Conjugate and Semi-Conjugate Direction Methods with Preconditioning Projectors

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The acceleration of the original projective iterative methods of multiplicative or additive type for solving systems of linear algebraic equations (SLAEs) by means of conjugate direction approaches is considered. The orthogonal and varitional properties of the preconditioned conjugate gradient, conjugate residual and semi-conjugate residual algorithms, as well as estimations of the number of iterations, are presented. Similar results were obtained for the dynamically preconditioned iterative process in Krylov subspaces. Application of discussed techniques for domain decomposition, Kaczmarz, and Cimmino methods is proposed.

1   Introduction

The aim of this paper is to analyze the iterative algorithms in the Krylov subspaces whose preconditioners are some kinds of projector operators. At first we consider the general approach for acceleration of some convergent iterations with a constant step matrix.

Let us have the system of linear algebraic equations:

$$Au = f, \quad u = \{u_i\}, \quad f = \{f_i\} \in R^N, \quad A = \{a_{i,j}\} \in R^{N,N}, \tag{1}$$

and the convergent stationary iterative process

$$u^{k+1} = Bu^k + g, \quad u^k \underset{k \to \infty}{\to} u, \quad g = (I - B)A^{-1}f. \tag{2}$$

Suppose that the step matrix B has eigenvalues $\lambda_q(B)$ and spectral radius $\rho = \max_q\{|\lambda_q(B)|\} < 1$. Then the vector u is the solution of system

$$\tilde{A}u \equiv (I - B)u = g, \tag{3}$$

where I is the identity matrix and $\tilde{A}$ is the preconditioned non-singular matrix. If $\tilde{A}$ is a symmetric positive definite (s.p.d) matrix, its spectral condition number is

$$æ = \|\tilde{A}\|_2 \|\tilde{A}^{-1}\|_2 = (1 + \rho)/(1 - \rho). \tag{4}$$

and to solve SLAE (3) we can apply some iterative conjugate direction methods (see [1] – [4]):

$$r^0 = g - \tilde{A}u^0, \quad p^0 = r^0; \quad n = 0, 1, \dots :$$
$$u^{n+1} = u^n + \alpha_n p^n, \quad r^{n+1} = r^n - \alpha_n \tilde{A}p^n, \tag{5}$$
$$p^{n+1} = r^{n+1} + \beta_n p^n,$$

which have the optimality property in the Krylov subspaces

$$\mathcal{K}_{n+1}(r^0, \tilde{A}) = Span\{p^0, p^1, \dots, p^n\} = Span\{p^0, \tilde{A}p^0, \dots, \tilde{A}^n p^0\}.$$

In conjugate direction (CG) and conjugate residual (CR) methods, $s = 0, 1$ respectively, the iterative parameters $\alpha_n^{(s)}$ and $\beta_n^{(s)}$ are defined as follows:

$$\alpha_n^{(s)} = (\tilde{A}^s r^n, r^n)/(\tilde{A}p^n, \tilde{A}^s p^n), \quad \beta_n^{(s)} = (\tilde{A}^s r^{n+1}, r^{n+1})/(\tilde{A}^s r^n, r^n). \tag{6}$$

These algorithms provide the residual and direction (correction) vectors r^n and p^n with the orthogonal peculiarities

$$(\tilde{A}^s r^n, r^k) = (\tilde{A}^s r^n, r^n)\delta_{n,k}, \quad (\tilde{A}p^n, \tilde{A}^s p^k) = (\tilde{A}p^n, \tilde{A}^s p^n)\delta_{n,k}. \tag{7}$$

Also, the functionals $\Phi_n^{(s)}(r^n) = (\tilde{A}^{s-1} r^n, r^n), \quad s = 0, 1$, are minimized in the Krylov subspaces, and the number of iterations necessary for satisfying the condition

$$(\Phi_n^{(s)}(r^n)/\Phi_0^{(s)}(r^0))^{1/2} \leq \varepsilon < 1,$$

is estimated by the value

$$n(\varepsilon) \leq 1 + \left(ln\frac{1 + \sqrt{1 - \varepsilon^2}}{\varepsilon}\right)/ln\gamma, \quad \gamma = (\sqrt{\ae} - 1)/(\sqrt{\ae} - 1). \tag{8}$$

It should be noted that matrix-vector multiplication in (5) presents the implementation of one iteration (2) that does not require explicit formulation of matrices $\tilde{A}$ and B, because, for example,

$$\tilde{A}p^n = p^n - Bp^n.$$

If martix $\tilde{A}$ is nonsymmetric and positive definite, i.e.

$$(\tilde{A}u, u) \geq \delta(u, u), \quad \delta > 0, \quad u \neq 0,$$

system (3) can be solved by means of the semi-conjugate residual (SCR) method realizing the stabilized version of the generalized conjugate residual (GCR) algorithm, which is described in [5] and has instability features in terms of truncation errors, see [4].

In SCR, the vectors u^{n+1} and r^{n+1} are computed according to formulas (5), with the coefficients $\alpha_n^{(s)}$ from (6) for $s = 1$, and the direction vectors p^{n+1} are defined as follows:

$$p^{n+1,0} = r^{n+1}, \quad p^{n+1,l} = p^{n+1,l-1} + \beta_{n,l} p^{l-1}, \quad l = 1, \dots, n,$$
$$\beta_{n,l} = -(\tilde{A}p^l, \tilde{A}p^{n+1,l-1})/(\tilde{A}p^l, \tilde{A}p^l), \quad p^{n+1} = p^{n+1,n}. \tag{9}$$

2

Relations (5), (9) realize the construction of $A^t A$-orthogonal (conjugate) vectors p^0, $p^1, ..., p^{n+1}$ by means of modified Gram–Schmidt orthogonalization [6]. In this case, the functional $\Phi_n^{(1)}(r^n) = (r^n, r^n)$ is minimized in the subspace $\mathcal{K}_{n+1}(r^0, \tilde{A})$ and the residual vectors are right semi-conjugate, in the sense of satisfaction of the equalities $(\tilde{A} r^k, r^n) = 0$ for $k < n$. Since SCR and GMRES methods (see [4]) have the same variational properties in the Krylov subspaces, similar estimate of the number of iterations $n(\varepsilon)$ is valid for them, and it will used below.

This paper is organized as follows. In Section 2, we describe projective methods of the multiplicative type using the conjugate direction and semi-conjugate direction approaches. The next Section is devoted to the additive type projective methods in the Krylov subspaces. Also, the application of dynamic preconditioners is discussed. This approach means using variable step matrix B_n at different iterations. This is the implementation requirement, for example, in many two-level iterative processes.

2 Multiplicative projector methods

Let $\Omega = \{i = 1, 2, ..., N\}$ denote a set of matrix row numbers and $\Omega_p, p = 1, 2, ..., l$, be its non-intersecting integer subsets, with the numbers m_p of their elements,

$$\Omega = \bigcup_{p=1}^{l} \Omega_p, \quad m_1 + ... + m_l = N.$$

Also, let us introduce subvectors $u_{(p)}, f_{(p)}, p = 1, ..., l$, of dimensions m_p and rectangular matrices $A_{(p)} \in R^{m_p \times N}$:

$$u_{(p)} = \{u_i, i \in \Omega_p\}, \quad f_{(p)} = \{f_i, i \in \Omega_p\}, \quad A_{(p)} = \{A_i, i \in \Omega_p\}, \tag{10}$$

where A_i is the i-th row of matrix A. Then SLAE (1) can be rewritten as

$$A_{(p)} u = f_{(p)}, \quad p = 1, 2, ..., l. \tag{11}$$

To solve (11), we consider an iterative process in which the computing of each n-th approximation step consists of the following stages:

$$u^{n,p} = u^{n,p-1} + \omega A_{(p)}^+ r_{(p)}^{n,p-1}, \quad n = 1, 2, ..., \quad p = 1, 2, ..., l, \quad u^n = u^{n,l}. \tag{12}$$

Here $u^{0,0} = \{u_i^0, i = 1, 2, ..., N\}$ is the initial guess, and ω is some iterative parameter,

$$r_{(p)}^{n,p-1} = f_{(p)} - A_{(p)} u^{n,p-1}$$

is the residual subvector of dimension m_p, and A_p^+ is pseudoinverse to matrix $A_{(p)}$ defined by the formula $A_{(p)}^+ = A_{(p)}^t (A_{(p)} A_{(p)}^t)^{-1}$ if $A_{(p)}$ has a full rank.

We have from the above that $I - A_{(p)}^+ A_{(p)}$ is a symmetric positive semi-definite matrix realizing orthogonal projection into the p-th subspace, which is presented geometrically by the union of subspaces described by the i-th equations, $i \in \Omega_p$.

Iterative method (12) can be written in the matrix form,

$$u^n = Bu^{n-1} + g, \quad B = (I - T_l) \cdots (I - T_1), \quad T_p = \omega A_{(p)}^+ A_{(p)}. \qquad (13)$$

Projective algorithm (12), (13) for $\omega = 1$ and $m_p = 1$ presents the "point-wise" method published by S.Kaczmarz in [7]. Its different generalizations and investigations were made by many authors, see [8], [9].

In [10] the following assertion was proved for abstract iterative projection method of the multiplicative type, with application to the domain decomposition approach:

Theorem 1. *Let $T_p, p = 1, ..., l$, be s.p.d. matrices, and the following inequalities be valid for any vector $v \in R^N$:*

$$(T_p v, v)/(v, v) \le \alpha < 2, \quad p = 1, 2, ..., l; \quad \|v\| \le \beta \sum_{p=1}^{l} (T_p v, v).$$

Then the estimate

$$\|B\|_2 \le \rho = 1 - (2 - \alpha)/\{\beta[l + \alpha^2 l(l - 1)/2]\}$$

is true for the Euclidian norm $\|B\|_2$. If the matrices $\bar{T}_p = \omega T_p$ for all p satisfy the conditions

$$(\bar{T}_p v, v)/(v, v) \le \bar{\alpha} < 2, \quad \|v\| \le \bar{\beta}[(\bar{T}_1 v, v) + ... + (\bar{T}_l v, v)],$$

then for $\omega = (\bar{\alpha}\sqrt{(l - 1)l})^{-1}$ we have $\rho = 1 - (3 \bar{\alpha} \bar{\beta} l)^{-1}$.

It should be noted that step matrix B in iterative process (13) is non-symmetric, because matrices T_p are not commutative in general.

Now we consider the alternative direction block version of the Kaczmarz method, in which each iteration consists of two stages. The first one realizes conventional formulas (12) or (13), and the second stage implements similar computations but in the backward ordering on the number p:

$$\begin{aligned}
u^{n+1/2,p} &= u^{n,p-1} + \omega A_{(p)}^+ r_{(p)}^{n,p-1}, \\
p &= 1, 2, ..., l, \quad u^{n+1/2} = u^{n+1/2,l} = u^{n+1/2,l+1}, \\
u^{n+1,p} &= u^{n+1/2,p+1} + \omega A_{(p)}^+ r_{(p)}^{n+1/2,p+1}, \\
p &= l, ..., 2, 1, \quad u^{n+1} = u^{n+1,1}.
\end{aligned} \qquad (14)$$

The step matrix in iterations (14) is the matrix product $B = B_2 B_1$, where B_1 coincides with B from (13) and B_2 has a similar form. Thus,

$$u^{n+1} = B_2 B_1 u^n + g, \quad B_2 = (I - T_1)(I - T_2) \cdots (I - T_l) = B_1^t. \qquad (15)$$

Under conditions of Theorem 1, the estimate $\|B_k\|_2 \le \rho$ is valid for each matrix B_1, B_2, and for the step matrix of the alternative direction method we have an inequality $\|B\| \le \|B_1\| \cdot \|B_2\| \le \rho^2 < 1$.

Since method (14), (15) can be presented in the form (2) with s.p.d. matrix B, it is possible to accelerate the convergence of iterations by means of conjugate direction

methods, applied formally for solving preconditioned SLAE (3), and the following result is true.

Theorem 2. *The iterations of the alternative direction multiplicative projective conjugate gradient* (ADMPCG) *and conjugate residual* (ADMPCR) *methods defined by relations* (3), (5), *and* (6) *for $s = 0, 1$ respectively, are convergent under conditions of Theorem 1, and the estimate* (8) *is valid for the number of iterations $n(\varepsilon)$, where $æ = (1 + \rho^2)/(1 - \rho^2)$ and the value ρ is determined in Theorem 1.*

Now let us consider the successive multiplicative projective semi-conjugate residual (SMPSCR) method in the Krylov subspaces which is an alternative to the above ADM-PCR algorithm. The new approach is based on the acceleration of iterative process (13) with non-symmetric step matrix B by means of formulas (5) and (9) where preconditioned matrix $\bar{A}$ is described by (3), (13). The SMPSCR procedure requires, for computing u^{n+1}, to save in memory all previous direction vectors $p^0, ..., p^n$, similarly to the GMRES method [4]. These two approach have the same convergent property because they provide minimization of the functional (r^n, r^n) in the subspace $\mathcal{K}_{n+1}(r^0, \tilde{A})$. The following result is true for the successive multiplicative method.

Theorem 3. *Suppose, that the SMPSCR algorithm, defined by formulas* (3), (5),(6) *and* (9),(11)–(13) *for $s = 1$, has diagonalizable matrix $\tilde{A} = X\Lambda X^{-1}$, $\Lambda = diag(\lambda_1, ..., \lambda_N)$, where λ_i are eigenvalues of $\tilde{A}$ and X is a square matrix whose columns are corresponding eigenvectors. Then this method is convergent under conditions of Theorem 1, and the following estimate is valid for the number of iterations:*

$$n(\varepsilon) \leq 1 + \Big(ln\frac{1 + \sqrt{1 - \varepsilon_1^2}}{\varepsilon_1}\Big)/ln\gamma, \quad \varepsilon_1 = \varepsilon/(\|X\|_2 \cdot \|X^{-1}\|_2),$$

Here $\gamma_1 = a + \sqrt{a^2 - d^2}, \gamma_2 = c + \sqrt{c^2 - d^2}$, where a, d are the semi-major axis and the focal distance $(d^2 < c^2)$ for the ellipse $E(a, d, c)$ which includes all values λ_i, excludes origin, and is centered at c.

It should be noted that for the SMPSCR method, as for GMRES, different reduced versions with a bounded number of saved direction vectors p^n can be constructed. This will decrease the computational resources for the implementation of the algorithm, but the quantities $n(\varepsilon)$ will increase in these cases.

3   Additive projective methods

Let us recall that the Kaczmarz method is based on successive projection of the points from the space R^N onto the hyperplates which are described by the corresponding equations of the algebraic system. A similar idea is used in the Cimmino algorithm (see [11]–[13] and its references). But here projections of the given point u^n onto all hyperplates are made simultaneously, and the next step of the iterative approximation is chosen by means of some averaging procedure, or linear combination, with projective points $u^{n,i}$, $i = 1, ..., N$. Such an additive type iterative process to solve SLAE (11) can be presented

in a generalized block version as

$$u^{n,p} = u^{n-1} + A_{(p)}^{+} r_{(p)}^{n-1}, \quad p = 1, 2, ..., l, \quad u^n = (u^{n,1} + u^{n,2} + ... + u^{n,l})/l, \qquad (16)$$

These relations can be written in the following matrix form:

$$u^n = Bu^{n-1} + g, \quad B = I - l^{-1} \sum_{p=1}^{l} A_{(p)}^{+} A_{(p)} =$$

$$= I - l^{-1} \sum_{p=1}^{l} T_p, \quad g = l^{-1} \sum_{p=1}^{l} A_{(p)}^{+} f_{(p)}, \qquad (17)$$

where matrices T_p are defined in (13).

Obviously, the limit vector of this sequence $u = \lim_{n \to \infty} u^n$, if it exists, satisfies the preconditioned system of equations

$$\tilde{A}u = \tilde{f}, \quad \tilde{A} = \sum_{p=1}^{l} T_p, \quad \tilde{f} = \sum_{p=1}^{l} A_{(p)}^{+} f_{(p)}. \qquad (18)$$

If matrix $\tilde{A}$ of system (18) is a s.p.d. one, its spectral properties are obtained from the following result [10].

Theorem 4. *Let the quantities $0 < \alpha < 2$ and $0 < \rho < 1$ be defined from Theorem 1. Then the spectral radius $\lambda(\tilde{A})$ of s.p.d. matrix $\tilde{A}$ from system (18) satisfies the inequalities*

$$(2 - \alpha)(1 - \rho)/4 \le \lambda(\tilde{A}) \le \alpha l.$$

Now we can estimate the convergence rate of the additive projective approach.

Theorem 5. *Estimate (8) for the number of iterations $n(\varepsilon)$ is valid for the conjugate gradient and conjugate residual methods to solve the SLAE (18), i.e. to accelerate the additive projective algorithm (17). In this case the condition number satisfies the estimate $æ(\tilde{A}) \le 4\alpha l(2 - \alpha)^{-1}(1 - \rho)^{-1}$.*

Remark 1. It follows from Theorems 1 and 5 that the multiplicative method is faster, in comparison to a similar additive procedure. However the letter has a considerable advantage for parallel implementation on a multi-processor computer, because the calculation of each projection at the subspace can be done independently.

Remark 2. Theorems 1 and 4 were proved in [10] to analyse convergence properties of the multiplicative and additive domain decomposition methods. It is evident that Theorems 2, 3 and 5 on the accelerations of projective iterative methods by means of conjugate direction or semi-conjugate direction algorithms in the Krylov subspaces can be used successively in these applications. Thus, the block variant of SLAE (11) can be interpreted as a matrix representation of the algebraic domain decomposion (ADD) formulation.

4 Iterations in Krylov subspaces with dynamic preconditioning

If we have a large problem, i.e. the original algebraic system (1) has a dimensionality of several millions or hundreds of millions, then it is natural to use some iterative procedure for solving auxiliary SLAEs at each step of block projection method (12) or (17).

In this case we obtain a two level iterative approach: at the external level we have iterative method of the form

$$u^{n+1} = B_n u^n + g^n = u^n + C_n^{-1}(f - Au^n), \quad B_n = I - C_n^{-1}A, \tag{19}$$

with variable (dynamic) step matrices B_n and preconditioning matrices C_n, and at the internal level the subsystems of dimensionality m_p are solved iteratively.

The acceleration of iterative process (19) in the Krylov subspaces

$$\mathcal{K}_{n+1}(r^0, C_n^{-1}A) = span\{C_0^{-1}r^0, AC_1^{-1}r^0, ..., A^n C_n^{-1}r^0\}$$

can be done by the following dynamically preconditioned semi-conjugate residual (DP-SCR) method:

$$
\begin{aligned}
&r^0 = f - Au^0, \quad p^0 = C_0^{-1}r^0, \quad n = 0, 1, .. : \\
&u^{n+1} = u^n + \alpha_n p^n, \quad r^{n+1} = r^n - \alpha_n Ap^n, \\
&p^{n+1} = C_{n+1}^{-1}r^{n+1} + \sum_{k=0}^{n} \beta_{n,k}p^k = p^{n+1,l} + \sum_{k=l}^{n} \beta_{n,k}p^k, \\
&p^{n+1,l} = p^{n+1,l-1} + \beta_{n,l-1}p^{l-1}, \quad p^{n+1,0} = C_{n+1}^{-1}r^{n+1}, \quad p^{n+1} = p^{n+1,n}, \\
&\alpha_n = (AC_n^{-1}r^n, r^n)/(Ap^n, Ap^n), \quad \beta_{n,k} = -(Ap^k, Ap^{n,k})/(Ap^k, Ap^k).
\end{aligned}
\tag{20}
$$

The algorithm DPSCR provides minimization of the residual norm $||r^{n+1}||$ in the subspace $\mathcal{K}_{n+1}(r^0, C_n^{-1}A)$, and the following equality is true:

$$||r^{n+1}||^2 = (r^0, r^0) - \frac{(AC_0^{-1}r^0, r^0)^2}{(Ap^0, Ap^0)} - \ldots - \frac{(AC_n^{-1}r^n, r^n)^2}{(Ap^n, Ap^n)}. \tag{21}$$

Thus, this method converges if matrices $C_n^{-1}A$ are positive definite. In order to decrease the computational complexity of the algorithm, for large n two reduced versions of method (20) can be applied. The first one is based on the procedure of periodical restarting after each m iterations. This means that for $n = ml, l = 1, 2, ...$, the residual vector r^n is computed not from the recurrent relation but from the original equation ($r^{ml} = f - Au^{ml}$), and subsequent calculations are performed in the conventional form. The second way consists in truncated orthogonalization, i.e. for $n > m$ only the last m direction vectors $p^n, ..., p^{n-m+1}$ and $Ap^n, ..., Ap^{n-m+1}$ are saved in the memory and used in the recursion.

The following combination of these two approaches can be proposed. Let m_1 be the restart period, m_2 be the number of saved orthogonal direction vectors, and $n' =$

$n - [\frac{n}{m_2}]m_2$, where [b] is the integer part of b. Then the unified reduced recursion for p^n is written as

$$p^{n+1} = C_{n+1}^{-1}r^{n+1} + \sum_{k=n-m+1}^{n} \beta_{n,k}p^k, \quad m = min\{n', m_1\}. \quad (22)$$

It is easy to show from (21) that the reduced versions of DPSCR converge also, if matrices $C_n^{-1}A$ are positive definite for all n.

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