A THEORETICAL OVERVIEW OF KRYLOV SUBSPACE METHODS

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Abstract. We survey Krylov subspace methods for the solution of linear systems with focus on commonly used and recently developed methods. The approach is theoretical and complementary to the engineering-based first article of this special issue. In particular convergence results are derived from a general theoretical framework, compiled and analyzed.

1. Background.

The purpose of this paper is to survey properties of commonly used and recently developed iterative methods for the solution of the linear system

$$Ax = b. \tag{1}$$

The matrix A is a real square matrix of dimension n, i. e. $A \in \mathbb{R}^{n\times n}$, and $x, b \in \mathbb{R}^n$. In general the matrix A is nonsymmetric and not positive definite.

There are many survey articles and books for modern iterative solvers. We confine us to name only a few recently published articles. An overview of generalized CG methods is given by Freund, Golub and Nachtigal [20]. Ashby, Manteuffel and Saylor [1] deliver a taxonomy. Many methods are analyzed by Barret, Berry, Chan, Demmel, Donato, Dongarra, Eijkhout, Pozo, Romine and van der Vorst. Their book is called templates [4] because they give recipes when a particular solver should be used. We also refer to the work of Axelsson [2], Gutknecht [28] and Joubert and Manteuffel in [33]. Meier Yang examines many methods in connection with incomplete LU preconditioning [36]. Historical overviews give Young [60] and Golub and O'Leary [24].

2. Iterative Methods.

We focus on parameter-free methods for practical applications, i. e. methods where no parameters depending on the inner properties of the matrix have to be estimated apriori. We give a definition that includes most of the modern iterative methods. In particular generalized CG methods [1, 3, 14, 15, 20, 27, 30, 31, 48, 53], error-minimizing methods [23, 54], conjugate Krylov subspace methods [55] and the (k,l)-step methods introduced by Gutknecht [26] fit into this class.

We use the following notations: A real matrix Z is called positive if the symmetric part is positive definite. Let Z be a positive real matrix, then the norm $||y||_Z$ of any vector $y \in \mathbb{R}^n$ is defined by $||y||_Z = \sqrt{y^T Z y}$. If Z is not positive real, then $||y||_Z^2$ is a mnemonic abbreviation for $y^T Z y$. $||y||$ is the Euclidean norm.

Definition 2.1. *Let x_0 be any initial guess and $r_0 = Ax_0 - b$ the starting residual. The following recurrence is called an orthogonalization method. For $k \geq 1$ let*

$$x_k \in \tilde{x}_k + span(q_{k-\sigma_k,k}, \ldots, q_{k-1,k}) \tag{2}$$

with $q_{k-i,k} \in \mathbb{R}^n$ and $\tilde{x}_k \in span(x_{k-\sigma_k}, \ldots, x_{k-1})$. Calculate the approximations so that the orthogonality condition

$$r_k^T Z_k q_{k-i,k} = 0 \tag{3}$$

is satisfied for $i = 1, \ldots, \sigma_k$. Z_k *are auxiliary, non-singular matrices. The method is called*

- *exact if* $\sigma_k = k$, *i. e.* k $q_{k-i,k}$ *are used for the calculation of the new iterate,*
- *restarted if* $\sigma_k = (k-1)$ *mod* σ_{res} $+1$, *i. e. a restart is made periodically after* σ_{res} *steps,*
- *truncated if* $\sigma_k = min(k, \sigma_{max})$ *with* σ_{max} *fixed, i. e. only* σ_{max} $q_{k-i,k}$ *are used for the calculation of the new iterate,*
- *combined if the truncated method is restarted,* *i. e.* $\sigma_k = min\left((k-1) \text{ mod } \sigma_{res} + 1, \sigma_{max}\right)$.

Let us introduce the abbreviations:

$$\tilde{r}_k = A\tilde{x}_k - b, \tag{4}$$
$$\tilde{e}_k = \tilde{x}_k - x. \tag{5}$$

It is quite clear that the approximations can be represented as

$$x_k = \sum_{i=1}^{\sigma_k} \gamma_{i,k} q_{k-i,k} + \tilde{x}_k. \tag{6}$$

The residuals and errors can be expressed as follows

$$r_k = \sum_{i=1}^{\sigma_k} \gamma_{i,k} A q_{k-i,k} + \tilde{r}_k, \tag{7}$$
$$e_k = \sum_{i=1}^{\sigma_k} \gamma_{i,k} q_{k-i,k} + \tilde{e}_k. \tag{8}$$

From (7) and (3) follows directly that the $\gamma_{i,k}$ can be determined from the solution of the linear system of dimension σ_k

$$\sum_{i=1}^{\sigma_k} \gamma_{i,k} q_{k-i,k}^T A^T Z_k q_{k-j,k} = -\tilde{r}_k^T Z_k q_{k-j,k}, \tag{9}$$

for $j = 1, \ldots, \sigma_k$.

As the choice of the $q_{k-i,k}$ is arbitrary the definition covers in fact many of the commonly used iterative methods. The methods distinguish by $q_{k-i,k}$, Z_k, σ_k and $\tilde{x}_k$ and can be easily classified by indicating these quantities. Note that Z_k is not unique. If Z_k fulfils (3), then any $\tilde{Z}_k$ fulfils (3) as well, where r_k is in the kernel of $(\tilde{Z}_k - Z_k)^T$. Despite the generality of the definition the following convergence result [56] can be proven.

THEOREM 2.2. *If* $Z_k A^{-1}$ *is positive real, i. e. the symmetric part of* $Z_k A^{-1}$ *is positive definite, then*

$$\|r_k\|_{Z_k A^{-1}} \leq \sqrt{1 + \frac{\rho^2(R)}{\mu_m(M)^2}} \min_{\eta_1, \ldots, \eta_{\sigma_k}} \left\| \sum_{i=1}^{\sigma_k} \eta_i A q_{k-i,k} + \tilde{r}_k \right\|_{Z_k A^{-1}}, \tag{10}$$
$$\|e_k\|_{A^T Z_k} \leq \sqrt{1 + \frac{\rho^2(R)}{\mu_m(M)^2}} \min_{\eta_1, \ldots, \eta_{\sigma_k}} \left\| \sum_{i=1}^{\sigma_k} \eta_i q_{k-i,k} + \tilde{e}_k \right\|_{A^T Z_k} \tag{11}$$

holds for orthogonalization methods. $\rho(R)$ is the spectral radius of the skew-symmetric part R of Z_kA^{-1}. $\mu_m(M)$ is the minimum eigenvalue of M, the symmetric part of Z_kA^{-1}. In particular if Z_kA^{-1} is symmetric, then

$$\|r_k\|_{Z_kA^{-1}} = \min_{\eta_1,\ldots,\eta_{\sigma_k}} \left\| \sum_{i=1}^{\sigma_k} \eta_i A q_{k-i,k} + \tilde{r}_k \right\|_{Z_kA^{-1}}, \tag{12}$$

$$\|e_k\|_{A^TZ_k} = \min_{\eta_1,\ldots,\eta_{\sigma_k}} \left\| \sum_{i=1}^{\sigma_k} \eta_i q_{k-i,k} + \tilde{e}_k \right\|_{A^TZ_k}. \tag{13}$$

This theorem is a generalization of the convergence results for generalized CG methods [53]. From this theorem follow the convergence investigations for conjugate Krylov subspace methods [55] and generalized minimum error methods [54]. From Theorem 2.2 follows immediately that the exact solution of the linear system is obtained at least in the iteration step n if the method is exact and the $q_{k-i,k}$ are linear independent because the whole space is spanned and the right-hand side of (11) is zero. Thus exact methods converge theoretically. The convergence of the restarted version is not guaranteed even if Z_kA^{-1} is positive real, because the right-hand side of the inequalities does not necessarily tend to zero. The same holds for truncated versions.

The most popular orthogonalization methods are *Krylov subspace methods.* The reason is that they are based on matrix-vector multiplications. Krylov subspace methods are orthogonalization methods with

$$q_{k-i,k} \in K_{k-i}(B,z) = span(z, Bz, \ldots, B^{k-i}z) \tag{14}$$

and

$$\tilde{x}_k = x_{k-\sigma_k}, \tag{15}$$

where $B \in \mathbb{R}^{n\times n}$ and $z \in \mathbb{R}^n$. If $B \neq A$, then in each iteration step two matrix-vector multiplications have to be performed, one by B to determine $q_{k-i,k}$ and one by A to calculate the residual r_k. If $B = A$, then in general one matrix-vector multiplication per iteration is sufficient.

3. Conjugate Krylov subspace methods (CKS).

Conjugate Krylov subspace methods (CKS) [55] are Krylov subspace methods with

$$B = A\ , \tag{16}$$

$$z = r_0\ . \tag{17}$$

Thus

$$q_{k-i,k} \in K_{k-i}(A, r_0)\ . \tag{18}$$

By (16) CKS methods can be formulated so that only one matrix-vector multiplication is needed per iteration step.

It is quite obvious that

$$x_k \in x_0 + K_{k-1}(A, r_0), \tag{19}$$

$$r_k \in r_0 + AK_{k-1}(A, r_0), \tag{20}$$

$$e_k \in e_0 + AK_{k-1}(A, e_0). \tag{21}$$

Thus

$$x_k = \sum_{i=1}^{k} \beta_{i,k} A^{i-1} r_0 + x_0 = \sum_{i=1}^{k} \eta_{i,k} r_{i-1} + x_0 \ . \tag{22}$$

For exact CKS methods we can consider the substitution

$$q_{k-i,k} \rightarrow r_{k-i} \ , \tag{23}$$

or

$$q_{k-i,k} \rightarrow A^{k-i} r_0 \ , \tag{24}$$

then the condition (3) is equivalent to

$$r_k^T Z_k r_{k-i} = 0 \ , \tag{25}$$

$$r_k^T Z_k A^{k-i} r_0 = 0 \ , \tag{26}$$

respectively, for $i = 1, \dots, k$.

A similar approach was introduced by Barth and Manteuffel [6], called variable metric conjugate gradient methods. In this approach the matrices Z_k do not depend on the iteration step but on the initial guess.

Generalized conjugate gradient (CG) methods are the subset of CKS methods with

$$Z_k = Z = const. \tag{27}$$

The method of steepest descent [49] and the classical CG method [30] are the origin of generalized CG methods. These two methods are suited for matrices that are diagonally dominant or symmetric and positive definite. Of course the methods can also be applied to other systems, but the convergence is not guaranteed or may be very slow. Starting from the 1970s the classical CG method has been generalized in order to obtain convergence techniques for non-symmetric and non-positive definite systems. A whole family of methods results from this generalization; see e. g. [3, 15, 20, 27, 30, 48]. For practical problems it is important that generalized CG methods can be formulated with a short recurrence if

$$A^T Z = ZA. \tag{28}$$

3.1. The Lanczos connection.

In 1950, Lanczos introduced a method for the successive transformation of a given matrix to a tridiagonal matrix [34]. The purpose was to calculate the eigenvalues by a successive procedure. This algorithm was reformulated by Lanczos himself [35] and later by Fletcher [16] for the solution of linear systems. If we apply the nonsymmetric Lanczos process to the Krylov spaces generated by A applied to r_0 and A^T applied to r_0^*, then the algorithm constructs the two vector sequences v_k and w_k with

$$span(v_0, \dots, v_k) = K_k(A, r_0), \tag{29}$$

$$span(w_0, \dots, w_k) = K_k(A^T, r_0^*), \tag{30}$$

and

$$w_i^T v_j \ = \ \begin{cases} 0 \ for \ i \neq j \\ d_i \ for \ i = j \end{cases} \tag{31}$$

for $i, j = 0, \ldots, k$. If we start with $\bar{v}_0 = r_0$, $\bar{w}_0 = r_0^*$, $v_0 = \frac{\bar{v}_0}{\eta_0}$, $w_0 = \frac{\bar{w}_0}{\mu_0}$, then the vectors can be calculated by a 3-term recurrence for $k \geq 2$

$$\bar{v}_k = Av_{k-1} - \alpha_k v_{k-1} - \beta_k v_{k-2}, \tag{32}$$

$$\bar{w}_k = A^T w_{k-1} - \alpha_k w_{k-1} - \gamma_k w_{k-2}, \tag{33}$$

$$v_k = \frac{1}{\eta_k}\bar{v}_k, \tag{34}$$

$$w_k = \frac{1}{\mu_k}\bar{w}_k. \tag{35}$$

For $k = 1$ use the same formulas but omit the terms with β_1 and γ_1. Here the coefficients are determined from (31)

$$\alpha_k = \frac{w_{k-1}^T A v_{k-1}}{w_{k-1}^T v_{k-1}}, \tag{36}$$

$$\beta_k = \frac{w_{k-2}^T A v_{k-1}}{w_{k-2}^T v_{k-2}}, \tag{37}$$

$$\gamma_k = \frac{v_{k-2}^T A^T w_{k-1}}{v_{k-2}^T w_{k-2}}. \tag{38}$$

η_k and μ_k can still be freely chosen resulting in different scalings of the vectors v_k and w_k. In general

$$\eta_k = \frac{1}{||\bar{v}_k||}, \tag{39}$$

resulting in

$$||v_k|| = 1. \tag{40}$$

The algorithms break down if $\bar{w}_k^T \bar{v}_k = 0$ because then a division by zero occurs in (34), (35), (36), (37) or (38), depending on the choice of η_k and μ_k. Remedies to avoid breakdowns were proposed by Parlett, Taylor and Liu [38]. They are based on so called look-ahead strategies. These strategies were investigated by Gutknecht [27], Brezinski, Redivo-Zaglia and Sadok [7, 8, 9], by Freund, Gutknecht and Nachtigal [21] and by many others, see also [58].

If A is symmetric, then the two sequences v_k and w_k coincide for $r_0^* = r_0$, resulting in the symmetric Lanczos process that requires the half of operations and storage. It is equivalent to the Arnoldi process.

Let us introduce the matrices

$$V_k = (v_0, \ldots, v_k) \in I\!R^{n\times(k+1)}, \tag{41}$$

$$W_k = (w_0, \ldots, w_k) \in I\!R^{n\times(k+1)}, \tag{42}$$

and the tridiagonal Hessenberg matrices $H_k, \tilde{H}_k \in \mathbb{R}^{(k+2)\times(k+1)}$:

$$(43) \qquad H_k = \begin{pmatrix} \alpha_1 & \beta_2 & 0 & \dots & \dots & \dots & 0 \\ \eta_1 & \alpha_2 & \beta_3 & 0 & & & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & 0 & \eta_{k-2} & \alpha_{k-1} & \beta_k & 0 \\ \vdots & & & 0 & \eta_{k-1} & \alpha_k & \beta_{k+1} \\ \vdots & & & & 0 & \eta_k & \alpha_{k+1} \\ 0 & \dots & \dots & \dots & \dots & 0 & \eta_{k+1} \end{pmatrix},$$

$$(44) \qquad \tilde{H}_k = \begin{pmatrix} \alpha_1 & \gamma_2 & 0 & \dots & \dots & \dots & 0 \\ \mu_1 & \alpha_2 & \gamma_3 & 0 & & & \vdots \\ 0 & \ddots & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & 0 & \mu_{k-2} & \alpha_{k-1} & \gamma_k & 0 \\ \vdots & & & 0 & \mu_{k-1} & \alpha_k & \gamma_{k+1} \\ \vdots & & & & 0 & \mu_k & \alpha_{k+1} \\ 0 & \dots & \dots & \dots & \dots & 0 & \mu_{k+1} \end{pmatrix}.$$

The equations (32) - (35) can be reformulated as

$$(45) \qquad AV_k = V_{k+1}H_k,$$

$$(46) \qquad A^TW_k = W_{k+1}\tilde{H}_k.$$

Equation (31) is equivalent to

$$(47) \qquad W_k^TV_k = D_k,$$

where

$$(48) \qquad D_k = diag(d_0, \dots, d_k).$$

We obtain by (40)

$$(49) \qquad \|V_k\| \leq \sqrt{k+1}.$$

From (19) - (21) follows for any CKS that

$$(50) \qquad x_k = x_0 + V_{k-1}\bar{z}_k,$$

$$(51) \qquad r_k = r_0 + AV_{k-1}\bar{z}_k = r_0 + V_kH_{k-1}\bar{z}_k = V_k(\eta_0\bar{u}_1^{k+1} + H_{k-1}\bar{z}_k),$$

$$(52) \qquad e_k = e_0 + AV_{k-1}\bar{z}_k = e_0 + V_kH_{k-1}\bar{z}_k,$$

where $\bar{z} \in \mathbb{R}^k$ and $\bar{u}_1^{k+1}$ is the first unit vector in $\mathbb{R}^{k+1}$. Note that for $i = 0, \dots, k$

$$\begin{aligned} r_{k-i} &= r_0 + AV_{k-i-1}\bar{z}_{k-i} = V_{k-i}(\eta_0\bar{u}_1^{k+1-i} + H_{k-i-1}\bar{z}_{k-i}) \\ (53) \qquad &= r_0 + AV_{k-1}z_{k-i} = V_k(\eta_0u_1 + H_{k-1}z_{k-i}) \end{aligned}$$

where $z_{k-i} = (\bar{z}_{k-i}^T, 0, \ldots, 0)^T \in I\!R^k$ and $u_1 = \bar{u}_1^{k+1}$ is the first unit vector in $I\!R^{k+1}$. Thus the orthogonality relation (25) is transformed for exact CKS's to

$$(\eta_0 u_1 + H_{k-1} z_k)^T V_k^T Z_k V_k (\eta_0 u_1 + H_{k-1} z_{k-i}) = 0 \tag{54}$$

for $i = 1, \ldots, k$. The components of z_k can be calculated by the solution of the linear system (54). As the vectors w_k are not needed explicitely for the calculation of x_k and r_k they are called shadow vectors.

Similarly to the above described orthogonal Lanczos process we introduce the conjugate Lanczos process. This algorithm constructs two vector sequences spanning the spaces in (29) and (30) with

$$[W_k^*]^T A V_k^* \quad = \quad D_k^*, \tag{55}$$

where V_k^* and W_k^* are defined accordingly to (41) and (42) and D_k^* is a diagonal matrix. We can introduce similarly to the orthogonal Lanczos process the tridiagonal Hessenberg matrices $H_k^*, \tilde{H}_k^*$ and we obtain (45) and (46) for these $*$-quantities. Moreover, we can express the iterates, residuals and errors as in (50), (51) and (52) by using V_k^* instead of V_k and H_k^* instead of H_k.

For exact CKS methods we can consider the substitution

$$q_{k-i,k} \longrightarrow v_{k-i} \ , \tag{56}$$

or

$$q_{k-i,k} \longrightarrow v_{k-i}^* \ , \tag{57}$$

then the condition (3) is equivalent to

$$r_k^T Z_k v_{k-i} = 0 \ , \tag{58}$$

$$r_k^T Z_k v_{k-i}^* = 0 \ , \tag{59}$$

respectively, for $i = 1, \ldots, k$.

3.2. Convergence Properties.

The convergence behavior of CKS methods can be investigated by applying Theorem 2.2, see also [53]. Simply substitute $Aq_{k-i,k}$ by $A^i r_0$ and $\tilde{r}_k$ by r_0 in (10) and (12), $q_{k-i,k}$ by $A^i e_0$ and $\tilde{e}_k$ by e_0 in (11) and (13). CKS methods describe CG methods as special case, where $Z_k = Z = const$. Thus the analysis is also valid for generalized CG. The convergenge behavior can be estimated more specificly.

THEOREM 3.1. *Let $Z_k A^{-1}$ be positive real, $\rho(R)$ be the spectral radius of the skew-symmetric part R of $Z_k A^{-1}$. Let $\mu_m(M)$ be the minimum eigenvalue of M, the symmetric part of $Z_k A^{-1}$. Let S be the square root of M and T the square root of the symmetric part of $A^T Z_k$, $\kappa(S)$, $\kappa(T)$ their condition numbers, then the following inequalities are satisfied for exact CKS methods.*

$$||r_k|| \ \leq \ \sqrt{1 + \frac{\rho^2(R)}{\mu_m^2(M)}}\ \kappa(S) \min_{\theta_1,\ldots,\theta_k} ||\sum_{i=1}^{k} \theta_i A^i + I||\ ||r_0||, \tag{60}$$

$$||e_k|| \ \leq \ \sqrt{1 + \frac{\rho^2(R)}{\mu_m^2(M)}}\ \kappa(T) \min_{\theta_1,\ldots,\theta_k} ||\sum_{i=1}^{k} \theta_i A^i + I||\ ||e_0||. \tag{61}$$

Let J be the Jordan canonical form of A, i. e. $A = C^{-1}JC$ with a non-singular C, then

$$(62) \qquad ||r_k|| \;\le\; \sqrt{1+\frac{\rho^2(R)}{\mu_m^2(M)}}\;\kappa(C)\;\kappa(S)\min_{\theta_1,\dots,\theta_k}||\sum_{i=1}^{k}\theta_i J^i + I||\;||r_0||,$$

$$(63) \qquad ||e_k|| \;\le\; \sqrt{1+\frac{\rho^2(R)}{\mu_m^2(M)}}\;\kappa(C)\;\kappa(T)\min_{\theta_1,\dots,\theta_k}||\sum_{i=1}^{k}\theta_i J^i + I||\;||e_0||,$$

where $\kappa(C)$ is the condition number of C. If A is similar to the diagonal matrix D, i. e. $A = C^{-1}DC$ with a non-singular C, then

$$(64) \qquad ||r_k|| \;\le\; \sqrt{1+\frac{\rho^2(R)}{\mu_m^2(M)}}\;\kappa(C)\;\kappa(S)\min_{\theta_1,\dots,\theta_k}\max_{\lambda}|\sum_{i=1}^{k}\theta_i\lambda^i + 1|\;||r_0||,$$

$$(65) \qquad ||e_k|| \;\le\; \sqrt{1+\frac{\rho^2(R)}{\mu_m^2(A)}}\;\kappa(C)\;\kappa(T)\min_{\theta_1,\dots,\theta_k}\max_{\lambda}|\sum_{i=1}^{k}\theta_i\lambda^i + 1|\;||e_0||,$$

where λ is an eigenvalue of A. If A is normal, then

$$(66) \qquad ||r_k|| \;\le\; \sqrt{1+\frac{\rho^2(R)}{\mu_m^2(M)}}\;\kappa(S)\min_{\theta_1,\dots,\theta_k}\max_{\lambda}|\sum_{i=1}^{k}\theta_i\lambda^i + 1|\;||r_0||,$$

$$(67) \qquad ||e_k|| \;\le\; \sqrt{1+\frac{\rho^2(R)}{\mu_m^2(M)}}\;\kappa(T)\min_{\theta_1,\dots,\theta_k}\max_{\lambda}|\sum_{i=1}^{k}\theta_i\lambda^i + 1|\;||e_0||.$$

Proof. See for example [53] and [55]. □

From theorem 3.1 follows directly that for normal matrices , i. e. $AA^T = A^TA$, with a small symmetric part and a small condition number of S, the convergence is depending on the eigenvalue distribution of A. For clustered eigenvalues the convergence is fast, while for scattered eigenvalues the convergence may be very slow. There are more detailed investigations of the convergence for generalized CG methods, i. e. for methods with $Z_k = Z = const$ based on the eigenvalue distribution, see [2]. For nonnormal matrices the factor

$$\sqrt{1+\frac{\rho^2(R)}{\mu_m^2(M)}}\;\kappa(C)\;\kappa(S)$$

may be so large that even for a fast decrease of the norms in (60) or (61), respectively, the upper bound is as large as $||r_0||$ or $||e_0||$ until the iteration step n. There is an excellent investigation by Greenbaum and Strakoš [25] showing that arbitrary eigenvalue distributions of A can generate any convergence behavior of GMRES. Thus for nonnormal matrices the convergence does not depend exclusively on the eigenvalues.

We can apply theorem 2.2 to CKS methods by using the representation of the Lanczos process.

Corollary 3.2. *If Z_kA^{-1} is positive real, then*

$$(68) \qquad ||r_k||_{Z_kA^{-1}} \;\le\; \sqrt{1+\frac{\rho^2(R)}{\mu_m^2(M)}}\min_{z_k\in I\!R^k}||r_0 + AV'_{k-1}z_k||_{Z_kA^{-1}}\;,$$

$$(69) \qquad ||e_k||_{A^TZ_k} \;\le\; \sqrt{1+\frac{\rho^2(R)}{\mu_m^2(M)}}\min_{z_k\in I\!R^k}||e_0 + V'_{k-1}z_k||_{A^TZ_k}$$

holds for exact CKS methods. $\rho(R)$ *is the spectral radius of the skew-symmetric part* R *of* $Z_k A^{-1}$. μ_m *is the minimum eigenvalue of* M, *the symmetric part of* $Z_k A^{-1}$. V'_{k-1} *is the matrix of the orthogonal Lanczos vectors (41), i. e.*

$$V'_{k-1} = V_{k-1}$$

or conjugate Lanczos vectors, i. e.

$$V'_{k-1} = V^*_{k-1}.$$

In particular if $Z_k A^{-1}$ *is symmetric, then*

$$||r_k||_{Z_k A^{-1}} = \min_{z_k \in \mathbb{R}^k} ||r_0 + AV'_{k-1} z_k||_{Z_k A^{-1}} \,, \tag{70}$$

$$||e_k||_{A^T Z_k} = \min_{z_k \in \mathbb{R}^k} ||e_0 + V'_{k-1} z_k||_{A^T Z_k}. \tag{71}$$

Proof. Apply Theorem 2.2 to CKS methods using (56) or (57). □

3.3. Special CKS methods.

In this section we will survey commonly used methods and derive the special convergence properties by applying Theorems 2.2 and 3.1 and Corollary 3.2. In addition we refer recently obtained convergence estimates.

3.3.1. Biconjugate Gradient-Based Methods.

BCG. The *biconjugate gradients* (BCG) are based on the Lanczos algorithm [16, 34]. BCG can be considered as CG method applied to a double system. This approach will be discussed later. Here we consider BCG as exact method using

$$Z = W^*[D^*]^{-T}\Omega^T\Omega[D^*]^{-1}[W^*]^T A, \tag{72}$$

where $W^* = W^*_{n-1} \in \mathbb{R}^{n\times n}$ is the matrix consisting of the shadow vectors and $D^* = D^*_{n-1} \in \mathbb{R}^{n\times n}$ is the diagonal matrix generated by the conjugate Lanczos process. $\Omega = diag(\omega_0, \ldots, \omega_{n-1}) \in \mathbb{R}^{n\times n}$ is an arbitrary diagonal matrix. This viewpoint was introduced by Barth and Manteuffel [6]. As ZA^{-1} is symmetric the following minimization properties can be derived from theorem 3.1.

$$\|r_k\| \le \kappa(\Omega[D^*]^{-1}[W^*]^T) \min_{\beta_1,\ldots,\beta_k} ||\sum_{i=1}^k \beta_i A^i r_0 + r_0||, \tag{73}$$

$$\|e_k\| \le \kappa(\Omega[D^*]^{-1}[W^*]^T A) \min_{\beta_1,\ldots,\beta_k} ||\sum_{i=1}^k \beta_i A^i e_0 + e_0||. \tag{74}$$

These results were also obtained by Barth and Manteuffel [6]. We can estimate the condition numbers because $\Omega[D^*]^{-1}[W^*]^T AV^*_{n-1}\Omega^{-1} = I$ by (55).

$$\kappa(\Omega[D^*]^{-1}[W^*]^T) = \kappa(AV^*_{n-1}\Omega^{-1}) \le \kappa(A)\kappa(V^*_{n-1})\kappa(\Omega), \tag{75}$$

$$\kappa(\Omega[D^*]^{-1}[W^*]^T A) = \kappa(V^*_{n-1}\Omega^{-1}) \le \kappa(V^*_{n-1})\kappa(\Omega). \tag{76}$$

Finally, if we choose $\Omega = I$ such that $\kappa(\Omega) = 1$, then

$$\|r_k\| \le \kappa(A)\ \kappa(V^*_{n-1}) \min_{\beta_1,\ldots,\beta_k} ||\sum_{i=1}^k \beta_i A^i r_0 + r_0||, \tag{77}$$

$$\|e_k\| \le \kappa(V^*_{n-1}) \min_{\beta_1,\ldots,\beta_k} ||\sum_{i=1}^k \beta_i A^i e_0 + e_0||. \tag{78}$$

Let us write the BCG residual in terms of the conjugate Lanczos process, where O_j is the zero vector in $\mathbb{R}^j$,

$$r_k = r_0 + AV_{n-1}^* \begin{pmatrix} z_k \\ O_{n-k} \end{pmatrix}, \tag{79}$$

then we get by Corollary 3.2

$$\begin{aligned}
&\|r_k\|^2_{W^*[D^*]^{-T}\Omega^T\Omega[D^*]^{-1}[W^*]^T} \\
&= \min_{z_k \in \mathbb{R}^k} \left\| r_0 + AV_{n-1}^* \begin{pmatrix} z_k \\ O_{n-k} \end{pmatrix} \right\|^2_{W^*[D^*]^{-T}\Omega^T\Omega[D^*]^{-1}[W^*]^T} \\
&= \min_{z_k \in \mathbb{R}^k} \left\| \Omega[D^*]^{-1}[W^*]^T \left(r_0 + AV_{n-1}^* \begin{pmatrix} z_k \\ O_{n-k} \end{pmatrix} \right) \right\|^2 \\
&= \min_{z_k \in \mathbb{R}^k} \left\| \Omega[D^*]^{-1}[W^*]^T r_0 + \Omega \begin{pmatrix} z_k \\ O_{n-k} \end{pmatrix} \right\|^2 \\
&\mathit{by}\ (55) \\
&= \left\| \begin{pmatrix} O_k \\ \omega_k d_k^{-1}[w_k^*]^T r_0 \\ \vdots \\ \omega_{n-1} d_{n-1}^{-1}[w_{n-1}^*]^T r_0 \end{pmatrix} \right\|^2 \\
&= \sum_{i=k}^{n-1} (\omega_i d_i^{-1}[w_i^*]^T r_0)^2.
\end{aligned}$$

BCG produces component by component zeros in the vector $\Omega[D^*]^{-1}[W^*]^T r_0$. This result is of its own interest.

The algorithm can be formulated with a short recurrence. To show this the formulation of BCG with the double system is quite more elegant. Let us consider the system

$$\hat{A}\hat{x} = \hat{b}, \tag{80}$$

where

$$\hat{A} = \begin{pmatrix} A & 0 \\ 0 & A^T \end{pmatrix}, \hat{x} = \begin{pmatrix} x \\ x^* \end{pmatrix}, \hat{b} = \begin{pmatrix} b \\ b^* \end{pmatrix}. \tag{81}$$

b^* is arbitrary. The residuals have the form

$$\hat{r}_k \; = \; \begin{pmatrix} r_k \\ r_k^* \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & A^T \end{pmatrix} \begin{pmatrix} x_k \\ x_k^* \end{pmatrix} - \begin{pmatrix} b \\ b^* \end{pmatrix} = \begin{pmatrix} Ax_k - b \\ A^T x_k^* - b^* \end{pmatrix}. \tag{82}$$

The errors are

$$\hat{e}_k = \begin{pmatrix} e_k \\ e_k^* \end{pmatrix} = \begin{pmatrix} x_k - x \\ x_k^* - x^* \end{pmatrix}. \tag{83}$$

Choose

$$Z = Z_B = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}. \tag{84}$$

BCG can be formulated with a short recurrence because

$$\begin{aligned}\hat{A}^T Z_B &= \begin{pmatrix} A^T & 0 \\ 0 & A \end{pmatrix}\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} = \begin{pmatrix} 0 & A^T \\ A & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}\begin{pmatrix} A & 0 \\ 0 & A^T \end{pmatrix} = Z_B \hat{A}\end{aligned}$$

and (28) applies.

$$Z_B \hat{A}^{-1} = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}\begin{pmatrix} A^{-1} & 0 \\ 0 & A^{-T} \end{pmatrix} = \begin{pmatrix} 0 & A^{-T} \\ A^{-1} & 0 \end{pmatrix}$$

is symmetric, but indefinite so that Theorem 3.1 cannot be applied. However, we can prove a similar result.

$$(85) \qquad \|\hat{r}_k\|^2_{Z_B\hat{A}^{-1}} = \begin{pmatrix} r_k \\ r_k^* \end{pmatrix}^T \begin{pmatrix} 0 & A^{-T} \\ A^{-1} & 0 \end{pmatrix}\begin{pmatrix} r_k \\ r_k^* \end{pmatrix} = 2(r_k^*)^T A^{-1} r_k.$$

Moreover,

$$\|\hat{r}_k\|^2_{Z_B\hat{A}^{-1}} = \hat{r}_k^T Z_B \hat{A}^{-1}\Phi_k(\hat{A})\hat{r}_0$$

for any matrix polynomial

$$\Phi_k(\hat{A}) = \sum_{i=1}^{k} \beta_i \hat{A}^i + I;$$

see for example [55]. Let Π_k be the polynomial with $r_k = \Pi_k(A)r_0$ and $r_k^* = \Pi_k(A^T)r_0^*$, then

$$\begin{aligned}\|\hat{r}_k\|^2_{Z_B\hat{A}^{-1}} &= \begin{pmatrix} r_k \\ r_k^* \end{pmatrix}^T \begin{pmatrix} 0 & A^{-T} \\ A^{-1} & 0 \end{pmatrix}\begin{pmatrix} \Phi_k(A)r_0 \\ \Phi_k(A^T)r_0^* \end{pmatrix} \\ &= r_k^T A^{-T}\Phi_k(A^T)r_0^* + (r_k^*)^T A^{-1}\Phi_k(A)r_0 \\ &= r_0^T \Pi_k(A^T)A^{-T}\Phi_k(A^T)r_0^* + (r_k^*)^T A^{-1}\Phi_k(A)r_0 \\ &= r_0^T \Phi_k(A^T)A^{-T}\Pi_k(A^T)r_0^* + (r_k^*)^T A^{-1}\Phi_k(A)r_0 \\ &= (r_0^*)^T \Pi_k(A)A^{-1}\Phi_k(A)r_0 + (r_k^*)^T A^{-1}\Phi_k(A)r_0 \\ &= 2(r_k^*)^T A^{-1}\Phi_k(A)r_0.\end{aligned}$$

Putting this result together with (85), taking moduli and choosing Φ_k accordingly finally leads to

$$(86) \qquad \left|(r_k^*)^T A^{-1} r_k\right| = \min_{\Phi_k} \left|(r_k^*)^T A^{-1}\Phi_k(A)r_0\right|,$$

$$(87) \qquad \left|(e_k^*)^T A e_k\right| = \min_{\Phi_k} \left|(e_k^*)^T A\Phi_k(A)e_0\right|,$$

respectively.

The algorithm produces highly oscillating residuals. Equation (87) does not guarantee that $e_k \to 0$. In particular $\left|(e_k^*)^T A e_k\right| = 0$ is possible without $e_k = 0$. The equations (86) and (87) can be considered as weak formulation of a minimization property. The method may break down. In this case look-ahead strategies can avoid breakdowns, see the section on the Lanczos connection. A simple method to overcome breakdowns is to restart the algorithm. This remedy is according to our experience in many practical cases sufficient.

BICO. It is known from practice that the convergence behavior of BCG in the Euclidean norm can be very erratic. In order to obtain a better behavior Schönauer applied minimal residual smoothing to BCG. This algorithm is called BICO [41].

Let r_k^{BCG} be the residual and x_k^{BCG} be the iterate resulting from BCG. Set $x_0 = x_0^{BCG}$, $r_0 = r_0^{BCG}$ and calculate for $k \geq 1$:

$$\begin{aligned}
\gamma_k &= -\frac{(r_{k-1})^T(r_k^{BCG} - r_{k-1})}{\|r_k^{BCG} - r_{k-1}\|^2}, \\
x_k &= x_{k-1} + \gamma_k(x_k^{BCG} - x_{k-1}), \\
r_k &= r_{k-1} + \gamma_k(r_k^{BCG} - r_{k-1}).
\end{aligned}$$

Thus we obtain

$$\|r_k\| = \min_{\gamma_k} \|r_{k-1} + \gamma_k(r_k^{BCG} - r_{k-1})\|, \tag{88}$$

$$\|e_k\|_{A^TA} = \min_{\gamma_k} \|e_{k-1} + \gamma_k(e_k^{BCG} - e_{k-1})\|_{A^TA}. \tag{89}$$

Clearly, BICO can be considered as truncated orthogonalization method with $Z_k = A$, $\sigma_k = 1$, $q_{k-1,k} = x_k^{BCG} - x_{k-1}$ and $\tilde{x}_k = x_{k-1}$.

A direct result of the residual-minimizing smoothing , see [53], is that the BICO residual is a function of the iteration index, with a non-increasing norm, i. e.

$$\|r_k\| \leq \|r_{k-1}\|, \tag{90}$$

and

$$\|r_k\| \leq \|r_k^{BCG}\|. \tag{91}$$

In [57] it is shown that

$$||r_k|| \quad \leq \quad \sqrt{k+1}\, \frac{1}{\sqrt{\sum_{i=0}^{k} \frac{1}{\|r_i^{BCG}\|^2}}}. \tag{92}$$

If V_k, H_k result from the orthogonal Lanczos process, see (41) and (43), we can prove

$$\|r_k\| \quad \leq \quad \sqrt{k+1}\, \min_{z_k \in I\!R^k} \|\eta_0 u_1 - H_{k-1} z_k\|, \tag{93}$$

where u_1 is the first unit vector. The equivalence of the right-hand sides of (92) and (93) is proven in [61]. Moreover, let

$$r_k^{min} = V_k(\eta_0 u_1 + H_{k-1} z_k^{min}), \tag{94}$$

where $z_k^{min} \in I\!R^k$ be such that

$$\|V_k(\eta_0 u_1 + H_{k-1} z_k^{min})\| = \min_{z_k \in I\!R^k} \|V_k(\eta_0 u_1 + H_{k-1} z_k)\|. \tag{95}$$

Thus r_k^{min} is the residual with the smallest possible Euclidean norm in the spanned Krylov space. We obtain

$$\|r_k\| \leq \sqrt{k+1}\; \|D_k^{-1} W_k^T\|\; \|r_k^{min}\|, \tag{96}$$

because by (93)

$$\begin{aligned}
\|r_k\| &\leq \sqrt{k+1}\ \min_{z_k \in \mathbb{R}^k} \|\eta_0 u_1 + H_{k-1} z_k\| \\
&\leq \sqrt{k+1}\ \|\eta_0 u_1 + H_{k-1} z_k^{min}\| \\
&= \sqrt{k+1}\ \|D_k^{-1} W_k^T V_k (\eta_0 u_1 + H_{k-1} z_k^{min})\| \\
&\quad \textit{by } (47) \\
&= \sqrt{k+1}\ \|D_k^{-1} W_k^T r_k^{min}\| \\
&\quad \textit{by } (94) \\
&\leq \sqrt{k+1}\ \|D_k^{-1} W_k^T\|\ \|r_k^{min}\|.
\end{aligned}$$

CGS. The *conjugate gradient squared* method (CGS) was introduced by Sonneveld [47]. The idea is to square the BCG matrix polynomial Π_k. Thus we get

$$e_k = \Pi_k^2(A) e_0, \tag{97}$$

$$r_k = \Pi_k^2(A) r_0. \tag{98}$$

If Π_k tends to zero, then a faster convergence is obtained by Π_k^2. Indeed, in many cases CGS converges twice as fast as BCG, but the convergence may be more erratic than for BCG. CGS has the additional advantage that no matrix-vector multiplication by A^T is necessary. Thus it is suited for problems, where the matrix A and, therefore, A^T are not available or where on massively parallel computers A^T cannot be easily accessed even if A is available. There are recent convergence estimates by Chan and Szeto [10] based on the BCG result, equation (73). Fokkema, Sleijpen and van der Vorst [17] give a unifying theoretical framework, called *generalized CGS*, that includes CGS, BiCGSTAB, BiCGSTAB(ℓ) and other methods as special cases.

BiCGSTAB. The *biconjugate gradients stabilized* (BiCGSTAB) were introduced by van der Vorst [50]. The idea is to substitute the squared matrix polynomial Π_k^2 of CGS, see (97) and (98), by the product of the matrix polynomials $\Psi_k \Pi_k$ in order to get a smoother convergence and to stabilize the iteration. Thus we get

$$e_k = \Psi_k(A) \Pi_k(A) e_0, \tag{99}$$

$$r_k = \Psi_k(A) \Pi_k(A) r_0. \tag{100}$$

Ψ_k is recursively defined by

$$\Psi_k(A) = (\gamma_k A + I) \Psi_{k-1}(A), \tag{101}$$

where γ_k is determined from a 1-dimensional minimization

$$\|r_k\| = \min_{\gamma_k} \|(\gamma_k A + I) \Psi_{k-1}(A) \Pi_k(A) r_0\|. \tag{102}$$

There are recent convergence estimates by Chan and Szeto [10] based on the BCG result, equation (73). Sleijpen and van der Vorst investigated the behavior for finite precision arithmetic and proposed techniques to maintain the convergence [45].

Gutknecht [29], Sleijpen and Fokkema [44] and Sleijpen, van der Vorst and Fokkema [46] generalized BiCGSTAB so that Ψ_k is determined by an ℓ-dimensional minimization. These methods are called *BiCGSTAB(ℓ)*.

QMR. The *quasi-minimal residual method* (QMR) was developed by Freund and Nachtigal [22]. It uses

$$Z_k = W_k D_k^{-T} \Omega_k^T \Omega_k D_k^{-1} W_k^T A, \tag{103}$$

where W_k is the matrix consisting of the shadow vectors generated by the nonsymmetric orthogonal Lanczos process, see (42), D_k is the diagonal or block diagonal matrix in (48) and Ω_k is a diagonal scaling matrix that can be freely chosen. As $Z_k A^{-1} = W_k D_k^{-T} \Omega_k^T \Omega_k D_k^{-1} W_k^T$ is symmetric, the following minimization properties can be derived from theorem 2.2.

$$\begin{aligned}
&\|r_k\|_{W_k D_k^{-T} \Omega_k^T \Omega_k D_k^{-1} W_k^T} \\
&\qquad = \min_{\beta_1, \ldots, \beta_k} \|\sum_{i=1}^{k} \beta_i A^i r_0 + r_0\|_{W_k D_k^{-T} \Omega_k^T \Omega_k D_k^{-1} W_k^T}, &(104)\\
&\|e_k\|_{A^T W_k D_k^{-T} \Omega_k^T \Omega_k D_k^{-1} W_k^T A} \\
&\qquad = \min_{\beta_1, \ldots, \beta_k} \|\sum_{i=1}^{k} \beta_i A^i e_0 + e_0\|_{A^T W_k D_k^{-T} \Omega_k^T \Omega_k D_k^{-1} W_k^T A}. &(105)
\end{aligned}$$

A similar result was obtained by Barth and Manteuffel [5], who consider instead of Z_k the constant matrix $Z = W_{n-1} D_{n-1}^{-T} \Omega_{n-1}^T \Omega_{n-1} D_{n-1}^{-1} W_{n-1}^T A$ that produces the same ortogonalities as Z_k. Let us write the QMR residual in terms of the Lanczos process, see equation (53),

$$r_k = V_k(\eta_0 u_1 + H_{k-1} z_k^{QMR}), \tag{106}$$

then equation (104) is equivalent to

$$\begin{aligned}
\|r_k\|^2_{W_k D_k^{-T} \Omega_k^T \Omega_k D_k^{-1} W_k^T} &= \min_{z_k \in \mathbb{R}^k} \|V_k(\eta_0 u_1 + H_{k-1} z_k)\|^2_{W_k D_k^{-T} \Omega_k^T \Omega_k D_k^{-1} W_k^T} \\
&= \min_{z_k \in \mathbb{R}^k} \|\Omega_k D_k^{-1} W_k^T V_k(\eta_0 u_1 + H_{k-1} z_k)\|^2 \\
&= \min_{z_k \in \mathbb{R}^k} \|\Omega_k(\eta_0 u_1 + H_{k-1} z_k)\|^2 \\
&\quad by\ (47).
\end{aligned}$$

Therefore, the residual of QMR fulfils (106) with z_k^{QMR} such that

$$\|\Omega_k(\eta_0 u_1 + H_{k-1} z_k^{QMR})\| = \min_{z_k \in \mathbb{R}^k} \|\Omega_k(\eta_0 u_1 + H_{k-1} z_k)\|. \tag{107}$$

Thus (104) coincides with the original approach of Freund and Nachtigal [22] who start with (107) for the definition of QMR.

We obtain the well known result from [22]

$$\|r_k\| \le \sqrt{k+1}\, \|\Omega_k^{-1}\| \min_{z_k \in \mathbb{R}^k} \|\Omega_k(\eta_0 u_1 + H_{k-1} z_k)\| \tag{108}$$

by applying (49)

$$\begin{aligned}
\|r_k\| &= \|V_k \Omega_k^{-1} \Omega_k(\eta_0 u_1 + H_{k-1} z_k^{QMR})\| \\
&\le \|V_k\|\, \|\Omega_k^{-1}\|\, \|\Omega_k(\eta_0 u_1 + H_{k-1} z_k^{QMR})\| \\
&\le \sqrt{k+1}\, \|\Omega_k^{-1}\| \min_{z_k \in \mathbb{R}^k} \|\Omega_k(\eta_0 u_1 + H_{k-1} z_k)\|.
\end{aligned}$$

Moreover, let

$$r_k^{min} = V_k(\eta_0 u_1 + H_{k-1} z_k^{min}), \tag{109}$$

where $z_k^{min} \in I\!R^k$ be such that

$$\|V_k(\eta_0 u_1 + H_{k-1} z_k^{min})\| = \min_{z_k \in I\!R^k} \|V_k(\eta_0 u_1 + H_{k-1} z_k)\|. \tag{110}$$

Thus r_k^{min} is the residual with the smallest possible Euclidean norm in the spanned Krylov space. We obtain

$$\|r_k\| \leq \sqrt{k+1}\ \kappa(\Omega_k)\ \|D_k^{-1} W_k^T\|\ \|r_k^{min}\|, \tag{111}$$

because

$$\begin{aligned}
\|\Omega_k(\eta_0 u_1 + H_{k-1} z_k^{QMR})\| &= \min_{z_k \in I\!R^k} \|\Omega_k(\eta_0 u_1 + H_{k-1} z_k)\| \\
&\leq \|\Omega_k(\eta_0 u_1 + H_{k-1} z_k^{min})\| \\
&= \|\Omega_k D_k^{-1} W_k^T V_k(\eta_0 u_1 + H_{k-1} z_k^{min})\| \\
&\quad by\ (47) \\
&= \|\Omega_k D_k^{-1} W_k^T r_k^{min}\| \\
&\quad by\ (109) \\
&\leq \|\Omega_k\|\ \|D_k^{-1} W_k^T\|\ \|r_k^{min}\|.
\end{aligned}$$

The statement follows by applying (108).

Zhou and Walker [61] show that quasi-residual smoothing transforms BCG into QMR: We can obtain QMR from BCG by the following technique if we omit Ω_k for simplicity. Let r_k^{BCG} be the residual and x_k^{BCG} be the iterate resulting from BCG. Set $x_0 = x_0^{BCG}$, $r_0 = r_0^{BCG}$, $\tau_0^2 = \|r_k^{BCG}\|^2$. Calculate for $k \geq 1$:

$$\begin{aligned}
\tau_k^2 &= \frac{1}{\frac{1}{\tau_{k-1}^2} + \frac{1}{\|r_k^{BCG}\|^2}}, \\
\gamma_k &= \frac{\tau_k^2}{\|r_k^{BCG}\|^2}, \\
x_k &= x_{k-1} + \gamma_k(x_k^{BCG} - x_{k-1}), \\
r_k &= r_{k-1} + \gamma_k(r_k^{BCG} - r_{k-1}).
\end{aligned}$$

From these equations follows [61] that

$$r_k = \frac{1}{\sum_{i=0}^{k} \frac{1}{\|r_i^{BCG}\|^2}} \sum_{i=0}^{k} \frac{1}{\|r_i^{BCG}\|^2} r_i^{BCG}. \tag{112}$$

TFQMR. The *transpose-free quasi-minimal residual method* (TFQMR) [19] by Freund is based on CGS . The quasi-minimal residual approach is applied to an auxiliary sequence y_m resulting from CGS. Let Π_k be the BCG polynomial and let us define

$$t_m = \begin{cases} r_k^{CGS} = \Pi_k^2(A) r_0 & if \quad m = 2k-1 \\ \Pi_k(A)\Pi_{k-1}(A) r_0 & if \quad m = 2k \end{cases}. \tag{113}$$

Let

$$Y_m = (y_0, \ldots, y_{m-1}) \in I\!R^{n\times m},$$
$$T_m = (t_0, \ldots, t_{m-1}) \in I\!R^{n\times m},$$

and let $B_m \in I\!R^{(m+1)\times m}$ be a bidiagonal matrix, then

$$AY_m = T_{m+1}B_m. \tag{114}$$

Let

$$x_m = x_0 + Y_m z_m, \tag{115}$$

then

$$r_m = r_0 + AY_m z_m = r_0 + T_{m+1}B_m z_m = T_{m+1}(u_1 + B_m z_m). \tag{116}$$

For TFQMR choose z_m^{TFQMR} such that

$$\|\Omega_m(u_1 + B_m z_m^{TFQMR})\| = \min_{z_m \in I\!R^m} \|\Omega_m(u_1 + B_m z_m)\| \tag{117}$$

with an arbitrary diagonal matrix $\Omega_m \in I\!R^{m\times m}$. From (117) follows directly

$$\begin{aligned} \|r_m\| &= \|T_{m+1}\Omega_m^{-1}\Omega_m(u_1 + B_m z_m^{TFQMR})\| \\ &\leq \|T_{m+1}\|\,\|\Omega_m^{-1}\|\,\|\Omega_m(u_1 + B_m z_m^{TFQMR})\| \\ &\leq \sqrt{m+1}\,\|\Omega_m^{-1}\| \min_{z_m \in I\!R^m} \|\Omega_m(u_1 + B_m z_m)\|. \end{aligned} \tag{118}$$

Zhou and Walker [61] show that quasi-residual smoothing transforms an auxiliary sequence based on CGS into TFQMR.

3.3.2. Rank-j Updates.

In this section we discuss a method proposed in [55]. A condition for obtaining short recurrences can be fulfilled by choosing

$$Z_k = Z + D_k E_k^T \tag{119}$$

as rank-j update with $D_k, E_k \in I\!R^{n\times j}$, where the matrices D_k and E_k have special properties.

R3-CKS. The *rank-3 update CKS method* (R3-CKS) [55] uses $Z_k = I + D_k E_k^T$ with $D_k, E_k \in I\!R^{n\times 3}$. We obtain by Theorem 2.2

$$||r_k||_{Z_k A^{-1}} \leq \sqrt{1 + \frac{\rho^2(R)}{\mu_m^2(M)}} \min_{\beta_1,\ldots,\beta_k} ||\sum_{i=1}^{k} \beta_i A^i r_0 + r_0||_{Z_k A^{-1}}, \tag{120}$$

$$||e_k||_{A^T Z_k} \leq \sqrt{1 + \frac{\rho^2(R)}{\mu_m^2(M)}} \min_{\beta_1,\ldots,\beta_k} ||\sum_{i=1}^{k} \beta_i A^i e_0 + e_0||_{A^T Z_k}. \tag{121}$$

3.3.3. Residual-Minimizing CG.

If we choose $Z = A$, then $ZA^{-1} = I$ is symmetric and we obtain from Theorem 2.2

$$
\begin{aligned}
(122)\qquad ||r_k|| &= \min_{\beta_1,..,\beta_k} ||\sum_{i=1}^{k} \beta_i A^i r_0 + r_0||, \\
(123)\qquad ||e_k||_{A^TA} &= \min_{\beta_1,..,\beta_k} ||\sum_{i=1}^{k} \beta_i A^i e_0 + e_0||_{A^TA} \\
&\leq \kappa(A) \min_{\beta_1,..,\beta_k} ||\sum_{i=1}^{k} \beta_i A^i e_0 + e_0||.
\end{aligned}
$$

Thus for these methods the residuals are minimized in the Euclidean norm. One of the first realizations is *ORTHOMIN* by Vinsome [51] for symmetric positive definite matrices. Paige and Saunders proposed *MINRES* [37], a numerically stable implementation for symmetric matrices.

GMRES. The *generalized minimal residual method* (GMRES) was proposed by Saad and Schultz [40] and works for arbitrary matrices. There are various implementations of GMRES [39, 52]. The original implementation of Saad and Schultz [40] is based on the Arnoldi process including exact and restarted versions.

CGNR-ATPRES. If we apply a method with $Z = I$ (classical CG) to the normal equations of the first kind

$$(124)\qquad A^TAx = A^Tb,$$

then we get the residuals of the original system r_k from the residuals of (124) r_k^N by

$$(125)\qquad r_k^N = A^TAx_k - A^Tb = A^T(Ax_k - b) = A^Tr_k.$$

From Theorem 2.2 follows

$$||r_k^N||_{A^{-1}A^{-T}} = \min_{\beta_1,..,\beta_k} ||\sum_{i=1}^{k} \beta_i \left(A^TA\right)^i r_0^N + r_0^N||_{A^{-1}A^{-T}},$$

and from (125) we obtain for the original system

$$(126)\qquad ||r_k|| = \min_{\beta_1,..,\beta_k} ||\sum_{i=1}^{k} \beta_i \left(AA^T\right)^i r_0 + r_0||.$$

For the errors the follows

$$(127)\qquad ||e_k|| \leq \kappa(A) \min_{\beta_1,..,\beta_k} ||\sum_{i=1}^{k} \beta_i \left(A^TA\right)^i e_0 + e_0||.$$

Indead, the method can be reformulated such that only the approximations and residuals of the original system are used. This method is called CGNR (*CG Normal equations Residual minimizing*) There are various implementations. The ATPRES (*A Transposed Pseudo RESidual method*) [42] implementation results from applying residual-minimizing smoothing [53] to CGNE. The validity of this transformation follows from [53].

3.3.4. Energy Norm-Minimizing CG.

If $Z = I$ exact methods minimize the energy norm of the error by Theorem 2.2 in the following sense:

$$||r_k||_{A^{-1}} \leq \sqrt{1 + \frac{\rho^2(R)}{\mu_m^2(M)}} \min_{\beta_1,..,\beta_k} || \sum_{i=1}^{k} \beta_i A^i r_0 + r_0||_{A^{-1}}, \tag{128}$$

$$||e_k||_A \leq \sqrt{1 + \frac{\rho^2(R)}{\mu_m^2(M)}} \min_{\beta_1,..,\beta_k} || \sum_{i=1}^{k} \beta_i A^i e_0 + e_0||_A. \tag{129}$$

If A is symmetric and positive definite, then we obtain the classical CG method [30] by Hestenes and Stiefel. As A is symmetric and therefore normal we obtain by Theorem 3.1

$$\begin{aligned} ||r_k|| &\leq \kappa(S) \min_{\theta_1,\ldots,\theta_k} \max_{\lambda} | \sum_{i=1}^{k} \theta_i \lambda^i + 1| \; ||r_0||, \\ ||e_k|| &\leq \kappa(S) \min_{\theta_1,\ldots,\theta_k} \max_{\lambda} | \sum_{i=1}^{k} \theta_i \lambda^i + 1| \; ||e_0||, \end{aligned}$$

where S is the square root of A. By substituting the polynomial by a normalized Chebyshev polynomial we obtain the well-known estimate for classical CG:

$$||e_k|| \leq 2\kappa(S) \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^k ||e_0||,$$

where $\kappa(A)$ is the condition number of A.

Paige and Saunders proposed *SYMMLQ* [37], a numerical stable implementation for symmetric matrices.

ORTHORES. For positive real matrices we obtain ORTHORES (ORTHOgonal RESiduals) [59].

3.3.5. Error-Minimizing CG.

Error-minimizing CG methods can only be realized by using the normal equations.

CGNE. If we apply a method with $Z = I$ (classical CG) to the normal equations of the second kind

$$AA^T y = b, \tag{130}$$

then we get the solution of the original system x by

$$x = A^T y. \tag{131}$$

Similarly we get the errors of the original system e_k from the errors of (130) e_k^N by

$$e_k = x_k - x = A^T y_k - A^T y = A^T (y_k - y) = A^T e_k^N. \tag{132}$$

From Theorem 2.2 follows

$$||e_k^N||_{AA^T} = \min_{\beta_1,..,\beta_k} || \sum_{i=1}^{k} \beta_i \left(AA^T\right)^i e_0^N + e_0^N||_{AA^T},$$

and from (132) we obtain for the original system

$$||e_k|| = \min_{\beta_1\ ,..,\beta_k} ||\sum_{i=1}^{k} \beta_i \left(A^T A\right)^i e_0 + e_0||. \tag{133}$$

Thus the method minimizes the error in the Euclidean norm and is called CGNE (*CG Normal equations Error-minimizing*). Reformulated to the approximations and residuals of the original system it was proposed by Craig [12]. For the residuals the following is satisfied:

$$||r_k|| \leq \kappa(A) \min_{\beta_1\ ,..,\beta_k} ||\sum_{i=1}^{k} \beta_i (AA^T)^i r_0 + r_0||. \tag{134}$$

3.3.6. Truncated and Restarted Versions.

For exact methods the storage and computing requirements increase with the iteration step. For full matrices the storage increases for exact methods up to 2 times of the amount needed for the matrix itself. Thus for full matrices exact methods can be applied instead of preconditioning. For large and sparse systems the situation is different because the storage would increase so that even the capacity of today's supercomputers would be exceeded in later steps. Exact methods can only be reformulated as short recurrences if special conditions are satisfied, for example:

$$A^T Z = ZA$$

see (28). This means for GMRES and ORTHORES that A has to be symmetric. In general truncated and restarted versions of the above mentioned methods have to be applied to solve non-symmetric problems for large and sparse systems.

PRES20. (Pseudo-RESidual method 20) [41] is a special version of smoothed ORTHORES with an optimized value of the truncation parameter σ_{min}. The sequence is restarted every σ_{res} steps from the smoothed sequence. As a result of many tests with very large and sparse matrices where a large number of σ_{max} or σ_{res} is prohibitive because of storage reasons a version with $\sigma_{max} = 5$ and $\sigma_{res} = 20$, called PRES20, has been demonstrated to be very efficient.

4. Generalized Minimum Error Methods.

Generalized minimum error methods [54] are the subset of Krylov subspace methods with

$$B = A^T \ , \tag{135}$$

$$Z_k = A^{-T} = const \ , \tag{136}$$

$$z = A^T y_0 \ . \tag{137}$$

Thus

$$q_{k-i,k} \in K_{k-i}(A^T, A^T y_0) \ . \tag{138}$$

The methods can be realized without knowing $Z_k = A^{-T}$ by introducing

$$y_{k-i,k} \in K_{k-i}(A^T, y_0) \tag{139}$$

and by calculating the $q_{k-i,k}$ by

$$q_{k-i,k} = A^T y_{k-i,k}. \tag{140}$$

By (135) generalized minimum error methods can be formulated so that only one matrix-vector multiplication is needed per iteration step.

It is quite obvious that

$$x_k = \sum_{i=1}^{k} \delta_{i,k} \left(A^T\right)^i y_0 + x_0 \ , \tag{141}$$

$$r_k = \sum_{i=1}^{k} \delta_{i,k} A \left(A^T\right)^i y_0 + r_0 \ , \tag{142}$$

$$e_k = \sum_{i=1}^{\sigma_k} \delta_{i,k} \left(A^T\right)^i y_0 + e_0 \ . \tag{143}$$

If we apply Theorem 2.2 to these methods, then we obtain the error-minimizing property, see also [54].

THEOREM 4.1. *For exact generalized minimum error methods*

$$||r_k||_{A^{-T}A^{-1}} = \min_{\beta_1,\ldots,\beta_k} ||\sum_{i=1}^{k} \beta_i A \left(A^T\right)^i y_0 + r_0||_{A^{-T}A^{-1}} \ , \tag{144}$$

$$||e_k|| = \min_{\beta_1,\ldots,\beta_k} ||\sum_{i=1}^{k} \beta_i \left(A^T\right)^i y_0 + e_0|| \tag{145}$$

is valid.

Proof. Apply Theorem 2.2 to generalized minimum error methods. □

The optimal choice of y_0 would be $y_0 = A^{-T}e_0 = A^{-T}A^{-1}r_0$ because then the solution is obtained in the first step following from (145). The optimal y_0 would be the solution of the linear system

$$AA^T y_0 = r_0 \ . \tag{146}$$

The solution of (146) is a problem as difficult as the solution of the original system. A natural choice for y_0 is

$$y_0 = r_0 \ . \tag{147}$$

With this choice we get the classical algorithm of Fridman [23] if A is symmetric and positive definite. His implementaion turned out to be unstable, see [48]. A stable version was proposed by Stoer and Freund, also in [48], and by Freund [18]. Fletcher [16] showed that auxiliary iterates calculated by SYMMLQ [37] coincide mathematically with the approximations of Fridman's algorithm. Therefore, SYMMLQ generates a stable implementation of that method as well.

GMERR proposed in [54] is the extension of error-minimizing methods for arbitrary matrices. A problem for GMERR is the controlling of the convergence because the errors decrease but they cannot be calculated. If we observe the norm of the residuals, it may oscillate heavily. Moreover, an additional matrix-vector multiplication is needed for the calculation of the residuals. Therefore, we propose to calculate the residuals only every j-th step and to apply residual-minimizing smoothing [53]. The norm of the smoothed residuals can be used for control.

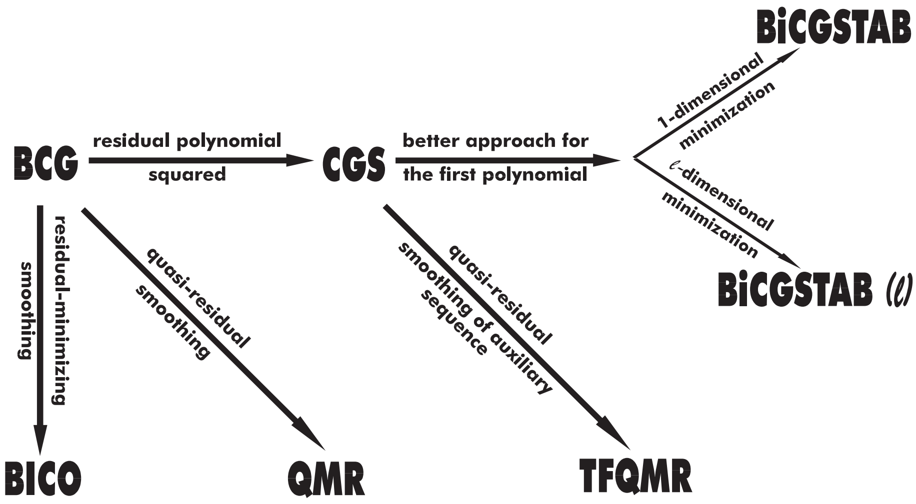

FIG. 1. *Relations between different BCG-based methods*

	original system	normal equations
error-minimizing	GMERR	CGNE
energy norm-minimizing	ORTHORES	
residual-minimizing	GMRES	CGNR-ATPRES

TABLE 1
Comparison of minimization properties for CG methods and GMERR

5. Discussion.
The BCG-based methods BCG, BICO, CGS, BiCGSTAB, QMR and TFQMR have the same origin BCG, see figure 1. Thus it is obvious that they are all closely related and it is confirmed by numerical tests, see for example the first article in this special issue. While the residuals and errors resulting from BCG and CGS oscillate heavily, all other methods produce a smoother convergence. The same convergence estimate applies for BICO, see (93) and (96), as for QMR, see (108) and (111). Numerical experiments show that the behavior of both methods is indeed very similar. The variants of BiCGSTAB are a combination of a Lanczos-based method with a residual-minimizing method, see (102). Numerical experiments indicate that BiCGSTAB takes advantage of the good properties of both. The BCG-based methods can be implemented with a short recurrence. Therefore, they have the advantage that the necessary computer resources are limited in cpu-time and storage. They have the disadvantage that they minimize the residuals and errors in norms different to the Euclidean norm.

The CG-based methods minimize the residuals or the errors in Euclidean norm or the energy norm. In table 1 the different methods are classified with respect to the particular minimization properties. These methods have the disadvantage that the length of the recurrence increases with the iteration step unless special conditions are valid. Thus they are not feasible as exact methods for large and sparse matrices because the required computer resources in cpu-time and storage exceed even the capabilities of today's supercomputers. Note that ORTHORES and GMRES can be computed simultaneously without additional costs by smoothing, see [53], and that

GMRES minimizes the residuals in the Euclidean norm while ORTHORES minimizes the error in the energy norm. GMRES guarantees monotonicly decreasing residuals. ORTHORES may be better as regards the decrease of the error because the minimization in the energy norm may be closer to the minimization in the Euclidean norm of the error. For both methods the convergence is only guaranteed if they are used as exact methods. Truncated and restarted versions are very efficient for matrices A with a single cluster of eigenvalues, but not very robust. Chin and Forsyth [11] compare GMRES with BiCGSTAB. For complex matrices a very elaborate comparison between complex generalized CG and complex BCG-based methods is given by Joly and Meurant [32].

The CG methods based on the solution of the normal equations, CGNR-ATPRES and CGNE, can be formulated with a short recurrence. Thus they have both advantages: a minimization property in the Euclidean norm, see (126) and (133), and limited requirements for computer resources. However, the eigenvalues of $A^T A$ can be more scattered than those of the original system matrix A. Then the convergence can be rather slow. Theoretically the methods converge always. Thus they are very robust but not very efficient.

For the error-minimizing methods the storage and the computing requirements increase with the iteration. Thus GMERR has the same disadvantage as GMRES or ORTHORES. The advantage is that the error is minimized in the Euclidean norm. From the point of the minimization property the methods should be optimal. However, the minimization property is connected to the choice of the vectors $q_{k-i,k}$, see (140), i. e. the $q_{k-i,k}$ cannot be freely chosen. Therefore, the convergence can be slower than the convergence of residual-minimizing CG. For symmetric matrices the convergence of the errors is comparable to the convergence of the GMRES errors, see [18]. For nonsymmetric matrices the speed of convergence is an open question.

R3-CKS can be implemented with a short recurrence. Very little is known about the convergence, except the minimization properties (120) and (121) involving a very strange norm. The potential of this method is that it can be combined with a step-depending preconditioner that eliminates the step-depending norm. This will be the topic of further research.

The investigation of the convergence results has been mainly confined to estimates that depend on Krylov spaces and on particular norms. While the global quantitative speed of convergence is determined by the minimization space, the qualitative convergence is given by the norm. Any more detailed analysis would involve inner properties of the matrices as for example eigenvalue distributions or speudo-spectra. These properties are in general unknown for practical applications. Moreover, the knowledge of the minimization space and the minimization norm already gives an insight into the relations between the different methods. For example the similar behavior of the residual and error norms of BICO and QMR, known from practice [43, 57, 61], is confirmed by the same convergence estimates (93) and (108), (96) and (111). The difference between BCG and QMR is the underlying Lanczos process that affects only the norm. Thus the qualitative behavior of both methods is quite different, but it seems that they fit into the same class as regards the quantitative residual and error reduction; for numerical tests see [43] in this special issue. An excellent theoretical investigation for the pair *BLanczos* and *BMinres* is given by Cullum in this special issue [13] confirming that different norms affect only the qualitative behavior. However, the quality of the convergence is as important as the quantity in order to get a reliable approximation in each iteration step.

Some properties cannot yet be explained by the convergence results. For example, the fast convergence of BiCGSTAB cannot be readily identified from the estimates. Moreover, in order to obtain more efficient and robust methods spaces different to Krylov subspaces have to be investigated. The concept of orthogonalization methods covers all possible spaces, but the choice of better approximation spaces is an open question. Therefore, further research is necessary.

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