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Strong Underrelaxation in Kaczmarz's Method for Inconsistent Systems*

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Summary. We investigate the behavior of Kaczmarz's method with relaxation for inconsistent systems. We show that when the relaxation parameter goes to zero, the limits of the cyclic subsequences generated by the method approach a weighted least squares solution of the system. This point minimizes the sum of the squares of the Euclidean distances to the hyperplanes of the system. If the starting point is chosen properly, then the limits approach the minimum norm weighted least squares solution. The proof is given for a block-Kaczmarz method.

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1. Introduction

In this paper we study the solution of the linear system of equations

$$Ax = b, \tag{1.1}$$

by Kaczmarz's method with relaxation. In particular, we consider what happens if the relaxation parameter is very small (strong underrelaxation). Kaczmarz's method for solving (1.1) is as follows. Let $A \in \mathbb{R}^{m \times n}$, (the space of $m \times n$ real matrices) and let a_i^T be the i'th row of A. A vector $x^0 \in \mathbb{R}^n$ (the real n-dimensional Euclidean space) is chosen arbitrarily, and is iteratively improved by the iteration process

$$x^{k+1} = x^k + \lambda_k \frac{b_i - a_i^T x^k}{\|a_i\|^2} a_i, \tag{1.2}$$

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where $i=k \bmod m+1$. The λ_k are relaxation parameters. It is no loss of generality to assume that the a_i are non-zero. Kaczmarz [7] proved that the sequence $\{x^k\}$ converges to the solution of (1.1) in the absence of relaxation, i.e., $\lambda_k=1$ for all k, assuming that A is square and non-singular. In this case, algorithm (1.2) performs successive orthogonal projections onto the hyperplanes

$$a_i^T x = b_i. \tag{1.3}$$

Herman et al. [6] proved convergence with arbitrary relaxation parameters satisfying

$$0 < \liminf_{k\to\infty} \lambda_k \leqq \limsup_{k\to\infty} \lambda_k < 2, \tag{1.4}$$

assuming (1.1) is consistent only (so A need not be non-singular and square). See also Censor [2] for some further comments and references.

In some significant practical cases, the method (1.2) is applied to *inconsistent* systems. In this case algorithm (1.2) cannot converge, but Tanabe [8] showed that in the absence of relaxation the subsequences

$$\{x^{km+i}\}_{k\geqq 0}, \quad 0 \leqq i \leqq m-1, \tag{1.5}$$

called *cyclic subsequences*, are convergent. This result of Tanabe was recently extended by Eggermont et al. [3]. A special case of their results shows that the cyclic subsequences converge in the inconsistent case if the relaxation parameters are *periodic*, i.e., $\lambda_k = \lambda_{i-1}$, $k \geqq 0$, and satisfy (1.4), [3, Theorem 1.1].

The use of relaxation parameters is important in practice. In the area of image reconstruction from projections it was demonstrated experimentally that small relaxation parameters significantly improve the practical performance of the algorithm (1.2), see Herman [5, Chap. 11.4–5], and in particular compare Figs. 11.4 and 11.5 against Figs. 11.2 and 11.3. So far, this phenomenon has not received a satisfactory explanation; the use of small relaxation parameters is still listed under the heading "Tricks" in [5]. We refer to the use of small relaxation parameters as "strong underrelaxation."

Inspired by this, we were led to investigate the effect of strong underrelaxation on Kaczmarz's method for *inconsistent* systems. We arrived at the following interesting mathematical result: as the relaxation parameters go to zero, the limits of the cyclic subsequences all approach the minimum norm (weighted) least squares solution of (1.1). The weighting matrix is presented. Geometrically, this particular weighted least squares solution minimizes the sum of the squares of the (Euclidean) distances to the hyperplanes determined by the equations.

We now summarize the paper. In Sect. 2 the matrix representation of a simple block-version of Kaczmarz's method is given. This simple version covers some important cases of the general block-Kaczmarz method of Eggermont et al. [3, Sect. 1]. In Sect. 3 we give sufficient conditions for the cyclic subsequences generated by this method to converge and derive a useful expression for their limits. We then investigate the behavior of the limits as the relaxation parameter goes to zero. In Sect. 4 we discuss the implications of this result to the Kaczmarz algorithm (1.2).

We use the following notations. I denotes the identity matrix, whose dimensions should be clear from the context. $\|\cdot\|$ denotes the Euclidean norm of vectors, in any real Euclidean vector space as well as the induced matrix norm (spectral norm). The Moore-Penrose inverse and transpose of a matrix A are denoted by $A^\dagger$ and A^T. $\mathcal{N}(A)$ and $\mathcal{R}(A)$ denote the nullspace and range of A. Finally, if $f(\lambda)$ is a matrix function depending on λ, and g is a nonnegative real function, then we write

$$f(\lambda)=O(g(\lambda)), \quad (\lambda \to 0) \tag{1.6}$$

to indicate that there exists a constant K such that for all λ small enough and positive,

$$\|f(\lambda)\| \leqq K g(\lambda). \tag{1.7}$$

2. Matrix Representation of the Block-Kaczmarz Method

In this section we present a simplified version of the block-Kaczmarz method, and give a matrix representation for a complete cycle of the iteration. At the end of this section we show that in most cases of interest, the simplified block-Kaczmarz method covers the general block-Kaczmarz method with relaxation matrices if we assume that the system has been scaled appropriately.

We consider the system

$$Ax=b \tag{2.1}$$

where $A \in \mathbb{R}^{LM \times N}$ and $b \in \mathbb{R}^{LM}$. We partition A and b as

$$A=\begin{pmatrix} A_1 \\ \hline A_2 \\ \hline \vdots \\ \hline A_M \end{pmatrix}, \quad b=\begin{pmatrix} b_1 \\ \hline b_2 \\ \hline \vdots \\ \hline b_M \end{pmatrix}, \tag{2.2}$$

with $A_i \in \mathbb{R}^{L \times N}$, $b_i \in \mathbb{R}^L$. We consider the following block-Kaczmarz method to solve (2.1), cf. [3, Sect. 1].

$$\begin{aligned} & x^0 \in \mathbb{R}^N, \quad \text{arbitrary}, \\ & x^{k+1}=x^k+\lambda A_i^T(b_i-A_i x^k), \\ & i=k \bmod M+1. \end{aligned} \tag{2.3}$$

In the special case $L=1$, and if the rows of A are scaled to have length one, this is Kaczmarz's algorithm with constant relaxation. Vasil'chenko and Svetlakov [9] study an orthogonal projections version of (2.3), i.e. λA_i^T replaced by $A_i^\dagger$, for a *nonsingular* system of equations.

Block-iterative methods of the Jacobi and SOR types for consistent and inconsistent systems of linear equations were carefully studied recently by Elfving [4].

Now we derive the matrix representation of one complete cycle of the algorithm (2.3), following closely Tanabe [8], cf. Elfving [4] and Eggermont et al. [3]. Writing the iterative step in (2.3) as

$$x^{k+1}=P_i x^k+\lambda A_i^T b_i \tag{2.4}$$

with

$$P_i=I-\lambda A_i^T A_i, \tag{2.5}$$

and $i=k \bmod M+1$, we obtain, by induction, that

$$x^{(k+1)M}=Qx^{kM}+Rb, \qquad k\geqq 0, \tag{2.6}$$

where

$$Q=P_M P_{M-1} \dots P_1, \tag{2.7}$$

$$Rb=\lambda \sum_{i=1}^{M} P_M \dots P_{i+1} A_i^T b_i. \tag{2.8}$$

Here, for $i=M$, $P_M \dots P_{i+1}$ is taken as I.

From (2.6) we have, again by induction, that

$$x^{(k+1)M}=\sum_{\ell=0}^{k} Q^{\ell} Rb+Q^{k+1}x^0. \tag{2.9}$$

This formula is the starting point for our analysis of strong underrelaxation. Similar formulas hold for the other cyclic subsequences $\{x^{kM+i}\}_{k\geqq 0}$, $1\leqq i\leqq M-1$.

We finish this section by discussing the generality of the iteration process (2.3). In Eggermont et al. [3], the convergence of the following block-Kaczmarz method is studied.

$$\begin{aligned} &x^0\in\mathbb{R}^N, \quad \text{arbitrary},\\ &x^{k+1}=x^k+A_i^T\Sigma^{(k)}(b_i-A_i x^k),\\ &i=k \bmod M+1. \end{aligned} \tag{2.10}$$

It is shown that a sufficient condition for convergence in case the system $Ax=b$ is consistent is that

$$\limsup_{k\to\infty} \|A_i^{\dagger} A_i(I-A_i^T\Sigma^{(k)}A_i)\|<1. \tag{2.11}$$

In case the system $Ax=b$ is inconsistent and if the method (2.10) is periodic, i.e.,

$$\Sigma^{(k)}=\Sigma^{(i-1)}, \tag{2.12}$$

where $i=k \bmod M+1$, then (2.11) is a sufficient condition for the convergence of the cyclic subsequences $\{x^{kM+i}\}_{k\geqq 0}$, $0\leqq i\leqq M-1$.

Numerically, the method (2.10) was used with the $\Sigma^{(i-1)}$ equal to a positive diagonal matrix, [3, Eq. (2.18)]. In this case, and other cases as well, $\Sigma^{(i-1)}$ may be written as

$$\Sigma^{(i-1)} = \Omega_i^T \Omega_i, \tag{2.13}$$

and the iterative step in (2.10) is of the form

$$x^{k+1} = x^k + B_i^T(\tilde{b}_i - B_i x^k), \tag{2.14}$$

where $B_i = \Omega_i A_i$. In other words, if (2.12–13) hold, then the algorithm (2.10) is of the same form as algorithm (2.3). By applying algorithm (2.3) to the scaled system

$$\Omega A x = \Omega b, \tag{1.15}$$

where Ω is the block-diagonal matrix with blocks $\Omega_1, \Omega_2, \ldots, \Omega_M$, we obtain algorithm (2.10, 12, 13) applied to the original system (2.1). So it is no great loss of generality to study (2.3) rather that (2.10).

3. The Effect of Strong Underrelaxation

In this section we investigate the effect of strong underrelaxation on the limits of the cyclic subsequencs generated by the block-Kaczmarz algorithm (2.3). As mentioned before, we consider only the cyclic subsequence $\{x^{kM}\}_{k \geqq 0}$. A similar analysis applies to the other subsequences. We prove the following result.

Theorem 1. *For all λ small enough,*

$$x^*(\lambda) = \lim_{k \to \infty} x^{kM} \tag{3.1}$$

exists, and

$$\lim_{\lambda \to 0} x^*(\lambda) = A^\dagger b + (I - A^\dagger A) x^0. \tag{3.2}$$

We divide the proof into a number of lemmas. Lemmas 1 and 2 follow closely Tanabe [8], cf. [3].

First we recall some results from [3].

Lemma 1. *Let*

$$\lambda_0 = \min_{1 \leqq i \leqq M} 2 \|A_i A_i^T\|^{-1}. \tag{3.3}$$

Then, for all $\lambda \in (0, \lambda_0)$,

(i) *Q is a contractive mapping of $\mathscr{R}(A^T)$ into itself;*

(ii) $\lim_{k \to \infty} Q^k = I - A^\dagger A$;

(iii) $\mathscr{R}(I - Q) = \mathscr{R}(I - Q^T) = \mathscr{R}(A^T)$.

Proof. We show that if $\lambda \in (0, \lambda_0)$, then

$$\|A_i^\dagger A_i (I - \lambda A_i^T A_i)\| < 1 \tag{3.4}$$

for all $1 \leqq i \leqq M$. This is condition (2.11) for the case

$$\Sigma^{(k)} = \lambda I, \quad k \geqq 0,$$

so that we then may appeal to the results of [3]. To show (3.4), let

$$A_i = U_i \Lambda_i V_i^T \tag{3.5}$$

be the singular value decomposition of A_i, with Λ_i a square, nonsingular matrix. Then

$$A_i^\dagger = V_i \Lambda_i^\dagger U_i^T$$

and so

$$\|A_i^\dagger A_i (I - \lambda A_i^T A_i)\| = \|I - \lambda \Lambda_i^2\|.$$

The condition

$$\|I - \lambda \Lambda_i^2\| < 1, \quad 1 \leqq i \leqq M,$$

is readily verified to be equivalent to $\lambda \in (0, \lambda_0)$.

Now (i) follows from [3, Lemma 5.4] and (ii) from [3, Theorem 5.5]. Also, from [3, Lemma 5.4],

$$\mathcal{N}(I - Q) = \mathcal{N}(A), \tag{3.6}$$

hence

$$\mathcal{R}(I - Q^T) = \mathcal{R}(A^T). \tag{3.7}$$

Since Q^T is the iteration matrix if in algorithm (2.3) we use the blocks A_i in reverse order, we have, similarly to (3.6),

$$\mathcal{N}(I - Q^T) = \mathcal{N}(A),$$

hence

$$\mathcal{R}(I - Q) = \mathcal{R}(A^T).$$

Together with (3.7), this proves (iii). □

Now we are ready to derive the convergence of $\{x^{kM}\}_{k \geqq 0}$, as well as a useful expression for its limit.

Lemma 2. *Let* $\lambda \in (0, \lambda_0)$, *with* λ_0 *given by* (3.3). *Then*

$$x^*(\lambda) = \lim_{k \to \infty} x^{kM}$$

exists and

$$x^*(\lambda) = (I - Q)^\dagger R b + (I - A^\dagger A) x^0. \tag{3.9}$$

Proof. From (2.8) we see that R_i, the i'th block of R where R is partitioned in the same way as A^T, is given by

$$R_i = \lambda P_M \dots P_{i+1} A_i^T$$

hence for an arbitrary vector $x \in \mathbb{R}^m$ we may write with the aid of (2.5),

$$Rx = \sum_{i=1}^{m} R_i x_i = \sum_{i=1}^{m} \lambda x_i (I - \lambda A_M^T A_M) \dots (I - \lambda A_{i+1}^T A_{i+1}) A_i^T.$$

The right hand side of the last equation is some linear combination of blocks of A^T, thus

$$\mathscr{R}(R) \subseteq \mathscr{R}(A^T),$$

hence

$$R = A^\dagger A R. \tag{3.10}$$

By Lemma 1 (i) we have then that

$$Q A^\dagger A = A^\dagger A Q A^\dagger A \tag{3.11}$$

so

$$\tilde{Q} = A^\dagger A Q A^\dagger A \tag{3.12}$$

has norm less that one. Also, by (3.10–12),

$$\sum_{\ell=0}^{k} Q^\ell R = \sum_{\ell=0}^{k} \tilde{Q}^\ell R.$$

Since the series on the right converges when $k \to \infty$, so does the series on the left. Hence, from (2.9)

$$\lim_{k \to \infty} x^{kM} = \sum_{\ell=0}^{\infty} \tilde{Q}^\ell R b + \lim_{k \to \infty} \tilde{Q}^{k+1} x^0.$$

Since $\|\tilde{Q}\| < 1$ the series on the right equals

$$(I - \tilde{Q})^{-1} R b,$$

and the limit on the right equals

$$(I - A^\dagger A) x^0,$$

by Lemma 1 (ii). So, for $\lambda \in (0, \lambda_0)$,

$$x^*(\lambda) = (I - \tilde{Q})^{-1} R b + (I - A^\dagger A) x^0. \tag{3.13}$$

The final step of the proof is to show that

$$(I - \tilde{Q})^{-1} R = (I - Q)^\dagger R.$$

Since $\mathscr{R}(R) \subset \mathscr{R}(A^T)$, it suffices to show that

$$(I - \tilde{Q})^{-1} A^T = (I - Q)^\dagger A^T.$$

For arbitrary y, consider the equation

$$(I - Q) x = A^T y.$$

By Lemma 1 (iii), this is a consistent system of equations, so its minimum norm least squares solution

$$\tilde{x} = (I - Q)^\dagger A^T y$$

is an exact solution. By Lemma 1 (iii), it follows that $\tilde{x} \in \mathscr{R}(A^T) = \mathscr{R}(A^\dagger A)$ so $\tilde{x} = A^\dagger A x$, and also that $(I-Q)\tilde{x} = A^\dagger A(I-Q)\tilde{x}$. Combining these two observations, we obtain

$$\begin{aligned}(I-Q)\tilde{x} &= A^\dagger A(I-Q)A^\dagger A\tilde{x}\\ &= (I - A^\dagger AQA^\dagger A)\tilde{x}.\end{aligned}$$

So,

$$(I-Q)\tilde{x} = A^T y = (I-\tilde{Q})\tilde{x}.$$

Since $I-\tilde{Q}$ is invertible, $\tilde{x}$ is also given by

$$\tilde{x} = (I-\tilde{Q})^{-1}A^T y,$$

and we are done. □

Now we are at the point where we can look what happens to $x^*(\lambda)$ as $\lambda \to 0$. The dependence of $x^*(\lambda)$ on λ is only in $(I-Q)^\dagger Rb$. It is readily verified, by inspection of (2.8), that

$$Rb = \lambda A^T b + O(\lambda^2), \quad (\lambda \to 0), \tag{3.14}$$

and that

$$I - Q = \lambda A^T A + O(\lambda^2), \quad (\lambda \to 0). \tag{3.15}$$

From (3.15) it is seen that we need to investigate perturbations of Moore-Penrose inverses. The following lemma is compiled from Ben-Israel and Greville [1, pp. 184–185].

Lemma 3. *If $m \times n$ matrices F and E satisfy*

$$\mathscr{R}(E) \subseteq \mathscr{R}(F), \quad \mathscr{R}(E^T) \subseteq \mathscr{R}(F^T) \tag{3.16}$$

and

$$\|F^\dagger E\| < 1 \tag{3.17}$$

then

$$\|(F+E)^\dagger - F^\dagger\| \leqq \frac{\|F^\dagger E\| \; \|F^\dagger\|}{1 - \|F^\dagger E\|}. \tag{3.18}$$

With this lemma in hand, we are ready to prove the following.

Lemma 4.

$$\|(I-Q)^\dagger - \lambda^{-1}(A^T A)^\dagger\| = O(1), \quad (\lambda \to 0).$$

Proof. Define the matrix E by

$$I - Q = \lambda(A^T A + E). \tag{3.19}$$

From (3.15) we have

$$\|E\| = O(\lambda), \quad (\lambda \to 0).$$

From Lemma 1 (iii) we obtain that

$$\mathscr{R}(E) = \mathscr{R}(E^T) = \mathscr{R}(A^T A). \tag{3.20}$$

Also

$$\|(A^T A)^\dagger E\| = O(\lambda), \quad (\lambda \to 0), \tag{3.21}$$

since $(A^T A)^\dagger$ does not depend on λ, so this is certainly less than one for λ small enough. Conditions (3.20–21) now allow us to conclude from Lemma 3 that

$$\|(A^T A + E)^\dagger - (A^T A)^\dagger\| = O(\lambda), \quad (\lambda \to 0). \tag{3.22}$$

From (3.19) we finally have

$$(I-Q)^\dagger = \lambda^{-1}(A^T A + E)^\dagger,$$

so that (3.22) proves the lemma. □

The proof of Theorem 1 now follows from the above analysis. We must show that

$$\lim_{\lambda \to 0} (I-Q)^\dagger R b = A^\dagger b. \tag{3.23}$$

We have

$$\begin{aligned}(I-Q)^\dagger R b &= [\lambda^{-1}(A^T A)^\dagger + O(1)]\,[\lambda A^T + O(\lambda^2)]\,b \\ &= (A^T A)^\dagger A^T b + O(\lambda).\end{aligned}$$

whence (3.23) follows. □

4. Discussion

In this section we discuss the effect of the (implicit) scaling in Kaczmarz's algorithm (1.2) and the block-Kaczmarz method (2.3).

It is easily seen that algorithm (1.2) is a special case of algorithm (2.3), with $L=1$, assuming that the rows of A have been scaled to have length one. Instead of system (1.1) we have the system

$$DAx = Db \tag{4.1}$$

where D is a diagonal matrix with

$$D_{i,i} = \|a_i\|^{-1}, \quad 1 \leqq i \leqq m, \tag{4.2}$$

cf. the discussion at the end of Sect. 2. Now Theorem 1 says that $z^* = \lim_{\lambda \to 0} x^*(\lambda)$ equals

$$z^* = (DA)^\dagger D b + (I - (DA)^\dagger (DA)) x^0. \tag{4.3}$$

It follows that

$$A^T D^2 A z^* = A^T D^2 b, \tag{4.4}$$

i.e., z^* is a weighted least squares solution of the system $Ax=b$. From (4.2) it is seen that z^* minimizes the sum of the squares of the (Euclidean) distances to the hyperplanes determined by the equations of the system.

Observe that since D is nonsingular $\mathscr{R}(A^T D)=\mathscr{R}(A^T)$, so if $x^0 \in \mathscr{R}(A^T)$, e.g., $x^0=0$, then (4.3) is equivalent to

$$z^* = (DA)^\dagger D b, \tag{4.5}$$

and z^* is the minimum norm weighted least squares solution.

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