Pseudoinverse-free randomized extended block Kaczmarz for solving least squares

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Abstract

Randomized iterative algorithms have recently been proposed to solve large-scale linear systems. In this paper, we present a simple randomized extended block Kaczmarz algorithm that exponentially converges in the mean square to the unique minimum $\ell_2$-norm least squares solution of a given linear system of equations. The proposed algorithm is pseudoinverse-free and therefore different from the projection-based randomized double block Kaczmarz algorithm of Needell, Zhao, and Zouzias. We emphasize that our method works for all types of linear systems (consistent or inconsistent, overdetermined or underdetermined, full-rank or rank-deficient). Moreover, our approach can utilize efficient implementations on distributed computing units, yielding remarkable improvements in computational time. Numerical examples are given to show the efficiency of the new algorithm.

Keywords: general linear systems, minimum $\ell_2$-norm least squares solution, randomized extended (block) Kaczmarz, exponential convergence

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1 Introduction

The Kaczmarz method [27] is a simple iterative method for solving a linear systems of equations

$$Ax = b, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^m.$$ 

Due to its simplicity and numerical performance, the Kaczmarz method has found many applications in many fields, such as computer tomography [33, 28, 24], image reconstruction [14, 25], digital signal processing [9, 32], etc. At each step, the method projects the current iterate onto one hyperplane defined by a row of the system. More precisely, assuming that the $i$th row $A_{i,:}$ has been selected at the $k$th iteration, then the $k$th estimate vector $x^k$ is obtained by

$$x^k = x^{k-1} - \alpha_k \frac{A_{i,:}x^{k-1} - b_i}{\langle A_{i,:}, (A_{i,:})^T \rangle} (A_{i,:})^T,$$

where $(A_{i,:})^T$ denotes the transpose of $A_{i,:}$, $b_i$ is the $i$th component of $b$, and $\alpha_k$ is a stepsize. Numerical experiments show that using the rows of the coefficient matrix in the Kaczmarz method in random order, rather than in their given order, can often greatly improve the convergence [26, 34]. In a seminal paper [17], Strohmer and Vershynin proposed a randomized Kaczmarz (RK) algorithm which exponentially converges in expectation to the solutions of consistent, overdetermined, full-rank linear systems. The convergence result was extended and refined in

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Let \( A^\dagger \) denote the Moore-Penrose pseudoinverse\(^1\) of \( A \). In this paper, we are interested in the vector \( A^\dagger b \). Here we would like to make clear what \( A^\dagger b \) stands for for different types of linear systems (see \[7\] [19]):

1. If \( Ax = b \) is consistent with full-column rank \( A \), i.e., \( \text{rank}(A) = n \), then \( A^\dagger b \) is the unique solution. In this case, we have \( m \geq n \) and the linear system is overdetermined when \( m > n \).

2. If \( Ax = b \) is consistent with \( \text{rank}(A) < n \), then \( A^\dagger b \) is the unique minimum \( \ell_2 \)-norm solution. In this case, we have \( m \geq n \) or \( m < n \), and the linear system is overdetermined (resp. underdetermined) when \( m > n \) (resp. \( m < n \)). The matrix \( A \) can be of full-row rank, i.e., \( \text{rank}(A) = m \), or rank-deficient, i.e., \( \text{rank}(A) < m \).

3. If \( Ax = b \) is inconsistent with \( \text{rank}(A) = n \), then \( A^\dagger b \) is the unique least squares solution. In this case, we have \( m \geq n \) and the linear system is overdetermined when \( m > n \).

4. If \( Ax = b \) is inconsistent with \( \text{rank}(A) < n \), then \( A^\dagger b \) is the unique minimum \( \ell_2 \)-norm least squares solution. In this case, we have \( m \geq n \) or \( m < n \), and the linear system is overdetermined (resp. underdetermined) when \( m > n \) (resp. \( m < n \)). The matrix \( A \) can be of full-row rank, i.e., \( \text{rank}(A) = m \), or rank-deficient, i.e., \( \text{rank}(A) < m \).

If \( Ax = b \) is inconsistent, Needell \[37\] showed that RK does not converge to \( A^\dagger b \). To resolve this problem, Zouzias and Freris \[50\] proposed a randomized extended Kaczmarz (REK) algorithm, which uses RK twice \[30\] \[13\] at each iteration and exponentially converges in the mean square to \( A^\dagger b \). More precisely, assuming that the \( j \)-th column \( A_{:,j} \) and the \( i \)-th row \( A_{i,:} \) have been selected at the \( k \)-th iteration, REK generates two vectors \( z^k \) and \( x^k \) via two RK updates (one for \( A^\dagger z = 0 \) from \( z^{k-1} \) and the other for \( Ax = b \) from \( x^{k-1} \)):

\[
\begin{align*}
    z^k &= z^{k-1} - \frac{(A_{:,j})^T z^{k-1}}{(A_{:,j})^T A_{:,j} A_{:,j}^T z^{k-1}} A_{:,j}, \\
    x^k &= x^{k-1} - \frac{A_{i,:} x^{k-1} - b_i + z_i^k}{A_{i,:} (A_{i,:})^T} (A_{i,:})^T.
\end{align*}
\]

For general linear systems (consistent or inconsistent, full-rank or rank-deficient), the vector \( x^k \) generated by REK exponentially converges to \( A^\dagger b \) if \( z^0 \in b + \text{range}(A) \) and \( x^0 \in \text{range}(A^T) \) \[30\] \[13\]. To accelerate the convergence, the following projection-based block variants \[39\] \[40\] of RK and REK were developed. For a subset \( \mathcal{I} \subset \{1, 2, \ldots, m\} \) and a subset \( \mathcal{J} \subset \{1, 2, \ldots, n\} \), denote by \( A_{\mathcal{I},:} \) and \( A_{:,\mathcal{J}} \) the row submatrix of \( A \) indexed by \( \mathcal{I} \) and the column submatrix of \( A \) indexed by \( \mathcal{J} \), respectively. Assuming that the subset \( \mathcal{I}_i \) has been selected at the \( k \)-th iteration, the randomized block Kaczmarz (RBK) algorithm \[39\] generates the \( k \)-th estimate \( x^k \) via

\[
x^k = x^{k-1} - (A_{\mathcal{I}_i,:})^T (A_{\mathcal{I}_i,:} x^{k-1} - b_{\mathcal{I}_i}).
\]

Assuming that the subsets \( \mathcal{J}_i \) and \( \mathcal{I}_i \) have been selected at the \( k \)-th iteration, the randomized double block Kaczmarz (RDBK) algorithm \[40\] generates the \( k \)-th estimate \( x^k \) via

\[
\begin{align*}
    z^k &= z^{k-1} - A_{:,\mathcal{J}_i} (A_{:,\mathcal{J}_i})^T z^{k-1}, \\
    x^k &= x^{k-1} - (A_{\mathcal{I}_i,:})^T (A_{\mathcal{I}_i,:} x^{k-1} - b_{\mathcal{I}_i} + z_{\mathcal{I}_i}^k).
\end{align*}
\]

\(^1\)Every \( m \times n \) matrix \( A \) has a unique Moore-Penrose pseudoinverse. In particular, in this paper we will use the following property of the pseudoinverse: \( A^T = A^\dagger A A^\dagger \).
Numerical experiments demonstrate that the convergence can be significantly accelerated if appropriate blocks of the coefficient matrix are used. The main drawback of projection-based block methods is that each iteration is expensive since one needs to apply pseudoinverses to vectors, or, equivalently, we must solve least-squares problems at each iteration. Moreover, projection-based block methods are not adequate for distributed implementations.

Recently, Necoara [35] proposed a randomized average block Kaczmarz (RABK) algorithm for consistent linear systems, which takes a convex combination of the projections of the current iterate onto several hyperplanes as a new direction with some stepsize. Assuming that the subset \( \mathcal{I} \) has been selected at the \( k \)th iteration, RABK generates the \( k \)th estimate \( x^k \) via

\[
x^k = x^{k-1} - \alpha_k \left( \sum_{i \in \mathcal{I}} \omega_i^k \frac{A_{i,:} x^{k-1} - b_i}{A_{i,:} (A_i^T)^T} \right),
\]

where the weights \( \omega_i^k \in [0,1] \) such that \( \sum_{i \in \mathcal{I}} \omega_i^k = 1 \), and the stepsize \( \alpha_k \in (0,2) \). The convergence analysis reveals that RABK is extremely effective when it is given a good sampling of the rows into well-conditioned blocks. Shortly afterwards, Du and Sun [15] proposed a doubly stochastic block Gauss-Seidel (DSBGS) algorithm, which uses a submatrix of the coefficient matrix at each iteration. Assuming that the subsets \( \mathcal{I} \) and \( \mathcal{J} \) have been selected at the \( k \)th iteration, DSBGS generates the \( k \)th estimate \( x^k \) via

\[
x^k = x^{k-1} - \alpha_k \frac{I_{\mathcal{I},\mathcal{J}} (A_{\mathcal{I},\mathcal{J}})^T (I_{\mathcal{I},\mathcal{J}})^T (A x^{k-1} - b)}{\| A_{\mathcal{I},\mathcal{J}} \|^2_F},
\]

where \( I \) denotes the identity matrix, \( A_{\mathcal{I},\mathcal{J}} \) denotes the submatrix that lies in the rows indexed by \( \mathcal{I} \) and the columns indexed by \( \mathcal{J} \), and \( \| \cdot \|_F \) is the Frobenius norm. Exponential convergence of DSBGS for consistent linear systems was proved. Setting \( \mathcal{I} \subset \{1,2,\ldots,m\} \) and \( \mathcal{J} = \{1,2,\ldots,n\} \), DSBGS recovers a special case of RABK, i.e., RABK with weight

\[
\omega_i^k = \frac{A_{i,:} (A_i^T)^T}{\| A_{i,:} \|^2_F}, \quad i \in \mathcal{I}.
\]

Note that both RABK and DSBGS are pseudoinverse-free and can utilize efficient implementations on distributed computing units, yielding remarkable improvements in computational time. We emphasize that convergence results in the mean square of RABK and DSBGS are obtained only for consistent linear systems.

In this paper, we present a pseudoinverse-free randomized extended block Kaczmarz (REBK) algorithm that exponentially converges in the mean square to the unique minimum \( \ell_2 \)-norm (least squares) solution of a given general linear system (full-rank or rank-deficient, overdetermined or underdetermined, consistent or inconsistent). Our method is different from those projection-based block methods, for example, those in [18] [1, 8, 42] [39] [40] [16]. At each step, REBK, as a direct extension of REK, uses two RABK (with special choice of \( \omega_i \)) updates (one for \( A_i^T z = 0 \) from \( z^{k-1} \) and the other for \( Ax = b - z^k \) from \( x^{k-1} \); see Section 2 for details). Compared with REK, REBK can exploit the high-level basic linear algebra subroutine (BLAS2), even fast matrix-vector multiplies (for example, if submatrices of \( A \) have circulant or Toeplitz structures, then the Fast Fourier Transform technique can be used), and therefore could be more efficient. We refer the reader to [39] for more advantages of block methods. Numerical examples are given to illustrate the efficiency of REBK.

Organization of the paper. In the rest of this section, we give some notation. In Section 2 we describe the pseudoinverse-free randomized extended block Kaczmarz algorithm and prove its convergence theory. Both the exponential convergence of the norm of the expected error and the exponential convergence of the expected norm of the error are discussed. In Section 3 we report the numerical results. Finally, we present brief concluding remarks in Section 4.
Notation. For any random variable $\xi$, let $E[\xi]$ denote its expectation. For an integer $m \geq 1$, let $[m] := \{1, 2, 3, \ldots, m\}$. Lowercase (upper-case) boldface letters are reserved for column vectors (matrices). For any vector $u \in \mathbb{R}^m$, we use $u_i$, $u^T$, and $\|u\|_2$ to denote the $i$th element, the transpose, and the $\ell_2$-norm of $u$, respectively. We use $I$ to denote the identity matrix whose order is clear from the context. For any matrix $A \in \mathbb{R}^{m \times n}$, we use $A^T$, $A^1$, $\|A\|_F$, range($A$), $\sigma_1(A) \geq \sigma_2(A) \geq \cdots \geq \sigma_r(A) > 0$ to denote the transpose, the Moore-Penrose pseudoinverse, the Frobenius norm, the column space, and all the nonzero singular values of $A$, respectively. Obviously, $r$ is the rank of $A$. For index sets $I \subseteq [m]$ and $J \subseteq [n]$, let $A_{I,:}$, $A_{:,J}$, and $A_{I,J}$ denote the row submatrix indexed by $I$, the column submatrix indexed by $J$, and the submatrix that lies in the rows indexed by $I$ and the columns indexed by $J$, respectively. We call $\{I_1, I_2, \ldots, I_s\}$ a partition of $[m]$ if $I_i \cap I_j = \emptyset$ and $\cup_{i=1}^s I_i = [m]$. Similarly, $\{J_1, J_2, \ldots, J_t\}$ denotes a partition of $[n]$ if $J_i \cap J_j = \emptyset$ and $\cup_{i=1}^t J_i = [n]$.

2 The randomized extended block Kaczmarz algorithm

Pseudoinverse-free block methods [35, 15] have been proposed to solve general consistent linear systems (full-rank or rank-deficient, overdetermined or underdetermined). Because of the efficient implementations, these block methods show better performance compared with their standard variants. It is natural to ask whether one can design a pseudoinverse-free block method for solving general inconsistent linear systems, that is, finding least squares solutions. In this section, based on given partitions of $[m]$ and $[n]$, we propose the following pseudoinverse-free randomized extended block Kaczmarz algorithm (see Algorithm 1) for solving consistent or inconsistent linear systems. We emphasize that, at each step, only matrix-vector products are involved, therefore the high-level basic linear algebra subroutine (BLAS2) even fast matrix-vector multiplies can be exploited.

\begin{algorithm}
Let $\{I_1, I_2, \ldots, I_s\}$ and $\{J_1, J_2, \ldots, J_t\}$ be partitions of $[m]$ and $[n]$, respectively. Let $\alpha > 0$. Initialize $z^0 \in b + \text{range}(A)$ and $x^0 \in \text{range}(A^T)$.

for $k = 1, 2, \ldots,$ do

Pick $j \in [t]$ with probability $\|A_{:,J_j}\|_F^2/\|A\|_F^2$

Set $z^k = z^{k-1} - \frac{\alpha}{\|A_{I,J_j}\|_F^2} A_{I,J_j}(A_{:,J_j})^T z^{k-1}$

Pick $i \in [s]$ with probability $\|A_{I_i,:}\|_F^2/\|A\|_F^2$

Set $x^k = x^{k-1} - \frac{\alpha}{\|A_{I_i,:}\|_F^2} (A_{I_i,:})^T (A_{I_i,:}x^{k-1} - b_{I_i} + z_{I_i}^k)$

end for

end Algorithm 1: Randomized extended block Kaczmarz (REBK)

Here we only consider constant stepsize for simplicity. By choosing the row partition parameter $s = m$, the column partition parameter $t = n$, and the stepsize $\alpha = 1$, we recover the well-known randomized extended Kaczmarz algorithm of Zouzias and Freris [50]. REBK uses two RABK updates (see [1]) at each step:

- RABK update for $A^T z = 0$ from $z^{k-1}$

$$z^k = z^{k-1} - \alpha \left( \sum_{l \in J_j} \omega_l^k (A_{l,J_j})^T z^{k-1} \right), \quad \omega_l^k = \frac{(A_{l,J_j})^T A_{l,J_j}}{\|A_{l,J_j}\|_F^2};$$

- RABK update for $Ax = b - z^k$ from $x^{k-1}$

$$x^k = x^{k-1} - \alpha \left( \sum_{l \in I_i} \omega_l^k A_{l,I_i} x^{k-1} - b_{I_i} + z_{I_i}^k \right) (A_{l,I_i})^T, \quad \omega_l^k = \frac{A_{l,I_i}(A_{l,I_i})^T}{\|A_{l,I_i}\|_F^2}. $$
Before proving the convergence theory of REBK for general linear systems, we give the following notation. Let $E_{k-1} [\cdot]$ denote the conditional expectation conditioned on the first $k - 1$ iterations of REBK. That is,

$$E_{k-1} [\cdot] = E [\cdot | j_1, i_1, j_2, i_2, \ldots, j_{k-1}, i_{k-1}],$$

where $j_l$ is the $l$th column block chosen and $i_l$ is the $l$th row block chosen. We denote the conditional expectation conditioned on the first $k - 1$ iterations and the $k$th column block chosen as

$$E_{k-1}^k [\cdot] = E [\cdot | j_1, i_1, j_2, i_2, \ldots, j_{k-1}, i_{k-1}, j_k].$$

Then by the law of total expectation we have

$$E_{k-1} [\cdot] = E_{k-1} [E_{k-1}^k [\cdot]].$$

### 2.1 The exponential convergence of the norm of the expected error

In this subsection we show the exponential convergence of the norm of the expected error, i.e.,

$$\|E [x^k - A^\dagger b]\|_2.$$

The convergence of the norm of the expected error depends on the positive number $\delta$ defined as

$$\delta := \max_{1 \leq i \leq r} 1 - \frac{\alpha \sigma^2(A)}{\|A\|_F^2}.$$

The following lemma will be used and its proof is straightforward (via singular value decomposition).

**Lemma 1.** Let $\alpha > 0$ and $A$ be any nonzero real matrix with $\text{rank}(A) = r$. For every $u \in \text{range}(A^T)$, it holds

$$\left\| \left( I - \frac{A^T A}{\|A\|_F^2} \right)^k u \right\|_2 \leq \delta k \|u\|_2.$$

We give the convergence of the norm of the expected error of REBK in the following theorem.

**Theorem 2.** For any given consistent or inconsistent linear system $Ax = b$, let $x^k$ be the $k$th iterate of REBK with $z^0 \in b + \text{range}(A)$ and $x^0 \in \text{range}(A^T)$. It holds

$$\|E [x^k - A^\dagger b]\|_2 \leq \delta^k \left( \|x^0 - A^\dagger b\|_2 + \frac{\alpha k \|A^T z^0\|_2}{\|A\|_F^2} \right).$$

**Proof.** By $A^T b = A^T A A^\dagger b$ and

$$x^k - A^\dagger b = x^{k-1} - A^\dagger b - \frac{\alpha}{\|A^T_{l_i} \|_F} (A^T_{l_i} x^{k-1} - b_{l_i} + z^k_{l_i}),$$
we have
\[
E_{k-1} \left[ x^k - A^I b \right] = E_{k-1} \left[ E_{k-1}^i \left[ x^k - A^I b \right] \right]
\]
\[
= x^{k-1} - A^I b - E_{k-1} \left[ \alpha \frac{A^T (A x^{k-1} - b + z^k)}{\|A\|_F^2} \right]
\]
\[
= x^{k-1} - A^I b - \alpha \frac{A^T A x^{k-1} - A^T b}{\|A\|_F^2} - \alpha \frac{A^T}{\|A\|_F^2} E_{k-1} \left[ z^k \right]
\]
\[
= \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right) (x^{k-1} - A^I b) - \alpha \frac{A^T}{\|A\|_F^2} \left( I - \alpha \frac{A A^T}{\|A\|_F^2} \right) z^{k-1}
\]
Taking expectation gives
\[
E \left[ x^k - A^I b \right] = E \left[ E_{k-1} \left[ x^k - A^I b \right] \right]
\]
\[
= \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right) E \left[ x^{k-1} - A^I b \right] - \alpha \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right)^k \frac{A^T z^0}{\|A\|_F^2}
\]
\[
= \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right)^2 E \left[ x^{k-2} - A^I b \right] - 2 \alpha \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right)^k \frac{A^T z^0}{\|A\|_F^2}
\]
\[
= \cdots
\]
\[
= \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right)^k (x^0 - A^I b) - \alpha k \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right)^k \frac{A^T z^0}{\|A\|_F^2}
\]
Applying the norms to both sides we obtain
\[
\|E \left[ x^k - A^I b \right]\|_2 = \left\| \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right)^k (x^0 - A^I b) - \alpha k \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right)^k \frac{A^T z^0}{\|A\|_F^2} \right\|_2
\]
\[
\leq \left\| \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right)^k (x^0 - A^I b) \right\|_2 + \alpha k \left\| \left( I - \alpha \frac{A^T A}{\|A\|_F^2} \right)^k \frac{A^T z^0}{\|A\|_F^2} \right\|_2
\]
\[
\leq \delta^k \left( \|x^0 - A^I b\|_2 + \frac{\alpha k \|A^T z^0\|_2}{\|A\|_F^2} \right).
\]
Here the last inequality follows from the fact that \(x^0 - A^I b \in \text{range}(A^T)\), \(A^T z^0 \in \text{range}(A^T)\), and Lemma [\(\square\)]

**Remark 3.** To ensure convergence of the expected error, it suffices to have
\[
\delta = \max_{1 \leq i \leq r} \left| 1 - \frac{\alpha \sigma_i^2(A)}{\|A\|_F^2} \right| < 1,
\]
which implies
\[
0 < \alpha < \frac{2\|A\|_F^2}{\sigma_r^4(A)}.
\]
2.2 The exponential convergence of the expected norm of the error

In this subsection we show the exponential convergence of the expected norm of the error, i.e.,

$$E \left[ \|z^k - A^*b\|_2^2 \right].$$

The convergence of the expected norm of the error depends on the positive number $\rho$ defined as

$$\rho := 1 - \frac{(2\alpha - \alpha^2)\sigma^2_F(A)}{\|A\|_F^2}.$$

The following lemmas will be used extensively in this paper. Their proofs are straightforward and we omit the details.

**Lemma 4.** Let $A$ be any nonzero real matrix with $\text{rank}(A) = r$. For every $u \in \text{range}(A)$, it holds

$$\|A^T u\|_2^2 \geq \sigma^2_F(A)\|u\|_2^2.$$

**Lemma 5.** Let $A$ be any nonzero real matrix. For every $u \in \mathbb{R}^m$, it holds

$$u^T A A^T u \leq \|A\|_F^2 u^T u.$$

In the following lemma we show that the vector $z^k$ generated in REBK with $z^0 \in b + \text{range}(A)$ converges to

$$b_\perp := (I - AA^\dagger)b,$$

which is the orthogonal projection of $z^0$ onto the set $\{ z \ | \ A^T z = 0 \}$.

**Lemma 6.** For any given consistent or inconsistent linear system $Ax = b$, let $z^k$ be the vector generated in REBK with $z^0 \in b + \text{range}(A)$. It holds

$$E \left[ \|z^k - b_\perp\|_2^2 \right] \leq \rho^k \|z^0 - b_\perp\|_2^2.$$

*Proof.* By $(A_i, J_i)^T b_\perp = 0$, we have

$$z^k - b_\perp = z^{k-1} - b_\perp - \frac{\alpha}{\|A_i, J_i\|_F^2} A_i, J_i (A_i, J_i)^T (z^{k-1} - b_\perp). \quad (2)$$

By $z^0 - b_\perp = AA^\dagger z^0 \in \text{range}(A)$, we can show that $z^k - b_\perp \in \text{range}(A)$ by induction. It follows from (2) that

$$\|z^k - b_\perp\|_2^2 = \|z^{k-1} - b_\perp\|_2^2 - \frac{2\alpha \| (A_i, J_i)^T (z^{k-1} - b_\perp)\|_2^2}{\|A_i, J_i\|_F^2}$$

$$+ \frac{\alpha^2}{\|A_i, J_i\|_F^2} (z^{k-1} - b_\perp)^T A_i, J_i (A_i, J_i)^T A_i, J_i (A_i, J_i)^T (z^{k-1} - b_\perp)$$

$$\leq \|z^{k-1} - b_\perp\|_2^2 - \frac{(2\alpha - \alpha^2) \| (A_i, J_i)^T (z^{k-1} - b_\perp)\|_2^2}{\|A_i, J_i\|_F^2}. \quad \text{(by Lemma 5)}$$

Taking the conditioned expectation on the first $k - 1$ iterations yields

$$E_{k-1} \left[ \|z^k - b_\perp\|_2^2 \right] \leq \|z^{k-1} - b_\perp\|_2^2 - \frac{(2\alpha - \alpha^2) \|A^T (z^{k-1} - b_\perp)\|_2^2}{\|A\|_F^2}$$

$$\leq \rho \|z^{k-1} - b_\perp\|_2^2. \quad \text{(by Lemma 4)}$$
Taking expectation again gives
\[
E \left[ \| z^k - b \|_2^2 \right] = E \left[ E_{k-1} \left[ \| z^k - b \|_2^2 \right] \right] \\
\leq \rho E \left[ \| z^{k-1} - b \|_2^2 \right] \\
\leq \rho^k \| x^0 - b \|_2^2.
\]
This completes the proof.  

We give the main convergence result of REBK in the following theorem.

**Theorem 7.** For any given consistent or inconsistent linear system $Ax = b$, let $x^k$ be the $k$th iterate of REBK with $z^k \in b + \text{range}(A)$ and $x^0 \in \text{range}(A^T)$. For any $\varepsilon > 0$, it holds
\[
E \left[ \| x^k - A^\dagger b \|_2^2 \right] \leq (1 + \varepsilon)^k \rho^k \left( \frac{(1 + \varepsilon)\| z^0 - b \|_2^2}{\varepsilon^2 \| A \|_F^2} + \| x^0 - A^\dagger b \|_2^2 \right).
\]

**Proof.** Let
\[
x^k - \hat{x}^k = \frac{\alpha}{\| A_{L_i} : \|_F^2} (A_{L_i})^T A_{L_i} : (x^{k-1} - A^\dagger b),
\]
which is actually one DSBGS update for the linear system $Ax = AA^\dagger b$ from $x^{k-1}$. It follows from
\[
x^k - \hat{x}^k = \frac{\alpha}{\| A_{L_i} : \|_F^2} (A_{L_i})^T (b_{L_i} - A_{L_i} : A^\dagger b - z^k_{L_i}),
\]
that
\[
\| x^k - \hat{x}^k \|_2^2 = \frac{\alpha^2}{\| A_{L_i} : \|_F^2} (b_{L_i} - A_{L_i} : A^\dagger b - z^k_{L_i})^T A_{L_i} : (x^{k-1} - A^\dagger b) \\
\leq \frac{\alpha^2 \| b_{L_i} - A_{L_i} : A^\dagger b - z^k_{L_i} \|_2^2}{\| A_{L_i} : \|_F^2}, \quad \text{(by Lemma 5)}
\]
It follows from
\[
E_{k-1} \left[ \| x^k - \hat{x}^k \|_2^2 \right] = E_{k-1} \left[ E_{k-1} \left[ \| x^k - \hat{x}^k \|_2^2 \right] \right] \\
\leq E_{k-1} \left[ \frac{\alpha^2 \| b - AA^\dagger b - z^k \|_2^2}{\| A \|_F^2} \right] \quad \text{(by 3)}
\]
that
\[
E \left[ \| x^k - \hat{x}^k \|_2^2 \right] \leq \frac{\alpha^2}{\| A \|_F^2} E \left[ \| b - AA^\dagger b - z^k \|_2^2 \right] \\
\leq \frac{\alpha^2 \rho^k \| z^0 - b \|_2^2}{\| A \|_F^2}. \quad \text{(by Lemma 6)}
\]
By $x^0 \in \text{range}(A^T)$ and $A^\dagger b \in \text{range}(A^T)$, we have $x^0 - A^\dagger b \in \text{range}(A^T)$. Then we can show that $x^k - A^\dagger b \in \text{range}(A^T)$ by induction. By
\[
\| \hat{x}^k - A^\dagger b \|_2^2 = \| x^{k-1} - A^\dagger b \|_2^2 - \frac{2\alpha \| A_{L_i} : (x^{k-1} - A^\dagger b) \|_2^2}{\| A_{L_i} : \|_F^2} \\
+ \frac{\alpha^2}{\| A_{L_i} : \|_F^2} (x^{k-1} - A^\dagger b)^T (A_{L_i})^T A_{L_i} : (A_{L_i})^T A_{L_i} : (x^{k-1} - A^\dagger b) \\
\leq \| x^{k-1} - A^\dagger b \|_2^2 - \frac{2(\alpha - \alpha^2) \| A_{L_i} : (x^{k-1} - A^\dagger b) \|_2^2}{\| A_{L_i} : \|_F^2}, \quad \text{(by Lemma 5)}
\]
we have
\[
\mathbb{E}_{k-1}\left[\|\hat{x}^k - A^\dagger b\|_2^2\right] \leq \|x^{k-1} - A^\dagger b\|_2^2 - \frac{(2\alpha - \alpha^2)\|A(x^{k-1} - A^\dagger b)\|_F^2}{\|A\|_F^2}
\]
\[
\leq \rho\|x^{k-1} - A^\dagger b\|_2^2, \quad \text{(by Lemma 4)}
\]
which yields
\[
\mathbb{E}\left[\|\hat{x}^k - A^\dagger b\|_2^2\right] \leq \rho\mathbb{E}\left[\|x^{k-1} - A^\dagger b\|_2^2\right].
\]
(5)

Note that for any \(\varepsilon > 0\), we have
\[
\|x^k - A^\dagger b\|_2^2 = \|x^k - \hat{x}^k + \hat{x}^k - A^\dagger b\|_2^2
\]
\[
\leq (\|x^k - \hat{x}^k\|_2 + \|\hat{x}^k - A^\dagger b\|_2)^2
\]
\[
\leq \|x^k - \hat{x}^k\|_2^2 + \|\hat{x}^k - A^\dagger b\|_2^2 + 2\|x^k - \hat{x}^k\|_2\|\hat{x}^k - A^\dagger b\|_2
\]
\[
\leq \left(1 + \frac{1}{\varepsilon}\right)\|x^k - \hat{x}^k\|_2^2 + (1 + \varepsilon)\|\hat{x}^k - A^\dagger b\|_2^2.
\]
(6)

Combining (4), (5), and (6) yields
\[
\mathbb{E}\left[\|x^k - A^\dagger b\|_2^2\right] \leq \left(1 + \frac{1}{\varepsilon}\right)\mathbb{E}\left[\|x^k - \hat{x}^k\|_2^2\right] + (1 + \varepsilon)\mathbb{E}\left[\|\hat{x}^k - A^\dagger b\|_2^2\right]
\]
\[
\leq \left(1 + \frac{1}{\varepsilon}\right)\frac{\alpha^2\rho^k}{\|A\|_F^2}\|z^0 - b\|_2^2 + (1 + \varepsilon)\rho\mathbb{E}\left[\|x^{k-1} - A^\dagger b\|_2^2\right]
\]
\[
\leq \left(1 + \frac{1}{\varepsilon}\right)\frac{(1 + 1 + \varepsilon)\alpha^2\rho^k}{\|A\|_F^2}\|z^0 - b\|_2^2
\]
\[
+ (1 + \varepsilon)^2\rho^2\mathbb{E}\left[\|x^{k-2} - A^\dagger b\|_2^2\right]
\]
\[
\leq \cdots
\]
\[
\leq \left(1 + \frac{1}{\varepsilon}\right)\frac{(1 + 1 + \varepsilon + \cdots + (1 + \varepsilon)^{k-1})\alpha^2\rho^k}{\|A\|_F^2}\|z^0 - b\|_2^2
\]
\[
+ (1 + \varepsilon)^k\rho^k\|x^0 - A^\dagger b\|_2^2
\]
\[
\leq (1 + \varepsilon)^k\rho^k\left(\frac{(1 + \varepsilon)\alpha^2\|z^0 - b\|_2^2}{\varepsilon^2\|A\|_F^2} + \|x^0 - A^\dagger b\|_2^2\right).
\]

This completes the proof. 

Remark 8. For the case REBK with \(s = m\), \(t = n\) and \(\alpha = 1\) (i.e., REK), by the orthogonality
\[(\hat{x}^k - A^\dagger b)^T(x^k - \hat{x}^k) = 0,
\]
the equation (6) becomes
\[
\|x^k - A^\dagger b\|_2^2 = \|x^k - \hat{x}^k\|_2^2 + \|\hat{x}^k - A^\dagger b\|_2^2,
\]
which yields the following convergence for REK:
\[
\mathbb{E}\left[\|x^k - A^\dagger b\|_2^2\right] \leq \rho^k\left(\frac{k\|z^0 - b\|_2^2}{\|A\|_F^2} + \|x^0 - A^\dagger b\|_2^2\right).
\]

Remark 9. Theorem 7 shows that REBK exponentially converges in the mean square to the minimum \(\ell_2\)-norm least squares solution of a given linear system of equations with the rate \((1 + \varepsilon)\rho\), which is a little worse than that of REK \(\frac{1}{\varepsilon^2}\) (the rate of REK is \(\rho\)). Although our theory does not yield higher rates of convergence, the numerical results show that the convergence
of REBK in terms of the number of iterations is much faster than that of REK (see numerical results in Section 3). The reason is the over amplification of Lemma 5 we used in the proof. We believe that a sharper convergence bound depending on the size of the blocks and the geometric properties of the matrix $A$ and its submatrices $A_{I,:}$ and $A_{:,J}$ can be obtained. Such kind of convergence result has been obtained for RABK [35, Theorems 4.1 and 4.2].

Remark 10. It was shown in [20] that the convergence of $x^k$ to $A^\dagger b$ under the expected norm of the error (Theorem 2) is a stronger form of convergence than the convergence of the norm of the expected error (Theorem 3), as the former also guarantees that the variance of $x^k_i$ (the $i$th element of $x^k$) converges to zero for $i = 1, \ldots, n$. By Remark 5 we know

$$0 < \alpha < \frac{2\|A\|_F^2}{\sigma_1^2(A)}$$

guarantees the convergence of the norm of the expected error. Recalling that

$$\rho = 1 - \frac{(2\alpha - \alpha^2)\sigma_2^2(A)}{\|A\|_F^2},$$

we know $0 < \alpha < 2$ guarantees the convergence of the expected norm of the error. However, since the convergence bound of Theorem 2 is not sharp, the stepsize $\alpha$ satisfying

$$2 \leq \alpha < \frac{2\|A\|_F^2}{\sigma_1^2(A)}$$

is possible to result in a faster convergence (see numerical results in Section 3). Convergence bounds like those for RABK obtained in [35, Theorems 4.1 and 4.2] could be useful for choosing optimal stepsize $\alpha$.

3 Numerical results

In this section, we compare the performance of the randomized extended block Kaczmarz (REBK) algorithm proposed in this paper against the randomized extended Kaczmarz (REK) algorithm [50] and the projection-based randomized double block Kaczmarz (RDBK) algorithm [40] on a variety of test problems. We do not claim optimized implementations of the algorithms, and only run on small or medium-scale problems. The purpose is only to demonstrate that even in these simple examples, REBK offers significant advantages to REK. All experiments are performed using MATLAB on a laptop with 2.7-GHz Intel Core i7 processor, 16 GB memory, and Mac operating system.

To construct a consistent linear system, we set $b = Ax$ where $x$ is a vector with entries generated from a standard normal distribution. To construct an inconsistent linear system, we set $b = Ax + r$ where $x$ is a vector with entries generated from a standard normal distribution and the residual $r \in \text{null}(A^\top)$. Note that one can obtain such a vector $r$ by the MATLAB function \texttt{null}. For all algorithms, we set $z^0 = b$ and $x^0 = 0$ and stop if the error $\|x^k - A^\dagger b\|_2 \leq 10^{-5}$. We report the average number of iterations (denoted as ITER) of REK, RDBK, and REBK. We also report the average computing time in seconds (denoted as CPU) and the speed-up of REBK against REK, which is defined as

$$\text{speed-up} = \frac{\text{CPU of REK}}{\text{CPU of REBK}}.$$
For the block methods, we assume that the subsets \( \{I_i\}_{i=1}^{s-1} \) and \( \{J_j\}_{j=1}^{t-1} \) have the same size \( \tau \) (i.e., \( |I_i| = |J_j| = \tau \)). We consider the row partition \( \{I_i\}_{i=1}^{s} \) and the column partition \( \{J_j\}_{j=1}^{t} \):

\[
I_i = \{(i-1)\tau + 1, (i-1)\tau + 2, \ldots, i\tau \}, \quad i = 1, 2, \ldots, s-1,
I_s = \{(s-1)\tau + 1, (s-1)\tau + 2, \ldots, m \},
\]

and

\[
J_j = \{(j-1)\tau + 1, (j-1)\tau + 2, \ldots, j\tau \}, \quad j = 1, 2, \ldots, t-1,
J_t = \{(t-1)\tau + 1, (t-1)\tau + 2, \ldots, n \}.
\]

### 3.1 Synthetic data

Two types of coefficient matrices are generated as follows.

- **Type I:** For given \( m, n, r = \text{rank}(A) \), and \( \kappa > 1 \), we construct a matrix \( A \) by
  \[
  A = UDV^T,
  \]
  where \( U \in \mathbb{R}^{m \times r} \) and \( V \in \mathbb{R}^{n \times r} \). Entries of \( U \) and \( V \) are generated from a standard normal distribution, and then, columns are orthonormalized,
  \[
  [U, \sim] = \text{qr}(\text{randn}(m, r), 0); \quad [V, \sim] = \text{qr}(\text{randn}(n, r), 0);
  \]
  The matrix \( D \) is an \( r \times r \) diagonal matrix whose diagonal entries are uniformly distributed numbers in \((1, \kappa)\),
  \[
  D = \text{diag}(1 + (\kappa - 1) \cdot \text{rand}(r, 1));
  \]
  So the condition number of \( A \) is upper bounded by \( \kappa \).

- **Type II:** For given \( m, n \), entries of \( A \) are generated from a standard normal distribution,
  \[
  A = \text{randn}(m, n);
  \]
  So \( A \) is a full-rank matrix with probability one.

In Tables 1-3, we report the numbers of iterations and the computing times for the REK, RDBK, and REBK algorithms. From these results we see: (i) the REBK algorithm vastly outperforms the REK algorithm in terms of both the numbers of iterations counts and CPU times with significant speed-ups, especially when the linear systems are overdetermined; (ii) the convergence rate of the RDBK and REBK algorithms are almost the same in terms of the numbers of iterations.

In Figures 1 and 2, we plot the error \( \|x^k - A^\dagger b\|_2 \) of REBK with different stepsizes and block sizes for rank-deficient inconsistent linear systems. From these figures, we observe: (i) appropriate stepsize and block size improve the convergence remarkably; (ii) increasing block size does not necessarily lead to a better convergence.

### 3.2 Real-world data

Finally, we test REK and REBK on eight real-world problems from the University of Florida sparse matrix collection [10]. The eight matrices are \( \text{abah1}, \text{cari}, \text{df2177}, \text{WorldCities}, \text{flower5_1}, \text{football}, \text{relat6}, \text{Sandi.authors} \). The first four matrices are of full-rank and the last four matrices are rank-deficient. For the full-rank cases, we construct consistent linear systems and for the rank-deficient cases, we construct inconsistent linear systems. In Table 4, we report the numbers of iterations and the computing times for the REK and REBK algorithms. We observe that REBK based on good choices of stepsize and block size significantly outperforms REK. Moreover, good stepsize and block size are problem dependent.
Table 1: The average (10 trials of each algorithm) ITER and CPU of REK, RDBK ($\alpha = 1, \tau = 10$), and REBK ($\alpha = 10, \tau = 10$) for consistent linear systems with random coefficient matrices $A$ of Type I: $A = UDV^T$.

| $m \times n$ | rank | $\kappa$ | ITER | CPU | speed-up |
|--------------|------|----------|-------|------|----------|
| 250 $\times$ 500 | 150 | 2 | 6,142 | 0.31 | 4.81 |
|               | 150 | 10 | 51,980 | 2.47 | 4.47 |
| 500 $\times$ 250 | 150 | 20 | 146,944 | 6.98 | 4.54 |
| 500 $\times$ 250 | 150 | 10 | 261,752 | 12.30 | 6.60 |
| 500 $\times$ 250 | 250 | 2 | 10,088 | 0.49 | 4.83 |
|               | 250 | 10 | 111,546 | 5.27 | 4.42 |
|               | 250 | 20 | 240,872 | 12.30 | 6.60 |

Table 2: The average (10 trials of each algorithm) ITER and CPU of REK, RDBK ($\alpha = 1, \tau = 10$), and REBK ($\alpha = 10, \tau = 10$) for inconsistent linear systems with random coefficient matrices $A$ of Type I: $A = UDV^T$.

| $m \times n$ | rank | $\kappa$ | ITER | CPU | speed-up |
|--------------|------|----------|-------|------|----------|
| 250 $\times$ 500 | 150 | 2 | 6,001 | 0.29 | 4.64 |
|               | 150 | 10 | 72,772 | 3.45 | 4.54 |
| 500 $\times$ 250 | 150 | 20 | 211,555 | 9.98 | 4.52 |
| 500 $\times$ 250 | 150 | 10 | 66,523 | 3.12 | 6.75 |
| 500 $\times$ 250 | 250 | 2 | 9,753 | 0.46 | 6.57 |
|               | 250 | 10 | 125,553 | 5.91 | 6.60 |
|               | 500 $\times$ 250 | 250 | 20 | 473,346 | 22.27 | 6.60 |

Table 3: The average (10 trials of each algorithm) ITER and CPU of REK, RDBK ($\alpha = 1, \tau = 10$), and REBK ($\alpha = 10, \tau = 10$) for linear systems with random coefficient matrices $A$ of Type II: $A = \text{randn}(m,n)$. The first three cases are consistent and the last three cases are inconsistent.

| $m \times n$ | rank | $\sigma_1(A)$ | $\sigma_r(A)$ | ITER | CPU | speed-up |
|--------------|------|---------------|---------------|-------|------|----------|
| 125 $\times$ 250 | 125 | 5.54 | 20,006 | 0.74 | 5.57 |
| 250 $\times$ 500 | 250 | 5.55 | 37,914 | 1.72 | 4.31 |
| 500 $\times$ 1000 | 500 | 5.84 | 84,880 | 5.34 | 3.95 |
| 500 $\times$ 250 | 250 | 5.68 | 40,862 | 1.84 | 6.56 |
| 1000 $\times$ 500 | 500 | 5.63 | 78,803 | 4.69 | 4.34 |
Figure 1: The error $\|x^k - A^*b\|_2$ of REBK with block size $\tau = 10$ and different stepsizes $\alpha = 1, 2, 5, 10, 15$ for a rank-deficient inconsistent linear system ($A = UDV^T$ with $m = 500$, $n = 250$, $r = 150$, $\kappa = 2$).

Figure 2: The error $\|x^k - A^*b\|_2$ of REBK with stepsize $\alpha = 10$ and different block size $\tau = 10, 25, 50$ for a rank-deficient inconsistent linear system ($A = UDV^T$ with $m = 500$, $n = 250$, $r = 150$, $\kappa = 10$).
Table 4: The average (10 trials of each algorithm) ITER and CPU of REK and REBK for linear systems with coefficient matrices from [10]: the first four cases are consistent and the coefficient matrices are of full-rank; the last four cases are inconsistent and the coefficient matrices are rank-deficient.

| Matrix          | m × n          | rank | \(\frac{\sigma_1(A)}{\sigma_r(A)}\) | REK ITER | CPU | \(\alpha\) | \(\tau\) | REBK ITER | CPU | speed-up |
|-----------------|----------------|------|--------------------------------------|-----------|-----|-----------|--------|-----------|-----|----------|
| abtahal         | 14596 × 209    | 209  | 12.23                                | 291,196   | 103.19 | 5         | 10     | 55,825    | 32.41 | 3.18     |
| car1            | 400 × 1200     | 400  | 3.13                                 | 11,025    | 0.75  | 2.5       | 5      | 3,517     | 0.55  | 1.36     |
| df2177          | 630 × 10358    | 630  | 2.01                                 | 21,508    | 10.38 | 5         | 10     | 3,256     | 7.41  | 1.40     |
| WorldCities     | 315 × 100      | 100  | 66.00                                | 102,577   | 4.02  | 2.5       | 10     | 39,979    | 2.30  | 1.75     |
| flower6          | 211 × 201      | 179  | 13.70                                | 131,512   | 5.41  | 2.5       | 5      | 50,782    | 2.83  | 1.91     |
| football         | 35 × 35        | 19   | 166.47                               | 967,062   | 28.91 | 2         | 4      | 480,969   | 20.50 | 1.41     |
| relat6           | 2340 × 157     | 137  | 7.74                                 | 35,502    | 2.73  | 2.5       | 10     | 14,104    | 2.08  | 1.31     |
| Sandi_authors   | 86 × 86        | 72   | 189.58                               | 2,386,773 | 75.90 | 2.5       | 5      | 967,308   | 45.47 | 1.67     |

4 Concluding remarks

We have proposed a pseudoinverse-free randomized extended block Kaczmarz (REBK) algorithm for solving general linear systems and prove its convergence theory. At each step, REBK uses two RABK (with special choice of weights) updates. The new algorithm can utilize efficient implementations on distributed computing units. Numerical experiments show that the crucial point for guaranteeing fast convergence is to obtain good stepsize and block size. We can design other variants of REBK based on different variants of RABK and the technique used in the proof of Theorem 7 still works for these variants. Finding appropriate variable stepsize by the adaptive extrapolation [35] and proposing more effective partitions based on the techniques of [39, 12, 48, 35] should be valuable topics in the future study.

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