Chapter 10

Iterative Methods for Nonsymmetric Linear Systems

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Dedicated to David M. Young, Jr., on the occasion of his sixty-fifth birthday.

Abstract

This paper will present a survey of polynomial methods for solving nonsymmetric linear systems. An emphasis will be placed on generalizations of the classical conjugate gradient method for symmetric problems. To provide a framework for these methods, we will first outline a general theory of projection methods. Then, the more specific class of Krylov projection methods will be presented, including examples such as the classical conjugate gradient method, normal equations methods, the GCW method and the biconjugate gradient method. After this, truncated and restarted Krylov space methods will be discussed. An attempt will be made to expose open questions.

1 Introduction

In this paper we are concerned with the solution of systems of the form

$$Au = b \tag{1.1}$$

where $A \in \mathbb{C}^{N \times N}$ is a large nonsingular matrix and b and u are column vectors.

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When A is large and sparse, iterative methods are usually necessary in order to solve this problem efficiently. In particular, when A is self-adjoint with respect to some inner product, then the conjugate gradient (CG) method in many cases is a useful and practical solution technique. However, for general A, no general-purpose short-recurrence iterative technique, other than forming the normal equations, is currently available.

The purpose of this paper is to establish a theoretical framework for iterative methods for non-Hermitian problems. We will be concerned mainly with generalizations of the conjugate gradient method which are applicable to the case when A is not Hermitian positive definite (HPD). This framework will attempt to give a systematic structure to the landscape of iterative methods. We will also prove certain results such as convergence results for various classes of methods, and suggest some open questions which merit further study.

Iterative Methods. An *iterative method* is defined by an initial guess $u^{(0)}$ to the exact solution $\bar{u} = A^{-1}b$, followed by a sequence of further approximations $\{u^{(i)}\}_{i>0}$. The error is given by $e^{(i)} = \bar{u} - u^{(i)}$ and the residual by $r^{(i)} = b - Au^{(i)} = Ae^{(i)}$.

Typically the system $Au = b$ is derived from the equivalent problem

$$\hat{A}\hat{u} = \hat{b} \tag{1.2}$$

by preconditioning: $A = Q_L^{-1}\hat{A}Q_R^{-1}$, $u = Q_R\hat{u}$, $b = Q_L^{-1}\hat{b}$, where $Q_L, Q_R \in \mathbb{C}^{N\times N}$, so that (1.1) becomes

$$(Q_L^{-1}\hat{A}Q_R^{-1})(Q_R\hat{u}) = (Q_L^{-1}\hat{b}).$$

We thus have the associated quantities for the system (1.2): $\hat{u}^{(n)} = Q_R^{-1}u^{(n)}$, $\hat{u} = \hat{A}^{-1}\hat{b}$, $\hat{r}^{(n)} = \hat{b} - \hat{A}\hat{u}^{(n)}$ and $\hat{e}^{(n)} = Q_R^{-1}e^{(n)}$. Note that the postconditioning Q_R^{-1} distinguishes $e^{(n)}$ from $\hat{e}^{(n)}$, resulting in differing norms for the two quantities. In many settings the postconditioning may be included within the preconditioning (see [1]).

For a given choice of $u^{(0)}$, we will say an that iterative method *converges* if $u^{(n)} \to \bar{u}$ in some norm as $n \to \infty$. We will say that the method experiences *finite termination* if for some d we have $u^{(n)} = \bar{u}$ for all $n \geq d$.

Polynomial Methods. A *polynomial method* is an iterative method satisfying

$$e^{(n)} = P_n(A)e^{(0)}$$

for some polynomial $P_n(z) = 1 - zQ_{n-1}(z)$ of degree no greater than n satisfying $P_n(0) = 1$. Equivalently,

$$u^{(n)} - u^{(0)} \in \mathbf{K}_n(r^{(0)}, A)$$

where $\mathbf{K}_n(v, A) = \text{span}\{A^i v\}_{i=0}^{n-1}$ is the Krylov space spanned by the n vectors $A^i v$, $0 \leq i \leq n-1$. Typically Q_{n-1} is chosen so that $Q_{n-1}(A)$ approximates A^{-1} in some sense.

It is possible to compute P_n in a number of ways. *Chebyshev-like* methods, for example, typically attempt to calculate P_n which in some sense is small on the

spectrum of A. On the other hand, *conjugate gradient-like* methods employ certain inner products of vectors from the Krylov space to attempt to reduce the error.

In the next section, we will define a class of methods that covers nearly all the existing conjugate gradient-like methods.

2 Projection Methods

We define a *projection method* to be an iterative method satisfying the following relations. For any n and initial guess $u^{(0)}$ let $\mathbf{L}_n$ be an l_n-dimensional and $\mathbf{R}_n$ an r_n-dimensional subspace. Assuming that $u^{(n-1)}$ exists, we define $u^{(n)}$ to be a vector satisfying

$$u^{(n)} - u^{(n-1)} \in \mathbf{R}_n, \qquad u^{(n)} - \bar{u} \perp \mathbf{L}_n. \tag{2.1}$$

Orthogonality is defined in the standard Euclidean sense, with inner products defined by $(x, y) = \sum x_i \bar{y}_i$ for vectors $x = [x_1, x_2, \ldots, x_N]^T$, $y = [y_1, y_2, \ldots, y_N]^T$. We note that such $u^{(n)}$ may not exist and may not be unique. In this setting $u^{(n-1)} + \mathbf{R}_n$ is called the *solution space*, and the orthogonality condition of (2.1) is called the *Petrov-Galerkin condition.*

We now consider the specific form such $u^{(n)}$ takes. Let L_n (R_n) be a $N \times l_n$ ($N \times r_n$) matrix whose columns form a basis for $\mathbf{L}_n$ ($\mathbf{R}_n$). Then for some $r_n \times 1$ vector α we have

$$u^{(n)} = u^{(n-1)} + R_n \alpha \tag{2.2}$$

or

$$e^{(n)} = e^{(n-1)} - R_n \alpha.$$

The Petrov-Galerkin condition (2.1) yields

$$L_n^* e^{(n)} = L_n^* e^{(n-1)} - L_n^* R_n \alpha = 0.$$

If $L_n^* R_n$ is square and nonsingular then

$$\alpha = (L_n^* R_n)^{-1} L_n^* e^{(n-1)}. \tag{2.3}$$

Thus,

$$\begin{aligned} u^{(n)} &= u^{(n-1)} + R_n (L_n^* R_n)^{-1} L_n^* e^{(n-1)}, \\ e^{(n)} &= \left[I - R_n (L_n^* R_n)^{-1} L_n^* \right] e^{(n-1)}. \end{aligned} \tag{2.4}$$

Let

$$P_n = I - R_n (L_n^* R_n)^{-1} L_n^*. \tag{2.5}$$

Clearly P_n is a projection; hence the name projection methods is appropriate.

We now examine some properties of projection methods. We will begin with some definitions and then prove several theorems.

It is desirable that $u^{(n)}$ exist and be unique for any n. Given a particular $u^{(n-1)}$, we will say that a given projection method *breaks down* at step n if $u^{(n)}$ as defined in (2.1) does not exist or is not unique. It is clear that if $l_n < r_n$ and $u^{(n)}$ satisfying (2.1) exists, then such $u^{(n)}$ cannot be unique. On the other hand, when $l_n = r_n$ we have the following result.

Theorem 2.1 (Existence/Uniqueness) *Suppose $l_n = r_n > 0$. Then breakdown occurs at step n if and only if $L_n^* R_n$ is singular.*

Proof: The proof follows from the discussion above. ∎

Corollary 2.2 (Finite Termination) *Suppose for a particular $e^{(0)}$ breakdown never occurs for any step of the projection method, and $u^{(n-1)} \neq \bar{u}$ implies $\dim \mathbf{R}_n \gneq \dim \mathbf{R}_{n-1}$ for any n. Then convergence is attained within N steps: $u^{(d)} = \bar{u}$ for some $d \leq N$.*

Proof: Suppose breakdown does not occur at step n. Then by uniqueness $u^{(n)} = \bar{u}$ if and only if $e^{(n-1)} \in \mathbf{R}_n$. Since $\dim \mathbf{R}_n$ is strictly increasing, $e^{(d-1)} \in \mathbf{R}_d$ for some $d \leq N$. ∎

Note that whenever $l_n = r_n \neq 0$, then it is possible to construct B_n such that $L_n = B_n^* R_n$. In particular, we define B_n by $B_n^* = L_n (R_n^* R_n)^{-1} R_n^*$. Thus (2.5) becomes

$$P_n = I - R_n (R_n^* B_n R_n)^{-1} R_n^* B_n. \tag{2.6}$$

The matrix B_n embodies the relation between L_n and R_n. If B_n is *definite* on the subspace $\mathbf{R}_n$, in the sense that $v^* B_n v \neq 0$ for all $v \in \mathbf{R}_n \setminus \{0\}$, then it follows that $L_n^* R_n = R_n^* B_n R_n$ is nonsingular and breakdown will not occur at step n. This motivates the following theorem.

Theorem 2.3 (Boundedness) *Suppose $l_n = r_n \neq 0$ and $L_n = B_n^* R_n$ for every n, where $\mathbf{L}_n$, $\mathbf{R}_n$ and B_n may depend on $e^{(0)}$. Suppose, furthermore, that there exists c_n independent of $e^{(0)}$ such that*

$$0 < ||B_n|| \cdot ||x||^2 \leq c_n \cdot |x^* B_n x|$$

for every $e^{(0)}$ and $x \in \mathbf{R}_n \setminus \{0\}$. Then breakdown is impossible at any step and

$$||u^{(n)}|| \leq ||u^{(n-1)}|| + c_n ||e^{(n-1)}||.$$

Proof: If $x = R_n v$, then $x^* B_n x = v^* L_n^* R_n v$. By hypothesis,

$$\frac{v^* L_n^* R_n v}{v^* v} \cdot \frac{||v||^2}{||R_n v||^2} = \frac{|x^* B_n x|}{||x||^2} \geq \frac{||B_n||}{c_n} > 0.$$

This implies $L_n^* R_n$ is definite, thus nonsingular, implying no breakdown at this step.

Continuing, we have

$$u^{(n)} = u^{(n-1)} + R_n (R_n^* B_n R_n)^{-1} R_n^* B_n e^{(n-1)}.$$

Now let $\tilde{R}_n = R_n Q$, where Q is square and $\tilde{R}_n^* \tilde{R}_n = I$. Then it is easily seen that

$$u^{(n)} = u^{(n-1)} + \tilde{R}_n (\tilde{R}_n^* B_n \tilde{R}_n)^{-1} \tilde{R}_n^* B_n e^{(n-1)}.$$

Then

$$||u^{(n)}|| \leq ||u^{(n-1)}|| + ||(\tilde{R}_n^* B_n \tilde{R}_n)^{-1}|| \cdot ||\tilde{R}_n^* B_n e^{(n-1)}||.$$

We seek an upper bound for $||u^{(n)}||$. We have

$$\begin{aligned}
||(\tilde{R}_n^* B_n \tilde{R}_n)^{-1}||^2 &= 1/\min_{||w||=1} ||\tilde{R}_n^* B_n \tilde{R}_n w||^2 \\
&= 1/\min_{||w||=1} w^* \tilde{R}_n^* B_n^* \tilde{R}_n \left[ww^* + (I - ww^*)\right] \tilde{R}_n^* B_n \tilde{R}_n w \\
&= 1/\min_{||w||=1} \left[|w^* \tilde{R}_n^* B_n \tilde{R}_n w|^2 + ||(I - ww^*) \tilde{R}_n^* B_n \tilde{R}_n w||^2 \right] \\
&\leq 1/\min_{||w||=1} |w^* \tilde{R}_n^* B_n \tilde{R}_n w|^2 \leq 1/\min_{x \in R_n, ||x||=1} |x^* B_n x|^2.
\end{aligned}$$

The last inequality follows from letting $x = \tilde{R}_n w$ and noting that $||\tilde{R}_n w|| = ||w||$. We have, therefore,

$$||u^{(n)}|| \leq ||u^{(n-1)}|| + \sup_{x \in R_n \setminus \{0\}} \frac{||x||^2}{|x^* B_n x|} \cdot ||B_n|| \cdot ||e^{(n-1)}||.$$

The hypothesis on B_n yields the result. ∎

Balanced Projection Methods

We say a projection method is *balanced* (a BPM) if there exists a fixed square matrix B such that $L_n = B^* R_n$ for all n and $e^{(0)}$.

Consider the sesquilinear form $(B\cdot, \cdot)$. The Petrov-Galerkin condition (3) is now equivalent to the condition

$$(Be^{(n)}, z) = 0 \qquad \forall z \in \mathbf{R}_n. \tag{2.7}$$

If B is *definite*, that is, $x^* Bx \neq 0$ for all $x \neq 0$, then the hypothesis of Theorem 2.3 is satisfied. Recall that a real matrix B is definite if and only if either its Hermitian part $B_H \equiv H(B) \equiv (B + B^*)/2$ or its negative $-H(B)$ is Hermitian positive definite (HPD) (see [12]).

We have then the following

Corollary 2.4 (Boundedness) *Let B be definite. Then a BPM based on B will not break down at any step. Furthermore, let*

$$\rho_{\min}(B) = \inf_{x \neq 0} \frac{|x^* B x|}{x^* x}.$$

Then

$$||u^{(n)}|| \leq ||u^{(n-1)}|| + \frac{||B||}{\rho_{\min}(B)} ||e^{(n-1)}||.$$

Proof: The proof is a direct application of Theorem 2.3. ∎

Theorem 2.5 (Uniform Boundedness) *Suppose the hypotheses of Corollary 2.4 are satisfied, and furthermore $\mathbf{R}_n \subseteq \mathbf{R}_{n+1}$ for every n. Then the following bound holds for every n:*

$$||u^{(n)}|| \leq ||u^{(0)}|| + \frac{||B||}{\rho_{\min}(B)} ||e^{(0)}||.$$

Proof: The proof is similar to the proof of Theorem 2.3 and follows from the fact that such $u^{(n)}$ may be equivalently defined by

$$u^{(n)} = u^{(0)} + R_n (R_n^* B R_n)^{-1} R_n^* B e^{(0)}.$$

∎

If a BPM satisfies the further criterion that the matrix B is HPD, then the projector

$$P_n = I - R_n (R_n^* B R_n)^{-1} R_n^* B$$

is orthogonal with respect to the B inner product, defined by $(\cdot, \cdot)_B \equiv (B\cdot, \cdot)$. Let $||v||_B = (Bv, v)^{1/2}$, the B norm of a vector v. Then we have

Theorem 2.6 (Minimization) *Suppose we have a BPM based on a matrix B which is HPD. Then $u^{(n)}$ is the unique minimizer of $||e^{(n)}||_B$ over the solution space, and $||e^{(n)}||_B \leq ||e^{(n-1)}||_B$.*

Proof: Now $e^{(n)}$ is the B-orthogonal projection of $e^{(n-1)}$ onto the complement of $\mathbf{R}_n$, and

$$\begin{aligned} e^{(n)*} B e^{(n)} &= e^{(n-1)*} B e^{(n-1)} - e^{(n-1)*} B R_n (R_n^* B R_n)^{-1} R_n^* B e^{(n-1)} \\ &\leq e^{(n-1)*} B e^{(n-1)} \end{aligned}$$

with R_n as above. Suppose $e' = \bar{u} - u'$ is the error arising from u', another element of the solution space. Then for some w,

$$e' = e^{(n)} + R_n w.$$

Using the properties of the projector yields

$$\begin{aligned} e'^* B e' &= e^{(n)*} B e^{(n)} + w^* R_n^* B R_n w \\ &> e^{(n)*} B e^{(n)} \text{ for } w \neq 0, \end{aligned}$$

showing $u^{(n)}$ gives the unique minimum. ∎

We also have the following sufficient condition for convergence, generalized from a theorem in [3]:

Theorem 2.7 (Convergence) *Suppose we have a BPM with B HPD. Suppose also that $Z = BA^{-1}$ is definite and $r^{(n-1)} \in \mathbf{R}_n$ for every n. Then there exists $\epsilon > 0$ independent of $e^{(0)}$ such that for all n,*

$$||e^{(n)}||_B \leq (1 - \epsilon)||e^{(n-1)}||_B.$$

Proof: Since B is HPD, the B norm of $e^{(n)}$ is minimized over the affine space $e^{(n-1)} + \mathbf{R}_n$. Let

$$\tilde{e}^{(n)} = e^{(n-1)} - \lambda A e^{(n-1)},$$

where λ is defined by the condition $B\tilde{e}^{(n)} \perp Ae^{(n-1)} = r^{(n-1)}$; note that since this causes a minimization over a smaller space, we must have

$$||e^{(n)}||_B \leq ||\tilde{e}^{(n)}||_B.$$

We obtain

$$\lambda = \frac{(Ae^{(n-1)})^* B(e^{(n-1)})}{(Ae^{(n-1)})^* B(Ae^{(n-1)})}.$$

Through the projection property we obtain

$$||\tilde{e}^{(n)}||_B^2 = ||e^{(n-1)}||_B^2 - \frac{|e^{(n-1)*} BAe^{(n-1)}|^2}{(Ae^{(n-1)})^* B(Ae^{(n-1)})}.$$

Dropping superscripts and letting $Ae = r$,

$$\begin{aligned} \frac{||\tilde{e}||_B^2}{||e||_B^2} &= 1 - \frac{|e^* BAe|^2}{(e^* Be)(e^* A^* BAe)} \\ &= 1 - \frac{|r^* A^{-*} Br|^2}{(r^* A^{-*} BA^{-1} r)(r^* Br)} \\ &= 1 - \frac{|r^* Zr|^2}{(r^* A^{-*} BA^{-1} r)(r^* Br)} \\ &\leq 1 - \frac{\rho_{\min}(Z)^2}{||A^{-1}||^2 \cdot ||B||^2} \end{aligned}$$

where

$$\rho_{\min}(M) = \min_{v \neq 0} \frac{|v^* M v|}{v^* v}$$

for any matrix M, so that M is definite if and only if $\rho_{\min}(M) \neq 0$. ∎

We remark that examples may be constructed of BPM's for which B is not HPD and the projection method diverges, i.e., $||e^{(n)}||_{B_H} \to \infty$, where $B_H = (B + B^*)/2$ is the Hermitian part of B (see [11]). However, if $r^{(n-1)} \in \mathbf{R}_n$, $Z = BA^{-1}$ is definite and the skew-Hermitian part $B_N \equiv (B - B^*)/2$ is sufficiently small, then convergence is assured. The following theorem gives a specific bound for this case of the form

$$||e^{(n)}||_{B_H}^2 \leq (1 - \epsilon + K)||e^{(n-1)}||_{B_H}^2,$$

where $\epsilon > 0$ and $K \geq 0$ is a constant which is small when B_N is small.

Theorem 2.8 (Convergence) *Consider a BPM based on B with the decomposition $B = B_H + B_N$ into its Hermitian and skew-Hermitian parts. If $r^{(n-1)} \in \mathbf{R}_n$, then*

$$\frac{||e^{(n)}||_{B_H}^2}{||e^{(n-1)}||_{B_H}^2} \leq 1 - \frac{(\rho_{\min}(BA^{-1}))^2}{||A^{-1}||^2 \cdot ||B_H||^2(1 + ||B_N||^2 \cdot ||B_H^{-1}||/||B_H||)}$$
$$+ 2||B_H^{-1}||^{3/2}||B_N||(||B_H||^{1/2} + ||B_H^{-1}||^{1/2} \cdot ||B_N||).$$

Proof: See [11]. ∎

3 Krylov Projection Methods

We will now begin to consider projection methods which are also polynomial methods.

A *(full) Krylov projection method* (KPM) is a balanced projection method satisfying $\mathbf{R}_n = \mathbf{K}_n(r^{(0)}, A)$. That is,

$$u^{(n)} - u^{(0)} \in \mathbf{K}_n(r^{(0)}, A), \qquad Be^{(n)} \perp \mathbf{K}_n(r^{(0)}, A).$$

The above theorems applied to Krylov projection methods yield the following very desirable properties:

- *Finite Termination.* If there is no breakdown at step n, then $u^{(n)} = \bar{u}$ if and only if $n \geq d(r^{(0)}, A)$. Here $d(v, A)$, the *degree* of a vector v with respect to A, is given by $d(v, A) = \min\{\deg P : P \text{ monic}, P(A)v = 0\}$. The *degree* of a matrix A is given by $d(A) = \min\{\deg P : P \text{ monic}, P(A) = 0\}$.

Class	B property
Idealized Generalized Conjugate Gradient (IGCG) Method [21]	B positive real
Orthogonal Error Method (OEM) [5]	B definite
Hermitian Krylov Projection Method (HKPM)	B Hermitian
Conjugate Gradient Method (CGM) [4]	B HPD

Table 10.1

- *No Breakdown for B Definite.* For fixed A and B, the KPM will not break down for any $r^{(0)}$ if and only if B is definite. (If B is not definite, breakdown is caused at step 1 if $r^{(0)} \neq 0$ is such that $r^{(0)^*} B r^{(0)} = 0$.)
- *Bounded Iterates for B Definite.* If B is definite and $u^{(0)}$ and $e^{(0)}$ are constrained to be in some bounded set, then the size of $u^{(n)}$ is bounded independent of n.
- *Minimization for B HPD.* If B is HPD, then $u^{(n)}$ is the unique element of $u^{(0)} + \mathbf{K}_n(r^{(0)}, A)$ to minimize $||e^{(n)}||_B$.

The choice of B and its associated sesquilinear form $(B\cdot, \cdot)$ is very strategic in terms of the properties of the method as well as the feasibility of implementing the method by some practical algorithm. Table 10.1 defines important classes of KPM's, based on the properties of B.

Most notable of these classes is the class of conjugate gradient methods (CGM), which possess a minimization property over the entire Krylov space due to B being HPD. Some examples of conjugate gradient methods are the classical conjugate gradient method (see [9]) ($B = A$ HPD), the preconditioned conjugate gradient method ($A = Q^{-1}\hat{A}$, $B = \hat{A}$, with Q and $\hat{A}$ HPD), and the conjugate residual method ($B = A^*A$, A Hermitian). (For a complete discussion of conjugate gradient methods, see [1].)

We now examine some common features of Krylov projection methods. Suppose no breakdown occurs up to step n. From (2.2) we have

$$u^{(n+1)} = u^{(n)} + \alpha_n p^{(n)}, \quad p^{(n)} \in \mathbf{K}_{n+1}(r^{(0)}, A) \tag{3.1}$$

where α_n is a scalar. This yields

$$e^{(n+1)} = e^{(n)} - \alpha_n p^{(n)}.$$

The orthogonality condition indicates that $e^{(n+1)} \perp B^*\mathbf{K}_{n+1}(r^{(0)}, A)$. Similarly, we have that $e^{(n)} \perp B^*\mathbf{K}_n(r^{(0)}, A)$. Thus, if such $\alpha_n p^{(n)}$ exists and $\alpha_n \neq 0$ then

$$p^{(n)} \in \mathbf{K}_{n+1}(r^{(0)}, A), \tag{3.2a}$$

$$p^{(n)} \perp B^*\mathbf{K}_n(r^{(0)}, A). \tag{3.2b}$$

An easy induction argument can be used to show that such a $p^{(n)}$ exists uniquely up to scaling if and only if $p^{(j)*}Bp^{(j)} \neq 0$, $j < n$. Furthermore, if $p^{(n)}$ exists uniquely, then it may be chosen nonzero if and only if $n < d(r^{(0)}, A)$. Since $p^{(n)} \in \mathbf{K}_{n+1}(r^{(0)}, A)$, the orthogonality condition yields

$$\alpha_n = \frac{p^{(n)*}Be^{(n)}}{p^{(n)*}Bp^{(n)}} \tag{3.3}$$

which exists uniquely if and only if $p^{(n)*}Bp^{(n)} \neq 0$. We sum up this discussion in the following theorem.

Theorem 3.1 *Suppose the Krylov projection method based on A and B with initial residual $r^{(0)}$ does not break down for steps $i = 1, 2, \ldots, n$, and $u^{(n)} \neq \bar{u}$. Then the KPM does not break down at step $n+1$ if and only if the unique (up to scaling) vector $p^{(n)}$ satisfying (3.2a,3.2b) has the property $p^{(n)*}Bp^{(n)} \neq 0$.*

Proof: The proof proceeds by induction. At each step the vector $p^{(i)} \in \mathbf{K}_{i+1}(r^{(0)}, A)$ such that $p^{(i)} \perp B^*\mathbf{K}_i(r^{(0)}, A)$ exists uniquely if and only if $p^{(j)*}Bp^{(j)} \neq 0$ for $j < i$. Then, α_i exists uniquely if and only if $p^{(i)*}Bp^{(i)} \neq 0$. ∎

We remark that it is possible to skip over several steps. That is, it may be possible to find $u^{(n+s)}$ satisfying

$$u^{(n+s)} - u^{(n)} \in \mathbf{K}_{n+s}(r^{(0)}, A)$$

and

$$e^{(n+s)} \perp B^*\mathbf{K}_{n+s}(r^{(0)}, A)$$

even if $p^{(n)*}Bp^{(n)} = 0$. This is the essence of the work on hyperbolic pairs given in [13]. For a further discussion of these ideas, see [11].

It is clear that in the absence of breakdown the direction vectors $\{p^{(i)}\}_{i=0}^{n}$ form a basis for the space $\mathbf{K}_{n+1}(r^{(0)}, A)$ and possess the property $p^{(j)*}Bp^{(i)} = 0$ for $j < i$. In the next section we discuss several algorithms for constructing these vectors.

3.1 Computational Schemes for Krylov Projection Methods

We will now examine practical algorithms for computing the KPM iterates. Practical algorithms hinge on the formation of a basis for the Krylov space which is well-conditioned as well as efficiently computed.

We will now introduce some further definitions. An *adjoint* (or *right adjoint*) of an arbitrary matrix A with respect to a matrix B is a matrix $A^\dagger$ satisfying $(Bu, A^\dagger v) = (BAu, v)$ for all u, v. If B is nonsingular, then $A^\dagger$ is given uniquely by $(BAB^{-1})^*$. The matrix A is said to be *B-self-adjoint* if $BA = A^*B$ (see [10]).

It should be noted that A may also have a *left adjoint* with respect to B, a matrix A^x satisfying $(BA^x u, v) = (Bu, Av)$ for every u and v. When B is nonsingular,

we have $A^x = B^{-1}A^*B$. Furthermore, when B is HPD, the adjoints are equal: $A^x = A^\dagger$; they are also equal if B is definite and A is B-normal (see [5]). Here we will be concerned only with $A^\dagger$, the right adjoint.

For a given matrix B, a matrix A is *B-normal* if $BA = q(A)^*B$ for some polynomial q. The *normal degree* of A with respect to B, given by $n(A) = n(A, B)$, is the lowest degree of any such polynomial. If $s = n(A, B)$, then A will be called *normal(s)* with respect to B or *B-normal(s)*.

When $B = I$, this definition of normal coincides with the classical definition of normal, that $AA^* = A^*A$. In fact, it is shown in [5] that for B definite the following are equivalent:

[1] A and $A^\dagger$ commute.

[2] A and $A^\dagger$ have the same complete set of B-orthogonal eigenvectors.

[3] $A^\dagger = q(A)$ for some polynomial q.

This equivalence does not hold for general nonsingular A and B, however.

We now present three principal algorithms for the computation of the KPM iterates. They are the Orthodir, Orthomin and Orthores algorithms (see [21]). The formulas for these KPM algorithms are given in Figures 10.1–10.3. Of these algorithms, the Orthomin algorithm is most widely used and in the case of $B = A$ HPD embodies the common two-term form of the conjugate gradient method of Hestenes and Stiefel. In the formulas that follow and throughout we will make the definition $Z = BA^{-1}$.

Breakdown. If B is definite, then the Krylov projection method is guaranteed not to break down. However, even when the iterates $\{u^{(i)}\}$ are uniquely defined by the KPM, it may be possible that one of the KPM algorithms reaches an impasse before convergence is attained. In particular, we will say that *the algorithm breaks down* at step n if iterates $\{u^{(i)}\}_{i=0}^{n-1}$ have been computed and $e^{(n-1)} \neq 0$ but the algorithm is unable to compute $u^{(n)}$. It is important to note that breakdown of the algorithm may occur even if the projection method itself does not break down.

The Orthodir algorithm is guaranteed not to break down whenever the KPM iterates exist and are unique. This is assured if B is definite. On the other hand Orthomin and Orthores are guaranteed not to break down if and only if both B and Z are definite.

Computability. A necessary condition for these algorithms to be practical is that B is chosen so that the necessary inner products are computable in a practical way. In particular, we require that inner products of the form $(Q_L^{-*}ZQ_L^{-1}\cdot, \cdot)$ of vectors in the space $\mathbf{K}_n(\hat{r}^{(0)}, \hat{A}Q_R^{-1}Q_L^{-1})$ be computable. This would exclude, for instance, the general case of methods with $B = I$, though it is possible to implement $B = I$ methods if special choices of Q_L and Q_R are made (see [1]).

Economical Computation. In general the recursions for Orthodir, Orthomin and Orthores given above are not practical, since the work per iteration increases for every iteration. However, when A and B satisfy certain relationships, the formulas

ORTHODIR

$$q^{(0)} = r^{(0)},$$

$$q^{(n)} = Aq^{(n-1)} + \sum_{i=\theta(n)}^{n-1} \beta_{n,i} q^{(i)}, \qquad n > 0. \qquad (\theta(n) = 0 \ \forall n)$$

$$\beta_{n,i} = \frac{-q^{(i)*} BAq^{(n-1)} - \sum_{j=\theta(n)}^{i-1} \beta_{n,j} q^{(i)*} Bq^{(j)}}{q^{(i)*} Bq^{(i)}}.$$

$$\begin{aligned} u^{(n+1)} &= u^{(n)} + \hat{\lambda}_n q^{(n)}, \\ r^{(n+1)} &= r^{(n)} - \hat{\lambda}_n Aq^{(n)}. \end{aligned}$$

$$\hat{\lambda}_n = \frac{q^{(n)*} Zr^{(n)}}{q^{(n)*} Bq^{(n)}}.$$

If B Hermitian : $\beta_{n,i} = -\dfrac{q^{(i)*} BAq^{(n-1)}}{q^{(i)*} Bq^{(i)}}$

If $n(A, B) = s$: $\beta_{n,i} = 0, \quad i < n - (s+1)$

Figure 10.1

ORTHOMIN

$$p^{(n)} = r^{(n)} + \sum_{i=\phi(n)}^{n-1} \alpha_{n,i} p^{(i)}, \qquad n \geq 0. \qquad (\phi(n) = 0 \ \forall n)$$

$$\alpha_{n,i} = \frac{-p^{(i)*} Br^{(n)} - \sum_{j=\phi(n)}^{i-1} \alpha_{n,j} p^{(i)*} Bp^{(j)}}{p^{(i)*} Bp^{(i)}}.$$

$$\begin{aligned} u^{(n+1)} &= u^{(n)} + \lambda_n p^{(n)}, \\ r^{(n+1)} &= r^{(n)} - \lambda_n Ap^{(n)}. \end{aligned}$$

$$\lambda_n = \frac{p^{(n)*} Zr^{(n)}}{p^{(n)*} Bp^{(n)}} = \frac{r^{(n)*} Zr^{(n)}}{p^{(n)*} Bp^{(n)}}.$$

If B Hermitian : $\alpha_{n,i} = -\dfrac{p^{(i)*} Br^{(n)}}{p^{(i)*} Bp^{(i)}}$

If $n(A, B) = s$: $\alpha_{n,i} = 0, \quad i < n - s$

Figure 10.2

ORTHORES

$$u^{(n+1)} = \lambda_n \left(r^{(n)} + \sum_{i=\theta(n+1)}^{n} \sigma_{n+1,i} u^{(i)} \right) \qquad (\theta(n) = 0 \ \forall n)$$

$$r^{(n+1)} = -\lambda_n \left(Ar^{(n)} - \sum_{i=\theta(n+1)}^{n} \sigma_{n+1,i} r^{(i)} \right)$$

$$\lambda_n = \left(\sum_{i=\theta(n+1)}^{n} \sigma_{n+1,i} \right)^{-1}$$

$$\sigma_{n+1,i} = \frac{r^{(i)*} Z A r^{(n)} - \sum_{j=\theta(n+1)}^{i-1} \sigma_{n+1,j} r^{(i)*} Z r^{(j)}}{r^{(i)*} Z r^{(i)}}.$$

If Z Hermitian : $\sigma_{n+1,i} = \dfrac{r^{(i)*} Z A r^{(n)}}{r^{(i)*} Z r^{(i)}}$

If $n(A,B) = s$: $\sigma_{n+1,i} = 0, \quad i < n - s$

Figure 10.3

for these three algorithms may be simplified to give short recurrences while still computing the true KPM iterates. The following theorems characterize these cases. Their proofs are found in [4, 5] and [12].

Theorem 3.2 (Simplification) *For the Orthodir algorithm to yield $\beta_{n,i} = 0$ for all $i < n-(s+1)$ and $n \leq d(r^{(0)}, A) - 1$ for all $r^{(0)}$, it is sufficient that $d(A) \leq s+2$ or that A be B-normal with $n(A,B) \leq s$. If B is definite, then the condition is also necessary.*

Proof: See [4, 5]. ∎

Theorem 3.3 (Simplification) *For the Orthomin and Orthores algorithms to yield $\alpha_{n,i} = 0$ and $\sigma_{n+1,i} = 0$ respectively for all $i < n - s$ and $n \leq d(r^{(0)}, A) - 1$ for all $r^{(0)}$, it is sufficient that $d(A) \leq s + 1$ or that A be B-normal with $n(A,B) \leq s$. If B and Z are definite, then the condition is also necessary.*

Proof: See [12]. ∎

Thus, if A is B-normal with $n(A,B) = s$ then, in the definition of the Orthodir algorithm, we may set $\theta(n) = \max(0, n-(s+1))$ and still obtain the KPM iterates.

In this case we may likewise set $\phi(n) = \max(0, n - s)$ in the Orthomin algorithm and $\theta(n+1) = \max(0, n - s)$ in the Orthores algorithm and still obtain the KPM iterates. The simplifications may also be accomplished when $d(A) \leq s+1$; however, this case is not very useful, since $d(A)$ is usually large for practical problems, which would require s to be large also.

The above simplifications of formulas for the KPM algorithms holds for an important but restrictive class of matrices. The next two results help define this class.

Theorem 3.4 (B-Normal(s) Matrices) *Suppose that B is definite and A is B-normal. If $s = n(A, B) > 1$, then $s \geq \sqrt{d(A)}$.*

Proof: The proof is a simple generalization of a result in [4]; see also [5] and [12]. ∎

Since $d(A)$ is typically large, this case is not practical. On the other hand,

Theorem 3.5 (B-Normal(1) Matrices) *Suppose that B is definite and A is B-normal. If $n(A, B) = 1$, then A is of the form*

$$e^{i\theta}(riI + G),$$

where r and θ are real and G is B-self-adjoint.

Proof: This proof is also a simple generalization of a result given in [4]; see also [5] and [12]. ∎

Note that A B-normal(1) with B definite requires that the spectrum of A be contained in a line in the complex plane (see [5]). Furthermore, B must be such that the necessary inner products are feasibly computable.

The above theorems show that when B is definite, short recurrences occur naturally for an important but restrictive class of matrices. Alternatively, one can artificially truncate the recursions in the case of more general matrices. However, the full orthogonality and optimality conditions are lost and with them finite termination. More will be said about truncated methods below.

If on the other hand B is allowed to be indefinite, short recurrences may be used to compute the full KPM iterates for a larger class of matrices A. However, breakdown may occur and the iterates may become unbounded. An important example of such a method is the biconjugate gradient method described in the next section.

3.2 Examples of Krylov Projection Method

Within the class of Krylov projection methods are three important subclasses, defined by restrictions applied to B. In this section we will consider particular methods in each of these subclasses.

Conjugate Gradient Methods. These methods are characterized by choosing B to be HPD. We have already mentioned several well-known methods in this class: the classical conjugate gradient method of Hestenes and Stiefel; the preconditioned conjugate gradient method; and the conjugate residual method. One further class of methods is the class of normal equations methods, which includes the methods defined by $A = \hat{A}^*\hat{A}$ with $B = I$ or $B = A$. Here $\hat{A}$ itself may be the result of a preconditioning. These cases are examined in detail in [1].

Orthogonal Error Methods. These methods are characterized by choosing B to be definite. A classic example of an OEM is the GCW method [2, 20]. Here we let $A = Q^{-1}\hat{A}$, $Q = \hat{A}_H \equiv (\hat{A} + \hat{A}^*)/2$ and $B = \hat{A}$, assuming $\hat{A}$ definite and $\hat{A}_H$ nonsingular. It is easily verified that the B-adjoint, $A^\dagger$, is a degree-1 polynomial in A. Since $(B\cdot, \cdot)$ is not in general an inner product, no obvious minimization property is satisfied. However, it is shown in [8] that when $\hat{A}$ is real, the even iterates of the GCW method are the same as the iterates of the CG method defined by $B = \hat{A}_H$ and $A = \hat{A}_H^{-1}\hat{A}^*\hat{A}_H^{-1}\hat{A}$.

Hermitian Krylov Projection Methods. These methods are characterized by restricting B to be Hermitian. Relaxing the constraint that B be definite is a drastic measure; the resulting methods may break down, and the iterates may be unbounded.

A classic example of an HKPM is the SYMMLQ method of [15], for which $B = A$ where A is Hermitian but possibly indefinite. Another example of an HKPM is the Lanczos or biconjugate gradient (BCG) method (Fig. 10.4). It is shown in [10] that when A, $u^{(0)}$, b, $\tilde{u}^{(0)}$ and $\tilde{b}$ are restricted to be real, then the biconjugate gradient iterates may be obtained by applying the Orthomin algorithm to the double system

$$\mathbb{A}\ \mathbb{u} = \mathbb{b}$$

with

$$\mathbb{A} = \begin{pmatrix} A & \\ & A^* \end{pmatrix}, \quad \mathbb{u} = \begin{pmatrix} u \\ \tilde{u} \end{pmatrix}, \quad \mathbb{b} = \begin{pmatrix} b \\ \tilde{b} \end{pmatrix}$$

and

$$\mathbb{Z} = \begin{pmatrix} & I \\ I & \end{pmatrix}, \qquad \mathbb{B} = \mathbb{Z}\,\mathbb{A} = \begin{pmatrix} & A^* \\ A & \end{pmatrix}.$$

The resulting iterates are

$$\mathbb{u}^{(n)} = \begin{pmatrix} u^{(n)} \\ \tilde{u}^{(n)} \end{pmatrix}$$

where $u^{(n)}$ is the same as the BCG iterate. Here $\tilde{r}^{(0)} \equiv \tilde{b} - A^*\tilde{u}^{(0)}$ is some arbitrary vector, typically set to $\tilde{Z}^*r^{(0)}$ for some fixed matrix $\tilde{Z}$, e.g. $\tilde{Z} = I$. The BCG method may also be seen as a polynomial projection method with $\mathbf{R}_n = \mathbf{K}_n(r^{(0)}, A)$ and $\mathbf{L}_n = \mathbf{K}_n(\tilde{r}^{(0)}, A^*)$.

THE BCG METHOD

$$p^{(0)} = r^{(0)}$$
$$\tilde{p}^{(0)} = \tilde{r}^{(0)}$$
$$p^{(n)} = r^{(n)} + \alpha_n p^{(n-1)}, \quad n > 0.$$
$$\tilde{p}^{(n)} = \tilde{r}^{(n)} + \alpha_n^* \tilde{p}^{(n-1)}, \quad n > 0.$$
$$\alpha_n = \frac{\tilde{r}^{(n)*} r^{(n)}}{\tilde{r}^{(n-1)*} r^{(n-1)}}$$

$$\begin{aligned} u^{(n+1)} &= u^{(n)} + \lambda_n p^{(n)}, \\ r^{(n+1)} &= r^{(n)} - \lambda_n A p^{(n)}, \\ \tilde{r}^{(n+1)} &= \tilde{r}^{(n)} - \lambda_n^* A^* \tilde{p}^{(n)}. \end{aligned}$$

$$\lambda_n = \frac{\tilde{r}^{(n)*} r^{(n)}}{\tilde{p}^{(n)*} A p^{(n)}}$$

Figure 10.4

The BCG method may break down unless certain very special conditions are satisfied, such as A HPD and $\tilde{r}^{(0)} = r^{(0)}$. Furthermore, the residuals may get arbitrarily large before convergence. However, for certain classes of problems, the set of initial residuals $r^{(0)}$ for which the BCG method breaks down is only a set of measure zero in the space of all real vectors [11]. It remains an open question of how likely it is that the method may "nearly" break down, in the sense that the residual becomes unacceptably large during the iteration process. Further work must be done to understand the convergence properties of BCG.

4 Semi-Krylov Projection Methods

Methods such as the normal equations methods, the GCW method and the BCG method attempt to embed the original problem (1.1) into a problem satisfying the B-normal(1) condition for some B. Another means to surmounting the problem of long recurrences is to define projection methods which use smaller subspaces than the whole Krylov space. This is the idea behind various truncated and restarted methods. These methods are more economical than the full-space methods; however, in general they do not possess certain desirable properties of KPM's, such as finite termination and minimization over the entire Krylov space when B is HPD.

In particular, we will define a *semi-Krylov projection method* (SKPM) to be

a projection method utilizing a portion of the Krylov space: $\mathbf{R}_n \subseteq \mathbf{K}_n(r^{(0)}, A)$ and $\mathbf{L}_n \subseteq B^*\mathbf{K}_n(r^{(0)}, A)$ for some matrix B. If an SKPM is also balanced (i.e., $\mathbf{L}_n = B^*\mathbf{R}_n$), we will say it is a *balanced* semi-Krylov projection method (BSKPM).

Some examples of SKPM's are the truncated Orthodir, Orthomin and Orthores algorithms. These are obtained from the above-stated KPM algorithms by a simple redefinition of the index functions θ and ϕ: Orthodir(s) ($\theta(n) = \max(0, n-s)$), Orthomin(s) ($\phi(n) = \max(0, n-s)$), and Orthores(s) ($\theta(n+1) = \max(0, n-s)$). Other truncated methods are documented in [16], including the Axelsson Least Squares ($B = A^*A$) and Axelsson Galerkin ($B = A$) methods. Restarted methods also fall into this category, including the GCR($s-1$) [3] and GMRES(s) [17] methods. These two restarted methods both utilize $B = A^*A$ and restart the full KPM every s steps. The GCR($s-1$) method, which is restarted Orthomin, is guaranteed not to break down for A definite; GMRES(s) will never break down but may stagnate for general nonsingular A.

Truncated and restarted methods do not in general possess all the useful KPM properties. However, certain desirable properties are possessed by some of the methods:

- *Behavior near the normal(1) case.* It is desirable that if A happens to be B-normal(1), then an adequate part of the Krylov space is saved in order to give the same iterate as the full KPM method. Likewise, by continuity, if A is a perturbation from a B-normal(1) matrix, it is hoped that nearly the KPM result will be given. This property is possessed by some truncated methods, e.g., Orthomin(s) with $s \geq 1$ and A nearly B-normal(1).

- *Minimization property.* It is hoped that the error $e^{(n)}$ is a minimization over some space, so that the error in some norm is nonincreasing.

- *Minimization over some Krylov space.* If each $e^{(n)}$ is minimized over an appropriate Krylov space, then certain error bounds may be invoked for the error, even though it is not a minimization over the entire Krylov space. In particular, we seek a balanced method with B HPD and $u^{(n)} \in u^{(n-k)} + \mathbf{K}_k(r^{(n-k)}, A)$ with k as large as possible. This property is possessed by restarted methods such as GCR($s-1$) and GMRES(s).

4.1 Balanced SKPM's: Truncated/Restarted Methods

Some truncated methods of the SKPM category satisfy the additional condition that they are balanced, in the sense that $\mathbf{L}_n = B^*\mathbf{R}_n$ for a fixed map B. Included are the truncated Orthodir and Orthomin methods, GCR($s-1$), GMRES(s), and the two methods of Axelsson mentioned above.

When B is HPD and $Z = B^{-1}A$ is definite, the Orthomin algorithm with the function $\phi(n)$ defined as an arbitrary nonnegative monotone function is guaranteed to converge (Theorem 2.7). Moreover, when A is definite, the restarted methods GCR($s-1$) and GMRES(s) (for which $B = A^*A$) will always converge (see [3], [17]).

Many open questions remain concerning these methods, such as necessary and sufficient conditions for $r^{(0)}$ and A for which the methods converge, as well as sharp error bounds. A few things are known, however.

We make the following definitions. Let $K_n(v, A) = (\, v \quad Av \quad A^2v \quad \ldots \quad A^{n-1}v\,)$, a matrix whose columns span $\mathbf{K}_n(v, A)$. Let $r^{(s)}$ be defined as a function of $r^{(0)}$ to be the residual at step s of the KPM with $B = A^*A$ applied to the initial residual $r^{(0)}$. Then let

$$\begin{aligned}\psi_s(A) &= \max_{r^{(0)}\neq 0} \frac{||r^{(s)}||}{||r^{(0)}||} = \max_{v\neq 0} \min_{P_s(0)=1} \frac{||P_s(A)v||}{||v||} \\ &= \max_{r:d(r,A)\geq s} \frac{1}{\|r\|} \{||r||^2 - r^*AK_s(r,A) \\ &\quad \cdot [(AK_s(r,A))^*(AK_s(r,A))]^{-1}(AK_s(r,A))^*r\}^{1/2}\end{aligned}$$

and let

$$\varphi_s(A) = \min_{P_s(0)=1} ||P_s(A)|| = \min_{P_s(0)=1} \max_{v\neq 0} \frac{||P_s(A)v||}{||v||}.$$

We will say a matrix A is *s-definite* if $\psi_s(A) < 1$. One can show (see [11]) that s-definiteness is a necessary and sufficient condition for a restarted method such as GMRES(s) to converge (i.e., not stagnate) for all $r^{(0)}$.

We note that for any n and A:

$$\psi_n(A) = \max_{v\neq 0} \min_{P_n(0)=1} \frac{||P_n(A)v||}{||v||} \leq \max_{v\neq 0} \min_{P_n(0)=1} ||P_n(A)|| = \varphi_n(A)$$

Thus GMRES(s) satisfies

$$\frac{||r^{(ms+s)}||}{||r^{(ms)}||} \leq \psi_s(A) \leq \varphi_s(A).$$

Also, $\varphi_s(A) \leq \text{cond}(P) \cdot \varphi_s(J)$, where $A = PJP^{-1}$ is a Jordan decomposition. It is known from complex analysis that for arbitrary nonsingular diagonal J, $\varphi_s(J)$ may be made arbitrarily small by s sufficiently large. Thus a bound may be established for GMRES(s) implying convergence for s sufficiently large, whenever A is diagonalizable. Computable and sharp bounds are still needed.

4.2 Balanced SKPM's: Generalized Minimal Error Methods

As a further class of BSKPM's, we now consider a class of generalizations of the minimal error method of [7] and [6]. Given B, let $A^\dagger$ be the B-adjoint of A. We define the iteration

$$u^{(n)} - u^{(0)} \in A^\dagger \mathbf{K}_n(r^{(0)}, A), \qquad e^{(n)} \perp B^*A^\dagger \mathbf{K}_n(r^{(0)}, A).$$

THE MINIMAL ERROR METHOD

$$p^{(0)} = Ar^{(0)},$$

$$p^{(n)} = Ap^{(n-1)} + \beta_{n,n-1}p^{(n-1)} + \beta_{n,n-2}p^{(n-2)},$$

$$\beta_{n,i} = -\frac{p^{(i)*}Ap^{(n-1)}}{p^{(i)*}p^{(i)}},$$

$$\begin{aligned} u^{(n+1)} &= u^{(n)} + \hat{\lambda}_n p^{(n)}, \\ r^{(n+1)} &= r^{(n)} - \hat{\lambda}_n Ap^{(n)}, \end{aligned}$$

$$\hat{\lambda}_n = \begin{cases} r^{(0)*}r^{(0)} \,/\, p^{(0)*}p^{(0)}, & n = 0, \\ p^{(n-1)*}r^{(n)} \,/\, p^{(n)*}p^{(n)}, & \text{else.} \end{cases}$$

Figure 10.5

This defines a balanced projection method with $\mathbf{R}_n = A^{\dagger}\mathbf{K}_n(r^{(0)}, A)$. If, furthermore, A is B-normal(1), we have a BSKPM and the method has a three-term Orthodir-like recurrence. It will be further noted that we also have a computable method in the case when $B = I$. If $A = A^*$, we obtain Fridman's minimal error method (Fig. 10.5).

For $A = A^*$ this method has the benefit of minimizing the 2-norm of the error $e^{(n)}$, which is useful when A is ill-conditioned or indefinite. However, convergence is hindered by numerical problems as well as the fact that $\mathbf{R}_n$ is not the entire Krylov space $\mathbf{K}_{n+1}(r^{(0)}, A)$; in fact, $r^{(n)} = P_{n+1}(A)r^{(0)}$ where $P_{n+1}(0) = 1$ and $P'_{n+1}(0) = 0$ (see [11]).

5 Non-polynomial Projection Methods

The class of methods we have herein called "projection methods" includes methods which are not, strictly speaking, polynomial methods. One example is the block conjugate gradient method [14] for which A is HPD and:

$$u^{(n)} - u^{(0)} \in \text{span} \bigcup_{i=1}^{k} \mathbf{K}_n(r_i^{(0)}, A), \qquad e^{(n)} \perp \text{span} \bigcup_{i=1}^{k} A^*\mathbf{K}_n(r_i^{(0)}, A)$$

for some set of vectors $\{r_i^{(0)}\}$, where $r_\ell^{(0)} = r^{(0)}$ for some ℓ.

The methods USYMLQ and USYMQR [18] are also non-polynomial projection methods. These methods are defined respectively by

$$u^{(n)} - u^{(0)} \in \tilde{\mathbf{K}}_n(r^{(0)}, A^*), \qquad e^{(n)} \perp A^*\tilde{\mathbf{K}}_n(r^{(0)}, A),$$

THE CGS METHOD

$$
\begin{aligned}
p^{(0)} &= f^{(0)} = r^{(0)} \\
u^{(n+1)} &= u^{(n)} + \lambda_n (f^{(n)} + h^{(n+1)}) \\
r^{(n+1)} &= r^{(n)} - \lambda_n A (f^{(n)} + h^{(n+1)}) \\
h^{(n+1)} &= f^{(n)} - \lambda_n A p^{(n)} \\
f^{(n+1)} &= r^{(n+1)} + \alpha_{n+1} h^{(n+1)} \\
p^{(n+1)} &= f^{(n+1)} + \alpha_{n+1} (h^{(n+1)} + \alpha_{n+1} p^{(n)}) \\
\lambda_n &= \frac{\tilde{r}^{(0)*} r^{(n)}}{\tilde{r}^{(0)*} A p^{(n)}}, \qquad \alpha_{n+1} = \frac{\tilde{r}^{(0)*} r^{(n+1)}}{\tilde{r}^{(0)*} r^{(n)}}.
\end{aligned}
$$

Figure 10.6

$$u^{(n)} - u^{(0)} \in \tilde{\mathbf{K}}_n(r^{(0)}, A^*), \qquad e^{(n)} \perp A^* A \tilde{\mathbf{K}}_n(r^{(0)}, A^*).$$

Here $\tilde{\mathbf{K}}_n$ indicates the quasi-Krylov space given as the linear span of the n vectors

$$\tilde{\mathbf{K}}_n(v, A) = \text{span}\{v, Av, AA^*v, AA^*Av, \ldots\}.$$

These methods are not in general based on a Krylov space. They do, on the other hand, possess an economical 3-term recurrence. The USYMQR method is a balanced projection method with $B = A^*A$ HPD, thus minimizing the 2-norm of the residual. The USYMLQ method can break down, however. For A not nearly Hermitian, these methods in practice appear to perform comparably to the normal equations.

6 Non-projection Polynomial Methods

Finally, we give an example of a conjugate gradient-like polynomial method which is not known to fit into the above setting of projection methods: the conjugate gradient squared (CGS) method of [19] (Fig. 10.6). This method is closely related to the BCG method: in particular, if the BCG residuals are given by

$$r^{(n)} = r^{(n)}_{BCG} = P_n(A) r^{(0)},$$

then the CGS residuals are given by

$$r^{(n)} = r^{(n)}_{CGS} = (P_n(A))^2 r^{(0)}.$$

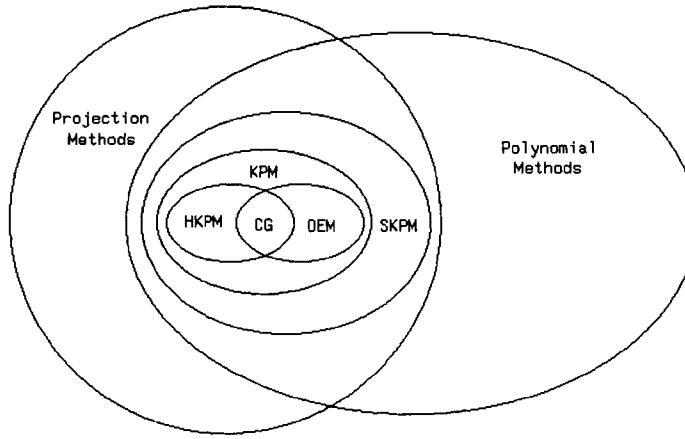

Figure 10.7 The landscape of iterative solvers.

Thus if $P_n(A)$ is a contraction, then its square is even more so; on the other hand, if $P_n(A)$ amplifies the error, as can happen in near-breakdown situations, the square can be even worse. In short, the CGS method shares a number of the convergence properties of the BCG method.

7 Conclusion

In this paper, we have suggested a structure for classifying and analyzing conjugate gradient-like iterative methods. The structure we have presented involves an "onion" of increasingly strong hypotheses. (See Fig. 10.7 for the landscape of iterative solvers.) The strengthening of these assumptions on the method, including the imposition of stronger properties on the generalized inner product matrix B, brings forth attractive features from the methods, such as assured convergence, minimization properties and error bounds. However, stronger assumptions also limit the domain of applicability of the methods to increasingly more specialized A. Further research is needed in order to study the implications of relaxing each of the assumptions, in the hope of better understanding the convergence properties of known and new methods. Further discussion of these issues may be found in [11].

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