \sum_{j=0}^{m} \left(\binom{m}{j} \sum_{i=1}^{n-j} \hat{b}_i \hat{a}_{i+j}\right) \lambda^{m-j}\Big) \\ &= \left(\lambda^m, \binom{m}{1}\lambda^{m-1}, \ldots, \binom{m}{m-1}\lambda, 1, 0, \ldots, 0\right)\hat{x} \end{aligned}$$

where $\hat{x} = (\hat{x}_1, \ldots, \hat{x}_n)$ $\quad \hat{x}_j = \sum_{i=1}^{n-j} \hat{b}_i \hat{a}_{j+i}$ (4.11)

Thus (4.4a) becomes

$$\hat{V}_\ell \hat{x} = 0$$

where $\hat{V}_\ell$ is the generalized Vandemonde matrix

$$\hat{V}_\ell = \begin{bmatrix} 1 & 0 & \cdots & & & 0 \\ \lambda & 1 & 0 & \cdots & & 0 \\ \vdots & & & & & \vdots \\ \lambda^{\ell-1} & \binom{\ell-1}{1}\lambda^{\ell-2} & \cdots & \binom{\ell-1}{k}\lambda^{\ell-k-1} & \cdots 1 \cdots & 0 \end{bmatrix}$$

so that

THEOREM 4.5. *Let* p^* *and* q *be defined by (4.5) and* B *by (4.8). Let* $\hat{b}_i$ *and* $\hat{a}_i$ *be defined by (4.10) and* $\hat{x}$ *by (4.11). Then curable breakdown of degree* ℓ *occurs at step* k *if and only if*

$$\hat{x} \in N(\hat{V}_\ell)$$
$$\hat{x} \notin N(\hat{V}_{\ell+1}) .$$

PROOF. The proof is completed by showing $\hat{x} \notin N(\hat{V}_{\ell+1})$. From (4.4b)

$$\begin{aligned} 0 \neq s_{k+1}^* B^\ell r_{k+1} &= (\lambda^\ell, \tbinom{\ell}{1}\lambda^\ell, \ldots, \tbinom{\ell}{m}\lambda^{\ell-m}, \ldots, 1, 0, \ldots, 0]\hat{x} \\ &= e_{\ell+1}^* \hat{V}_{\ell+1} \hat{x} \end{aligned}$$

where $e_{\ell+1}$ is the $(\ell+1)^{st}$ column of I_n. ∎

4.9 Summary

We now have the characterizations for serious breakdown in terms of the eigensystems. Further, we have that one form of serious breakdown can be remedied and that the other form is fortuitous in the search for eigenvalues.

Though the result of Theorem 4.2 is counter-intuitive at first, it becomes more tangible when we consider the case of only one residual vector becoming zero. The other residual vector does not interfere

with one important feature of the J-matrix (that is, each Ritz value of J being an eigenvalue of B). We only lose one set of eigenvectors.

In the case of incurable breakdown we preserve the relationship between Ritz values of J and some of the eigenvalues of B, but cannot extract either row or column eigenvectors directly from the subspaces generated.

Finally, we can characterize curable breakdown, from which we see that the curable breakdown of degree k becomes less likely as k increases. Thus the restrictions on pivot size due to practical considerations such as storage do not unduly restrict the effectiveness of the algorithm.

Appendix. Look-Ahead Lanczos Algorithm

The algorithm below leaves the 2×2 pivot factorization (i.e. U and V^*) arbitrary. Recall (section 2.8) that the step i corresponds to the number of pivots (1×1 or 2×2) used and ℓ corresponds to the number of bases vectors generated.

Step i:

Action 0: (Collect and evaluate data from the previous stpe, i-1)

On hand are r_ℓ, s_ℓ^*, $\|r_\ell\|$, $\|s_\ell^*\|$, P_{i-1}^*, Q_{i-1}, z_i, $\tilde{z}_i^*$, ω_i.

If $\|r_\ell\|$ or $\|s_\ell^*\|$ less than some tolerance, then exit with invariant subspace.

Check residual bounds for converged eigentriples.

Action 1: (Perform look-ahead to determine pivot size)

a: (Complete $R_i = [r_\ell, \tilde{r}_{\ell+1}]$ and $S_i^* = \begin{bmatrix} s_\ell^* \\ \tilde{s}_{\ell+1}^* \end{bmatrix}$ by generating $\tilde{r}_{\ell+1}$ and $\tilde{s}_{\ell+1}^*$ from r_ℓ and s_ℓ^* (see section 2.9))

$$\tilde{r}_{\ell+1} \leftarrow Br_\ell - Q_{i-1}z_i$$

$$\tilde{s}_{\ell+1}^* \leftarrow s_\ell^*B - \tilde{z}_i^*P_{i-1}^*$$

b: (Compute needed inner product matrices)

$$W_i \leftarrow S_i^*R_i$$

$$X_i \leftarrow R_i^*R_i$$

$$Y_i \leftarrow S_i^*S_i$$

(Six inner products are needed since the (1,1) element for each matrix comes from step i-1).

c: 1. (Compute cosines of important angles)

$$\phi_1 \ (= p_\ell^*q_\ell) = \omega_i/(\|r_\ell\|\|s_\ell^*\|)$$

$$\phi_2 \ (= \min \max \{|\tilde{p}_\ell^*\tilde{q}_\ell|, |\tilde{p}_{\ell+1}^*\tilde{q}_{\ell+1}|\}) = 0$$

(set for W_i singular)

If W_i cannot be factored skip to action 2.

Factor W_i into $V_i^{-*}U^{-1}$ and ω_ℓ into $\beta_\ell\gamma_\ell$.

(This version uses $p^*q = 1$)

2. (For norms of prospective bases vectors)

$$\|\tilde{q}_\ell\| \leftarrow (e_1^* U_i^* X_i U_i e_1)^{1/2}$$

$$\|\tilde{q}_{\ell+1}\| \leftarrow (e_2^* U_i^* X_i U_i e_i)^{1/2}$$

$$\|\tilde{p}_\ell^*\| \leftarrow (e_1^* V_i^* Y_i V_i e_1)^{1/2}$$

$$\|\tilde{p}_{\ell+1}^*\| \leftarrow (e_2^* V_i^* Y_i V_i e_2)^{1/2}$$

If any of the above norms is less than some tolerance, then skip to action 2.

3. (Form angles between prospective bases vectors)

$$\psi_1 \leftarrow \cos \angle(\tilde{p}_\ell^*, \tilde{q}_\ell) \equiv 1/(\|\tilde{p}_\ell^*\| \cdot \|\tilde{q}_\ell\|)$$

$$\psi_2 \leftarrow \cos \angle(\tilde{p}_\ell^*, \tilde{q}_\ell) = 1/(\|\tilde{p}_{\ell+1}^*\| \cdot \|\tilde{q}_{\ell+1}\|)$$

4. (Get the minimum angle for comparison)

$$\phi_2 \leftarrow \min\{|\psi_1|, |\psi_2|\}$$

Action 2: (Test for failure)

If $|\phi_1|$ and ϕ_2 are too small, exit with error.

(The look-ahead process with the 2×2 pivot is not guaranteed to work in all cases (see Chapter IV) and the only reasonable response is to flag these cases and exit.)

Action 3: (Select bases)

If $|\phi_1| >$ (some bias) $* \phi_2$ then take a single step (1×1 pivot), otherwise, take a double step (2×2 pivot).

	Single step		Double step
a.		(Form Q_i and P_i^*)	
	$q_\ell \leftarrow r_\ell/\beta_\ell$		$Q_i \leftarrow R_i U_i$
	$p_\ell^* \leftarrow s_\ell^*/\gamma_\ell$		$P_i^* \leftarrow V_i^* S_i^*$

	Single step	Double step
b.	(Form B_i and Γ_i)	
	$B_i \leftarrow \beta_\ell \tilde{z}^*$	$B_i \leftarrow (V_i^* S_i^*) r_k \tilde{z}$
	$\Gamma_i \leftarrow z_i \gamma_\ell$	$\Gamma_i \leftarrow z_i s_k^* (R_i U_i)$
	(Note that both B_i and Γ_i are rank 1 matrices)	
c.	(Form the new residuals)	
	$r_{\ell+1} \leftarrow r_{\ell+1} \beta_\ell^{-1}$	$r_{\ell+2} \leftarrow (BQ_i - Q_{i-1}\Gamma_i)x$
	$s_{\ell+1}^* \leftarrow \gamma_{\ell+1}^{-1} s_{\ell+1}$	$s_{\ell+2} \leftarrow y^*(P_i^* B - B_i P_{i-1}^*)$
		(x and y^* 2 element vectors)
d.	(Form A_i)	
	$A_i \leftarrow \alpha_\ell = e_1^* W_i e_2 / \omega_k$	$A_i \leftarrow P_i^* B Q_i$
		$= U_i^* [W_i e_2, S_i^* B r_{k+1}] V_i$
e.	(Orthogonalize)	
	$r_{\ell+1} \leftarrow r_{\ell+1} - q_\ell \alpha_\ell$	$r_{\ell+2} \leftarrow r_{\ell+2} - Q_i A_i x$
	$s_{\ell+1}^* \leftarrow s_{\ell+1}^* - \alpha_\ell p_\ell^*$	$s_{\ell+2}^* \leftarrow s_{\ell+1}^* - y^* A_i P_i^*$
f.	(Form inner products for next step)	
	$\|r_{\ell+1}\| \leftarrow ((-\alpha_\ell, 1) X_i \binom{-\alpha_\ell}{1})^{1/2} \beta_\ell^{-1}$	$\|r_{\ell+2}\| \leftarrow (r_{\ell+2}^* r_{\ell+2})^{1/2}$
	$\|s_{\ell+1}^*\| \leftarrow ((-\alpha_\ell, 1) Y_i \binom{-\alpha_\ell}{1})^{1/2} \gamma_\ell^{-1}$	$\|s_{\ell+2}^*\| \leftarrow (s_{\ell+2}^* s_{\ell+2})^{1/2}$
	$\omega_{\ell+1} \leftarrow \det(W_i) \omega_\ell^{-2}$	$\omega_{\ell+2} \leftarrow s_{\ell+2}^* r_{\ell+2}$
g.	(Set z_{i+1} and $\tilde{z}_{i+1}^*$)	
	$z_{i+1} = (1)$	$z_{i+1} = (V_i^* e_2)/(y^* V_i^* e_2)$
	$\tilde{z}_{i+1}^* = (1)$	$\tilde{z}_{i+1}^* = (e_2^* U_i)/(e_2^* U_i x)$
	end of step i	

NOTES

The above algorithm assumes that $p_\ell^* q_\ell = 1$ rather than $\|p_\ell^*\| = 1$, $\|q_\ell\| = 1$. Further, no assumption is made about the actual factorization

of ω_ℓ or W_i.

The vectors x and y^* (action 3c) allow flexibility in specifying the components of the new residuals strictly within $K^{\ell+2}$ and $K_*^{\ell+2}$, respectively.

The bias factor in action 3 is a programming device which permits the Look-Ahead Lanczos to implement standard Lanczos (bias = 0) or a sequence of double steps (2×2 pivots, bias = ∞).

The look-ahead process modifies the two-sided Lanczos algorithm to the extent that the next residuals are already being formed before the bases vectors of the previous step are set (action 1a). Further, if the 1×1 pivot is used (two-sided Lanczos) the norms of residual vectors and the 1×1 pivot are calculated without more vector inner products (action 3f).

Finally, note that the relevant cosines (see section 2.10, Chapter II) are calculated without calculating the bases vectors involved (actions 1b and 1c).

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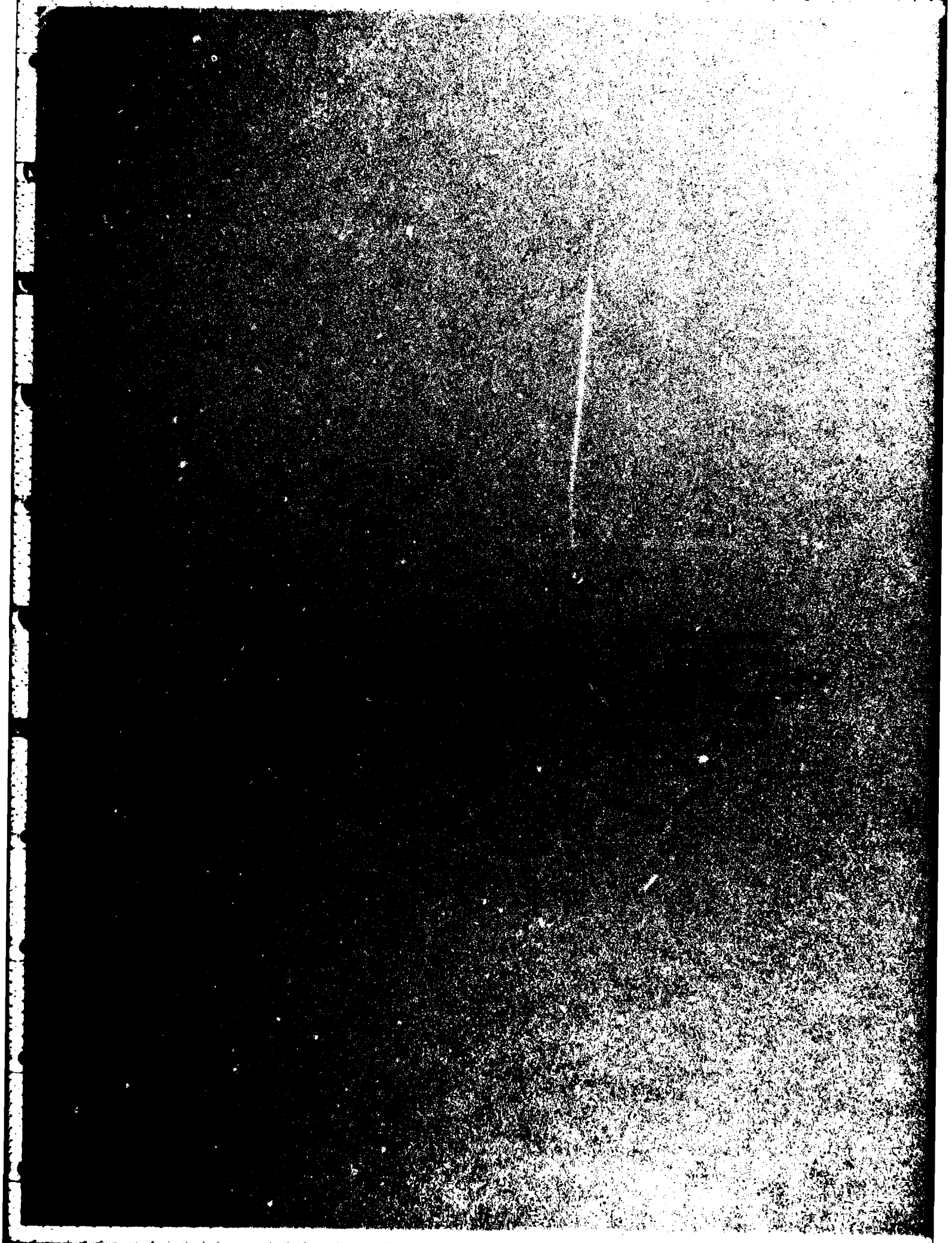

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