A TWIN ERROR GAUGE FOR KACZMARZ’S ITERATIONS

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Abstract. We propose two new methods based on Kaczmarz’s method that produce a regularized solution to noisy tomography problems. These methods exhibit semi-convergence when applied to inverse problems, and the aim is therefore to stop near the semi-convergence point. Our approach is based on an error gauge that is constructed by pairing Kaczmarz’s method with its reverse-ordered method; we stop the iterations when this error gauge is minimum. Our first proposed method stops when the error gauge is at a minimum, the second uses the error gauge to determine step sizes. Our numerical experiments demonstrate that our two methods are superior to the standard Kaczmarz method equipped with state-of-the-art statistical stopping rules. Even compared to Kaczmarz’s method equipped with an oracle that provides the exact error – and is thereby able to stop at the best possible iterate – our methods perform better in almost 90% of our test cases. In terms of computational cost, our methods are a little cheaper than standard Kaczmarz equipped with a statistical stopping rule.

Key word. Computed tomography, ART, Kaczmarz, stopping rules, error estimation, semi-convergence.

AMS subject classifications. 65F22, 65F10, 65R32, 65F15

1. Introduction. The image reconstruction problem in X-ray tomography can be formulated as a large, sparse linear system of equations, i.e.,

\begin{equation}
A x = b, \quad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^m, \quad x \in \mathbb{R}^n.
\end{equation}

Here, the vectors \( b \) and \( x \) represent the measured data (the sinogram) and the image to be reconstructed, respectively. The system matrix \( A \) represents a discretization of the forward problem \([11]\); there are no restrictions of its dimensions \( m \) and \( n \). There is inherently some noise present in the data \( b \), and one of the key challenges in tomographic reconstruction is to compute a good reconstruction in the presence of these errors.

Tomographic reconstruction problems are a type of inverse problems where the forward operator, in the continuous formulation, is a smoothing operation which leads to a poorly conditioned matrix \( A \). The continuous problem is mildly ill-posed and the singular values \( \sigma_i \) of the operator decay as \( i^{-1/2} \) \([2]\).

The system \((1.1)\) is usually too large to solve by factorization methods, and often iterative linear solvers are used. The commonly used iterative solvers exhibit semi-convergence \([18]\) in the presence of noise, meaning that initially the reconstruction error decreases but eventually it increases. This is due to the error consisting of two parts, the iteration error and the noise error. The iteration error decreases steadily, and in the case of error-free data the classical asymptotic convergence theory applies. Initially the noise error is small but it steadily increases until the iterative method has “inverted the noise” rather than the clean data; see, e.g., \([5, 6]\) for more details.

To obtain meaningful solutions to noisy problems we need to stop the iterations at the semi-convergence point where the reconstruction error is at a minimum. The

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iteration number therefore acts as a regularization parameter. There are various methods that estimate a good optimal regularization parameter and these can be used as stopping rules for the iterations \[1, 2]\). These methods aim to provide conditions under which semi-convergence is at least approximately attained.

Many of the parameter-choice/stopping rules are based on statistical properties of the noise, for instance when using generalized cross-validation \[30\] and unbiased predictive risk estimation \[29, Sec. 7.1\] and when fitting to the noise level by variations of the discrepancy principle \[12, Sec. 7.2\].

All these stopping rules may work well for simultaneous iterative reconstruction techniques such as Landweber or Cimmino \[13\]. The reason is that these methods tend to produce error histories that are very flat around the minimum. A few hundred iterations more or less often does not really matter, and the quality of the reconstruction is only little affected. This is not so for Kaczmarz’s method which tends to converge much faster \[6\] and thus has a fairly narrow window of opportunity around the minimum of the error history.

We propose a completely different approach, one without any statistical assumptions on the noise, which is motivated from general ideas in linear algebra and numerical analysis that pertain to error estimation. Using several numerical examples, we show that our stopping rules and algorithms perform very well. To illustrate the point, we compare our methods with an oracle that provides the true error and is therefore able to stop at the best possible iterate.

In our analysis of the proposed methods, we consider first consistent systems to prove that our approach is theoretically sound. In the numerical examples, however, we only consider the noisy case.

The rest of the paper is organized as follows. Section 2.1 introduces the necessary background theory for Kaczmarz’s method. In Section 3 we analyze the errors and use this analysis to propose a new way to estimate the estimate the error. The insight then leads to a new algorithm that is presented in Section 4. Finally, in Section 5 we present numerical examples that illustrate our theory and compare our new algorithm with existing ones. Throughout this work, we will use the following common notations:

- A column vector is denoted by a bold lower-case character, while a bold upper-case character is a matrix. Normal font is used for scalars and polynomials.
- We will use the 2-norm and denote it by \(\| \cdot \|\).
- The expectation operator is written as \(\mathbb{E}\).
- Exact quantities are marked with a superscript \(\star\), while objects marked with a tilde \(\sim\) are related to an alternative (up-sweep) version of Kaczmarz’s methods, cf. Section 3.1.
- The symbol \(\leftarrow\) in pseudocode means assignment.

2. Background theory.

2.1. Kaczmarz’s method. This work pertains to Kaczmarz’s method \[17\], also known as the algebraic reconstruction technique (ART) \[10, 28\]. Let \(k = 1, 2, 3, \ldots\) denote sweeps through the rows of \(A\), and let \(x_0\) denote the starting vector. Let \(\omega \in (0, 2)\) be a relaxation parameter, let \(a_j^T\) denote the \(j\)th row of \(A\), and let \(b_j\) denote the \(j\)th element of \(b\). Then, in the \(k\)th sweep we sequentially perform the
updates

\[(2.1a) \quad x_k^{(0)} = x_{k-1},\]
\[(2.1b) \quad x_k^{(i+1)} = x_k^{(i)} + \frac{b_j - a_j^T x_k^{(i)}}{\|a_j\|^2} a_j, \quad i = 1, 2, \ldots, m,\]
\[(2.1c) \quad x_k = x_k^{(m)} .\]

If \(\omega = 1\), Kaczmarz’s method has a nice geometrical interpretation: each update projects onto hyperplane represented by the \(j\)th equation. There are various strategies for picking the row index \(j\), for instance randomized or cyclic \([20]\); here we consider only cyclic down-sweeps \(j = i\) and up-sweeps \(j = m - i + 1\).

For the down-sweep version, the entire sweep \((2.1)\) of all equations in Kaczmarz’s method can be written as

\[(2.2) \quad x_{k+1} = x_k + A^T L^{-1} (b - Ax_k), \quad L = \text{slt}(AA^T) + \frac{1}{\omega} D ,\]

where \(\text{slt}(\cdot)\) extracts the strictly lower triangular part and \(D = \text{diag}(AA^T)\); as proved for the first time by Elfving and Nikazad in \([7]\).

There are some more elaborate versions of Kaczmarz method available, for instance using block row partitioning or variable relaxation parameters \([9, 6]\). For ease and simplicity of the presentation we use a simple, fully sequential version \((2.1)\) with a fixed relaxation parameter. However, we do not see any insurmountable barriers to extending our ideas to the more elaborate methods.

Using \((2.2)\) we can interpret Kaczmarz’s method as a fixed point method, since we have

\[(2.3) \quad x_{k+1} = G x_k + A^T L^{-1} b, \quad G = I - A^T L^{-1} A,\]

where \(I\) is the identity matrix. We emphasize that \(G\) depends on the relaxation parameter \(\omega\) via \(L\), cf. \((2.2)\). If the system is consistent, we can write \(b = A x^*\) and in this case

\[(2.4) \quad x_{k+1} - x^* = G x_k - x^* + A^T L^{-1} A x^* = G (x_k - x^*).\]

The up-sweep version of Kaczmarz’s method relates in a very nice way to the down-sweep method. The following result is implicit in Elfving and Nikazad \([7]\), we merely provide an explicit demonstration.

**PROPOSITION 2.1.** The up-sweep iteration matrix \(\tilde{G}\) is related to the down-sweep iteration matrix \(G\) \((2.2)\) by transposition, i.e.,

\[(2.5) \quad \tilde{G} = G^T .\]

**Proof.** Let \(R\) denote the reverse identity, i.e., the permutation matrix that reverses the ordering. We investigate what happens when we apply Kaczmarz’s method to the system \(R A x = R b\). Note first that \(R^T = R = R^{-1}\), so that

\[R A A^T R^T = R A A^T R,\]

where pre- and post-multiplying by \(R\) results in the flipping over of both the columns and the rows. From this, we see that

\[(2.6) \quad \tilde{D} = \text{diag}(R A A^T R) = R \text{diag}(A A^T) R,\]

...
since flipping over both columns and rows of a diagonal matrix yields a diagonal matrix with the entries reversed. Here, $\tilde{D}$ is the up-sweep analogue of $D$. Next, it may be checked that the strictly lower triangular part of some matrix $RM$ is the strictly upper triangular part of $M$, flipped over both columns and rows. Hence, the relation is exactly $\text{slt}(RM) = R\text{sut}(M)R$, where $\text{sut}$ takes the strictly upper triangular part. Applying this to the symmetric matrix $AA^T$, we obtain

\begin{equation}
\text{slt}(RAA^T) = R\text{sut}(AA^T)R = R\text{slt}(AA^T)^TR.
\end{equation}

Putting (2.6) and (2.7) together, we find that

$$
\bar{L} = R\left(\text{slt}(AA^T)^T + \frac{1}{\omega}\tilde{D}\right)R = RL^TR,
$$

where $\bar{L}$ is the up-sweep analogue of $L$. Thus, when we inspect the up-sweep iteration matrix $\bar{G}$, we find

$$
\bar{G} := I - (RA)^T(RL^{-T}R)(RA) = I - A^TL^{-T}A = G^T.
$$

**Key Point 1.** The iteration matrix of the up-sweep Kaczmarz method is the transpose of the down-sweep iteration matrix. Consequently, they have exactly the same spectrum.

We present the following well-known result from [15].

**Lemma 2.2.** Kaczmarz’s method is convergent for a consistent linear system (1.1) using any $\omega \in (0, 2)$.

We aim to restate this result in terms of the eigenvalues of the iteration matrix $G$. This provides a different perspective on this familiar result, which to the best of our knowledge is new. First, however, we need the following well-established result, which we adapted from [23, Thm. 4.1].

**Lemma 2.3.** Kaczmarz’s method is convergent if and only if $\rho(G) < 1$.

Note that the two lemmas say slightly different things. Lemma 2.2 pertains to system (1.1) and assures us that Kaczmarz will find a solution if the original system is consistent. Lemma 2.3, on the other hand, gives a slightly more general condition and introduces the possibility that Kaczmarz’s method is also convergent when (1.1) is inconsistent. In this case, Kaczmarz’s method is known to behave in a manner known as cyclic convergence [3]: the trajectory of updates from (2.1) through a sweep will converge to a limiting cycle. Fix some $i$ and consider $x_k^{(i)}$ as a sequence in $k$, then this sequence is convergent for any $i$. Here, however, we consider only full sweeps, which means we look only at $i = m$.

The two lemmas combine to inform us about an interesting property of the iteration matrix $G$ occurring in Kaczmarz’s method, for any matrix $A$ and any $0 < \omega < 2$.

**Theorem 2.4.** The iteration matrix $G = I - A^TL^{-1}A$ of Kaczmarz’s method satisfies $\rho(G) < 1$ for any $0 < \omega < 2$ and any $A$.

**Proof.** For any matrix $A$ we can find a consistent right-hand side $y$, simply take some $x$ and define $y = Ax$. If we solve the system $Ax = y$ for $x$ using Kaczmarz’s, it will converge to a solution by Lemma 2.2. Hence, we can invoke Lemma 2.3 to conclude the proof. \qed
From (2.2), Kaczmarz’s method can be seen to solve the following system

\[
A^T L^{-1} A x = A^T L^{-1} b,
\]

which will always be consistent, whether or not (1.1) is. Indeed, as \(x_{k+1}\) approaches \(x_k\) in the limit of large \(k\), we end up with \(A^T L^{-1}(b - Ax_k) = 0\), which is equivalent to (2.8). When (1.1) is consistent, this system is equivalent to (1.1). However, when (1.1) is inconsistent, the two will not be equivalent and (2.8) is a closely related square and consistent system.

We can also describe Kaczmarz’s method in terms of an iteration polynomial, which is a matrix polynomial; for some background on iteration polynomials see, e.g., [23, Ch. 6] or [24, Ch. 7]. The iterates of Kaczmarz’s method with down-sweeps, cf. (2.1), can be written in terms of a polynomial \(q_k\) of degree \(k - 1\),

\[
x_k = x_0 + q_k(G) r_0,
\]

where \(r_0 = AL^{-1}(b - Ax_0)\) is the initial residual of (2.8). To show this, first we rewrite (2.3) a little to read

\[
x_k - x_0 = G(x_{k-1} - x_0) + r_0.
\]

Rolling back this recurrence relation to the initial guess results in

\[
x_k - x_0 = G^2(x_{k-2} - x_0) + (I + G) r_0
\]

\[
= G^3(x_{k-3} - x_0) + (I + G + G^2) r_0
\]

\[
= (I + G + \cdots + G^{k-1}) r_0.
\]

The polynomial \(q_k\) is therefore given by

\[
q_k(t) = 1 + t + \cdots + t^{k-1} = \frac{1 - t^k}{1 - t}.
\]

It is well-known that such a geometric sum of matrices converges to \((I - G)^{-1}\) [16, Cor. 5.6.16], which is the inverse of \(A^T L^{-1} A\), i.e., the coefficient matrix occurring in (2.8). In this interpretation, we can see that Kaczmarz’s method constructs first a matrix with eigenvalues inside the complex unit circle, and consequently uses a truncated Neumann series to approach its inverse.

The residual of system (2.8) can also be expressed in terms of an iteration polynomial, given by

\[
r_k = p_k(G) r_0.
\]

This can be confirmed by calculation

\[
r_k = A^T L^{-1} b - A^T L^{-1} A(x_0 + q_k(G) r_0) = (I - (I - G)q_k(G)) r_0,
\]

where we used the fact that \(A^T L^{-1} A = I - G\). We can therefore identify \(p_k\) as

\[
p_k(t) = 1 - (1 - t)q_k(t) = t^k.
\]

According to Theorem 2.4, all eigenvalues \(\lambda\) of \(G\) are such that \(|\lambda| < 1\). Consequently, we can restrict the domains of both \(q_k\) and \(p_k\) to the open unit circle in the complex plane. The iteration polynomial approach to Kaczmarz’s method reveals something a little more profound than the simple statement of Theorem 2.4, as it tells us exactly how each eigencomponent of \(x_k\), the components of \(x_k\) expressed in the eigenvector basis, converges. This will form an important part of our analysis further on.
2.2. Statistical stopping rules. To use the semi-convergence of Kaczmarz’s method for noisy data we need a stopping rule for terminating the iterations near the point of semi-convergence. To set the stage we introduce the exact solution $x^\star$ and the corresponding exact (or noise-free) data vector $b^\star = A x^\star$. Moreover we write the empirical data vector as $b = b^\star + \delta b$, and we follow the literature and assume\(^3\) that the elements of $\delta b$ are Gaussian with zero mean and standard deviation $\sigma$.

Several statistical stopping rules seek to minimize the norm of the prediction error for the $k$th iteration, defined as
\[
    p_k = b^\star - A x_k .
\]

However, since this is unavailable, the methods work instead with the norm of the residual vector $b - A x_k$. One way to do so involves the trace of the influence matrix, which is defined as $A A_k^\#$. The trace of this matrix features in many stopping rules. For iterative regularization methods the trace is often estimated by means of a Monte Carlo approach as proposed in [8] and [25].

We can now summarize the three statistical stopping rules used in this work. In the unbiased predictive risk estimation (UPRE) method we find the $k$ that minimizes the expected prediction estimation error norm $E(\|p_k\|^2)$. This is done by minimizing the quantity
\[
    U_k = \|b - A x_k\|^2 + 2 \sigma^2 \text{tr}(A A_k^\#) - \sigma^2 m .
\]
The generalized cross validation (GCV) method also seeks to minimize the expected prediction error, and it does so without the need for the noise’s standard deviation $\sigma$. Here we find the $k$ that minimizes
\[
    G_k = \frac{\|b - A x_k\|^2}{(m - \text{tr}(A A_k^\#))^2} .
\]
The compensated discrepancy principle (CDP) was defined by Turchin [27] for Tikhonov regularization. The underlying idea is to determine the largest iteration number for which we cannot reject $x_k$ – computed from the noisy data – as a possible solution to the noise-free system, cf. [27, p. 93]. Here we stop at the first iteration $k$ for which
\[
    \|b - A x_k\|^2 \leq \sigma^2 (m - \text{tr}(A A_k^\#)) .
\]
A derivation of UPRE is given in [29, Sec. 7.1] while summaries of GCV and CDP can be found in [12, Sec. 7.2 and 7.4]. The methods we reviewed here require the assumption that $\delta b$ is white Gaussian noise. In the next section, we will develop alternatives that do not need these.

3. The Error Gauge and the Twin Method. Given two numerical methods designed to solve the same problem, a general approach to error estimation is to take the difference of the two numerical solutions. For simplicity, we assume there is a unique solution $x^\star$. One way, then, to reason about this is by adding and subtracting the exact solution,
\[
    \|x_k - \bar{x}_k\|^2 = \|x_k - x^\star + x^\star - \bar{x}_k\|^2
\]
\[
    = \|e_k - \bar{e}_k\|^2
\]
\[
    = \|e_k\|^2 + \|\bar{e}_k\|^2 - 2 \cos(\varphi_k) \|e_k\| \|\bar{e}_k\| ,
\]
\(^3\) This assumption is quite crude, as $\delta b$ contains all errors between the mathematical model and the actual measurements.
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where \( x_k \) and \( \tilde{x}_k \) are the numerical solutions, \( e_k \) and \( \tilde{e}_k \) are their respective errors, and \( \varphi_k \) is the angle between the two errors \( e_k \) and \( \tilde{e}_k \). When one solution is much more accurate than the other, the difference between the two is an error estimate for the less accurate solution; this is used in quadrature methods and numerical solvers for differential equations. It is also possible to use two methods with the same order of accuracy, but with different error constants; most famously this idea is used in Richardson extrapolation, provided the order is known \[22\]. One can interpret this technique as first approximating the lowest-order error term and subsequently subtracting it from the solution.

3.1. Analysis of an error gauge: the consistent case. Here, we use \((3.1)\) as an error gauge, which indicates the accuracy of the solution of the linear system. When the approximations are different, but converge to the same solution at the same rate, the difference between them will vanish at the same rate. Therefore this gives us a simple error gauge.

To obtain two different iterates \( x_k \) and \( \tilde{x}_k \) of Kaczmarz’s method to be used in \((3.1)\), we use down-sweeps and up-sweeps, respectively. The latter is simply obtained by reversing the row order in \((2.1)\), i.e., \( i = m, m-1, \ldots, 1 \). The iterates of the up-sweep version, or twin, can be written as

\[
x_{k+1} = x_k + A^T L^{-T} (b - Ax_k)
\]

and the iteration matrix of the up-sweep version is given by \( G^T \). Now the important observation is that the asymptotic convergence rates of the up-sweep Kaczmarz method and the down-sweep Kaczmarz method are the same. According to \((3.1)\), the only other ingredient we need to obtain a valid error gauge is that \( x_k \) and \( \tilde{x}_k \) are different for all \( k \); this will in general be the case for Kaczmarz’s method unless there is some stupefying coincidence. Comparing the iterates from up-sweeps and down-sweeps will therefore allow us to estimate the error.

**Key Point 2.** For Kaczmarz method, the iteration matrix \( G \) is not symmetric, even for symmetric \( A \).

Before stating the results, we recall that the condition number of a simple eigenvalue \( \lambda \) is given by

\[
\kappa(\lambda) = |u^H v|^{-1},
\]

where \( u \) and \( v \) are the left and right eigenvectors, respectively \([26, \text{Chap. 1, Sec. 3.2}]\), and \( u^H \) is the conjugate transpose of \( u \). An eigenvalue is called normal if its condition number is exactly equal to 1, which is the case if and only if \( u \) and \( v \) coincide.

**Proposition 3.1.** Suppose the iteration matrix \( G \in \mathbb{R}^{n \times n} \) has an isolated largest eigenvalue in modulus \( \lambda_1 \), that is, we label the eigenvalues such that

\[
|\lambda_n| \leq \cdots \leq |\lambda_2| < |\lambda_1| < 1.
\]

We furthermore assume that \( \lambda_1 \) is nonnormal and we denote its right and left eigenvector by \( v_1 \) and \( \tilde{v}_1 \), respectively. Suppose that \( e_0 \), the initial error for the up-sweep iterates, has a nonzero component \( d_1 \) in the direction of \( v_1 \), and that the same holds for \( \tilde{d}_1 \), the component of \( \tilde{e}_0 \) in the direction of \( \tilde{v}_1 \).

Then, for consistent systems, the error gauge \( \|x_k - \tilde{x}_k\| \) is asymptotically propor-
tional to the true error norms $\|e_k\|$ and $\|\tilde{e}_k\|$, i.e.,

$$
\|x_k - \tilde{x}_k\|^2 = \frac{\|d_1 v_1 - \tilde{d}_1 \tilde{v}_1\|^2}{|d_1|^2} \|e_k\|^2 + O (|\lambda_1|^k |\lambda_2|^k),
$$

(3.5)

$$
\|x_k - \tilde{x}_k\|^2 = \frac{\|d_1 v_1 - \tilde{d}_1 \tilde{v}_1\|^2}{|d_1|^2} \|\tilde{e}_k\|^2 + O (|\lambda_1|^k |\lambda_2|^k),
$$

for large $k$. Moreover, the proportionality constants will be strictly larger than zero.

Proof. The system is consistent, so that (2.4) holds, i.e.,

$$
e_k = Ge_k \quad \text{and} \quad \tilde{e}_k = G^T \tilde{e}_k.
$$

Since we assume that there is a unique largest eigenvalue in modulus $\lambda_1$, asymptotically the errors will point along the dominant eigenvector, i.e.,

$$
e_k = |\lambda_1|^k \left( d_1 v_1 + O \left( \frac{|\lambda_2|^k}{|\lambda_1|^k} \right) \right) \quad \text{and} \quad \tilde{e}_k = |\lambda_1|^k \left( \tilde{d}_1 \tilde{v}_1 + O \left( \frac{|\lambda_2|^k}{|\lambda_1|^k} \right) \right),
$$

for large $k$. It follows that

$$
\|x_k - \tilde{x}_k\|^2 = \|e_k - \tilde{e}_k\|^2 = |\lambda_1|^{2k} \left( \|d_1 v_1 - \tilde{d}_1 \tilde{v}_1\|^2 + O \left( \frac{|\lambda_2|^k}{|\lambda_1|^k} \right) \right).
$$

The assumption that $\lambda_1$ is nonnormal is equivalent to $v_1$ and $\tilde{v}_1$ being linearly independent. Consequently, we have $\|d_1 v_1 - \tilde{d}_1 \tilde{v}_1\| > 0$, since the only way to produce a zero constant is to have $d_1 = \tilde{d}_1 = 0$, which by assumption does not occur. Therefore, from this, we can conclude (3.5).

Remark 3.2. The assumptions of the proposition are practically speaking always satisfied. Barring pathological examples, it is extremely unlikely to ever encounter a matrix $G = I - A T L^{-1} A$ with $\kappa(\lambda_1) = 1$, even if $A$ is symmetric or normal itself. Also, for an arbitrary starting vector $x_0$ — including the zero vector — it is extremely unlikely that the initial error does not having a component in the dominant eigenvector.

In general, methods with a nonsymmetric iteration matrix are harder to understand theoretically, since they do not have the elegant and pleasant properties of symmetric iteration matrices. Such properties include real eigenvalues, orthogonal eigenvectors, and equal right and left eigenvectors. One approach would be to try and construct a symmetric iteration matrix such as, for instance, the symmetric SOR method [23, Section 4.1]. Here, on the contrary, we exploit the nonsymmetry of the iteration matrix. Since $G$ is not symmetric, its transpose will generate a different sequence of iterates, which is exactly what we need for our error gauge.

Key Point 3. The error gauge $\|x_k - \bar{x}_k\|$ depends crucially on the fact that $G$ is not symmetric.

Put in colloquial terms, Proposition 3.1 asserts that the error gauge $\|x_k - \bar{x}_k\|$ is a good estimate of the iteration error of a consistent system. In the consistent case the argument is simple: both methods converge to the same solution at the same speed, but along different paths, so that the difference vanishes at the same speed as the errors.
In the presence of noise, the story is a little different. However, for problems that exhibit semi-convergence the behavior is more or less the same up to the semi-convergence point. After that, the two iterates diverge and so we should look for a minimum in the error gauge.

3.2. Analysis of an error gauge: the noisy case. Heuristically, we can say that as long as the up-sweep and down-sweep iterates move closer together, the error with respect to the noise-free solution is decreasing, as both methods are moving towards to the same target. However, when the up-sweeps and down-sweeps start diverging, the noise error is driving both away from the noise-free solution and away from each other, see Figure 1. This behavior is bound to happen, since we restrict ourselves to problems that exhibit semi-convergence. We will now endeavor to make this argument more precise, though it will inevitably still involve some heuristics.

Recall that we split the empirical data vector according to $b = b^* + \delta b$, i.e., into an exact part $b^*$ and a noise part $\delta b$. We assume that there exists a unique exact solution $x^*$ satisfying $Ax^* = b^*$. Moreover, we stress that there are no assumptions on the behaviour of $\delta b$. When we use the empirical data vector $\tilde{b}$ instead of the exact data vector $b^*$ in Kaczmarz’s down-sweep method, we obtain from (2.9),

\begin{equation}
\tilde{x}_k = q_k(G) A^T L^{-1} (b^* + \delta b).
\end{equation}

The fact that $b^* = Ax^*$ allows us to write

\begin{equation}
x_k = p_k(G) A^T L^{-1} A x^* + q_k(G) A^T L^{-1} \delta b.
\end{equation}

Note that $A^T L^{-1} A = I - G$, so that we have the polynomial $(1-t)q_k(t) = 1 - p_k(t)$ acting on $G$ in the first term, yielding

\begin{equation}
x_k = (I - p_k(G)) x^* + q_k(G) A^T L^{-1} \delta b.
\end{equation}

This illustrates how the convenient splitting of the exact data vector from the empirical data vector allows us to separate the iteration error and the noise error. Evidently, the iteration error is associated with the polynomial $p_k$, while the noise error is associated with $q_k$ (in the consistent case, we only needed to deal with $p_k$, as $\delta b$ was assumed zero).
Intuitively, we understand that the interplay of these two components of the error lead to the phenomenon of semi-convergence, as is also discussed in [6]. Indeed, we have that $p_k(t) \to 0$ and $q_k(t) \to \frac{1}{t}$ as $k$ increases. Thus, as more iterations pass, the iteration error decreases, while the total error approaches inverted noise.

To progress, we assume that $G$ has an eigendecomposition $VAV^{-1}$, so that

$$x_k - x^* = -V p_k(\Lambda) V^{-1} x^* + V q_k(\Lambda) V^{-1} A^T L^{-1} \delta b.$$  \hspace{1cm} (3.9)

Rewriting this slightly, we see that

$$x_k - x^* = \sum_{j=1}^{n} (c_j q_k(\lambda_j) - d_j p_k(\lambda_j)) v_j,$$  \hspace{1cm} (3.10)

where $c = V^{-1} A^T L^{-1} \delta b$ and $d = V^{-1} x^*$. Hence, (3.9) and (3.10) express the error as a linear combination of the eigenvectors of $G$. This shows that we can analyze the behavior of the polynomials $q_k$ and $p_k$ on their whole domain, the open unit circle, instead of working with a discrete set of eigenvalues.

First, it is important to realize that $|p_k(\lambda)|$ decreases as $k$ increases for all $\lambda$ inside the unit circle. As we have already seen, in asymptotic convergence theory we only consider the eigenvalue for which $|p_k(\lambda)|$ converges slowest, i.e., Proposition 3.1. Previously, we called the largest in modulus eigenvalue $\lambda_1$, and we now write for brevity $\rho = |\lambda_1| < 1$. Hence, we see that for all $|\lambda| \leq \rho$, we have

$$|p_k(\lambda)| \leq \rho^k.$$  \hspace{1cm} (3.11)

Second, there are some values of $\lambda$ for which $|q_k(\lambda)|$ increases. To be sure, there are also values for which $|q_k(\lambda)|$ decreases, but these do not concern us, as their contribution to the error is negligible. The eigenvalues for which $|q_k(\lambda)|$ grows unbounded contribute most to the error; these occur near $\lambda = 1$. The absolute value $|q_k(\lambda)|$ around this point will be smaller than the limit

$$\lim_{\lambda \to 1} 1 + \lambda + \cdots + \lambda^{k-1} = k.$$  \hspace{1cm} (3.12)

Hence, we have

$$|q_k(\lambda)| < k,$$  \hspace{1cm} (3.13)

and for eigenvalues near $\lambda = 1$ the modulus of the polynomial will approximately attain the bound $k$. We point out that, under certain conditions, it is possible to obtain a more sophisticated bound which scales as $\sqrt{k}$ [6].

As asserted earlier, the interplay between the two polynomials results in the semi-convergence phenomenon. The iteration error vanishes exponentially, while the noise error increases linearly with the iteration number, i.e.,

$$\|e_k\| \leq \xi \rho^k + \zeta k,$$  \hspace{1cm} (3.14)

where $\xi$ and $\zeta$ are positive constants. For suitable values of $\xi$ and $\zeta$, there will be a $k^*$ at which the bound attains a minimum. Since we restrict our attention to problems that exhibit semi-convergence, we may assume that the values for $\xi$ and $\zeta$ do indeed admit this behavior.

We now have to argue that the error bound (3.14) is sharp. For the iteration error, this can be done rigorously, following the proof of Proposition 3.1. The noise
error does not admit such an argument, but intuitively a similar mechanism is at play. The eigencomponents with eigenvalues close to $\lambda = 1$ grow the most rapidly and will dominate the noise error. The bound should therefore be reasonably sharp.

Next, we apply the same arguments to the up-sweeps and of course find a completely analogous expression as (3.14) for $\|\tilde{e}_k\|$. The analogous constant $\tilde{\xi}$ will be equal to $\xi$, as both errors must be equal when $k = 0$. Moreover, the constant $\tilde{\zeta}$ will be very close to $\zeta$, though not necessarily equal. As a consequence, both $\|e_k\|$ and $\|\tilde{e}_k\|$ will have a minimum around the same iteration number. Next, we apply (3.1), and what results is a more complicated expression, which nonetheless exhibits roughly the same behavior as either error norms. Crucially, it will have a minimum close to the two minima of the true errors.

To conclude, we have argued, although admittedly not completely rigorously, that the error gauge should behave roughly the same as the true errors even in the face of noise. Indeed, it will decrease when the errors are dominated by the iteration error and it will increase when the errors are dominated by the noise. As a consequence, its minimum will provide a good estimate for the minimum of the true errors.

3.3. The Twin Algorithm. To summarize the above discussion of the error gauge, we now propose a new method that utilizes it as a stopping rule. We use here the shorthand $K^\downarrow(x)$ for a Kaczmarz down-sweep starting with $x$ and fixed parameter $0 < \omega < 2$ (it goes without saying that we use $A$ and $b = b^* + \delta b$). Likewise, $K^\uparrow(\tilde{x})$ denotes the twin Kaczmarz up-sweep. A possible implementation of the Twin Method in pseudocode is presented in Algorithm 1.

| Algorithm 3.1 Twin Algorithm |
|-------------------------------|
| **Require:** maxits, $0 < \omega < 2$, $A$, $b$ |
| **Output:** A regularized solution to (1.1). |
| 1: $x \leftarrow 0$, $\tilde{x} \leftarrow 0$ |
| 2: for $k = 1, \ldots, \text{maxits}$ do |
| 3: $x \leftarrow K^\downarrow(x)$ |
| 4: $\tilde{x} \leftarrow K^\uparrow(\tilde{x})$ |
| 5: if $\|x - \tilde{x}\|$ is at a minimum then break, end if |
| 6: end for |
| 7: return $\frac{1}{2}(x + \tilde{x})$. |

The algorithm requires some maximum number of iterations maxits, which is simply a convenience; e.g., to ensure the algorithm stops after a finite number of steps, or that it uses at most some preallocated amount of computational resources. The Twin Algorithm finds a minimum of the error gauge, which we have argued above amounts to finding approximately the minimum error of both up-sweeps and down-sweeps. How to find this minimum requires some more explanation, but there are various approaches one might try. Finally, the output of the Twin Algorithm is the average of the stopped down- and up-sweeps. This is because we do not have any method of preferring the one over the other. Taking the average then seems a reasonable thing to do.

One might think that finding the minimum of the error gauge is a trivial matter. Indeed, the true error should decrease monotonically until semi-convergence, after which it increases monotonically. Naively, one might then say that we should stop
when the error gauge increases. Surely\(^2\), the error gauge will be smooth too! Unfortunately the error gauge is a somewhat spasmodic function of \(k\). Although it is smooth asymptotically, in the initial iterations the error gauge can be quite irregular. Nonetheless, we should build in some robustness with respect to this behavior into our stopping rule.

An easy way to do so is with a user-specified slack, together with storing the best approximation so far. The slack is simply a number of iterations to keep running to accommodate any oscillations of the error gauge. We use 10 iterations, which is long enough for most oscillations, but not too long such that it wastes a lot of computational resources. Once a minimum has been found, the approximation is stored and the slack starts running. If a new minimum is found within the slack period, the slack is reset. In this way, oscillations in the error gauge are ignored, as long as they are shorter than the slack length.

There are alternative approaches to finding the minimum of a function that may have rapid variations as well as a global smooth trend. Such approaches may be valuable if memory is an issue or computing power is in short supply and the slack cannot be too long. One such approach is described in [14].

4. The Mutual-Step Method. Up till now we used our error gauge to select the best iteration while leaving the iterative method unaltered. Now, we use our error gauge to modify the method which, as we will see, precludes the necessity of a stopping rule altogether. Specifically, we will use the error gauge to determine step lengths, causing the method to converge to a good approximation of the noise-free solution.

4.1. Motivation for a new method. Let us define \(w_k\) and \(\tilde{w}_k\) as the search directions in the down-sweep and up-sweep versions of Kaczmarz’s method, respectively, i.e.,

\[
\begin{align*}
  w_k &= A^T L^{-1} (b - A x_k), \\
  \tilde{w}_k &= A^T L^{-T} (b - A \tilde{x}_k).
\end{align*}
\]

Note that this definition includes the relaxation parameter \(\omega \in (0, 2)\) via the matrix \(L\). Iteration \(k+1\) of the down-sweep method is then given by \(x_k + w_k\). A simple modification to the method allows for an iteration-dependent step size \(\alpha_k\), so that \(x_k + \alpha_k w_k\) is the next iteration. Similarly, we define \(\tilde{x}_k + \beta_k \tilde{w}_k\) as the next up-sweep iterate. Ideally, one wishes to plug these expressions into the exact error to find the optimal step sizes. However, the exact error is not available, so we use the error gauge instead. Hence, we aim to compute the step length parameters that solve the minimization problem

\[
\min_{\alpha, \beta} \frac{1}{2} \|x_k + \alpha w_k - \tilde{x}_k - \beta \tilde{w}_k\|^2,
\]

which is the error gauge of iteration \(k+1\). If we set the derivatives with respect to \(\alpha\) and \(\beta\) to zero, we obtain

\[
\begin{bmatrix}
  \|w_k\|^2 & -w^T_k \tilde{w}_k \\
  -w^T_k \tilde{w}_k & \|\tilde{w}_k\|^2
\end{bmatrix}
\begin{bmatrix}
  \alpha_k \\
  \beta_k
\end{bmatrix}
= \begin{bmatrix}
  -w^T_k (x_k - \tilde{x}_k) \\
  -\tilde{w}^T_k (x_k - \tilde{x}_k)
\end{bmatrix}.
\]

\(^2\)Dennett points out that the word surely usually signals the weakest point in someone’s argument [4].
We solve this linear system for $\alpha_k$ and $\beta_k$ to obtain the step sizes. It is important to note that this system is nonsingular when the vectors $\mathbf{w}_k$ and $\tilde{\mathbf{w}}_k$ are linearly independent. In this case, the $2 \times 2$ coefficient matrix in (4.3) is symmetric positive definite. Of course, since the two search directions come from up-sweeps and down-sweeps, they will generally be linearly independent. The step sizes obtained from this system will therefore be generally well-defined.

Because we are minimizing the distance between the up- and down-sweep iterates at every iteration by choosing suitable step sizes, the distance cannot increase. Therefore the error gauge, which is this distance, will form a monotonically decreasing sequence. This immediately leads to the following result.

**Proposition 4.1.** Suppose that $\mathbf{w}_k$ and $\tilde{\mathbf{w}}_k$ are linearly independent for all $k$. By using the step sizes from (4.3), the error gauge $\|\mathbf{x}_k - \tilde{\mathbf{x}}_k\|$ converges to a local minimum.

**Proof.** The error gauge is a monotonically decreasing sequence, while it is trivially bounded from below, i.e., $\|\mathbf{x}_k - \tilde{\mathbf{x}}_k\| \geq 0$.

**Corollary 4.2.** If $\mathbf{w}_k$ and $\tilde{\mathbf{w}}_k$ are linearly independent for all $k$, the step sizes $\alpha_k$ and $\beta_k$ converge to zero. Moreover, the limiting search directions $\mathbf{w}$ and $\tilde{\mathbf{w}}$ are related to the limiting approximations $\mathbf{x}$ and $\tilde{\mathbf{x}}$ by

$$\mathbf{w}^T(\mathbf{x} - \tilde{\mathbf{x}}) = 0, \quad \tilde{\mathbf{w}}^T(\mathbf{x} - \tilde{\mathbf{x}}) = 0. \quad (4.4)$$

**Proof.**
1. By assumption, $\mathbf{w}_k$ and $\tilde{\mathbf{w}}_k$ are linearly independent, so that there is no linear combination resulting in the zero vector other than $\alpha_k = \beta_k = 0$. Proposition 4.1 asserts that the error gauge converges. Therefore, the step sizes must vanish as well, otherwise the error gauge would change.
2. Since the system (4.3) is symmetric positive definite, again by the assumption that $\mathbf{w}_k$ and $\tilde{\mathbf{w}}_k$ are linearly independent, the zero solution can only occur when the right-hand side is zero.

The corollary provides several possible convergence criteria for an implementation of the Mutual-Step Method. For example, we can inspect $|\alpha_k| + |\beta_k|$ and stop when it falls below a certain threshold. There is no real point in choosing the tolerance close to machine precision; it is sufficient to choose the tolerance a little smaller than the noise level. Alternatively, we can demand that the step sizes are positive, since the standard Kaczmarz method has $\alpha_k = \beta_k = 1$, and a negative step size would mean a step in the wrong direction for the consistent case. We stop when either one of these conditions is satisfied.

**Key Point 4.** The Mutual-Step Method is convergent. Moreover, it converges to a regularized solution of (1.1).

The step sizes will be chosen in such a way that the up-sweep and down-sweep iterates are kept as close as possible to each other. The intuition is the same as previously explained: when the iteration error is dominant the two approximations converge, while they diverge when the noise error dominates. Therefore, the point where the two iteration vectors are closest is going to be a good guess for the semi-convergence point. Corollary 4.2 expresses this idea in a rigorous way, as there are only two ways in which the right-hand side of (4.3) can be zero. Either the two approximations are equal, meaning the methods have converged, or the search directions have no component in the error gauge. In short, Corollary 4.2 expresses the fact that locally the error gauge can be reduced no further by Kaczmarz sweeps.
Work load of the various methods for a 2D problem; for a 3D problem replace $\sqrt{n}$ with $3\sqrt{n}$. A work unit is defined as the work in a single Kaczmarz sweep.

| Method                        | Operations                  | Work units |
|-------------------------------|----------------------------|------------|
| Standard Kaczmarz             | $4m\sqrt{n}$               | 1          |
| Idem + trace-estimate stopping rules | $10m\sqrt{n} + 2n + 3m\frac{5}{2} + \frac{1}{2}\sqrt{\frac{n}{m}} + \frac{3}{4}\frac{1}{\sqrt{n}}$ |            |
| Twin Method                   | $8m\sqrt{n} + 3n$          |            |
| Mutual-Step Method            | $8m\sqrt{n} + 11n$         |            |

4.2. The algorithm. We present here a possible implementation of the Mutual-Step Method in pseudocode, see Algorithm 2. Unlike the Twin Method, the Mutual-Step Method should be considered as different from Kaczmarz’s method, although it is related.

Algorithm 4.1 Mutual-Step Algorithm

Require: maxits, tol, $0 < \omega < 2$, $A$, $b$

Output: A regularized solution to (1.1)

1. $x_0 \leftarrow K^\downarrow(0)$, $\tilde{x}_0 \leftarrow K^\uparrow(0)$
2. $x \leftarrow x_0$, $\tilde{x} \leftarrow \tilde{x}_0$
3. for $k = 1, \ldots, \text{maxits}$ do
4. $w \leftarrow K^\downarrow(x) - x$
5. $\tilde{w} \leftarrow K^\uparrow(\tilde{x}) - \tilde{x}$
6. Solve (4.3) to determine $\alpha$ and $\beta$.
7. if $|\alpha| + |\beta| < \text{tol}$ or $(\alpha < 0$ and $\beta < 0)$ then
8. break
9. end if
10. $x \leftarrow x + \alpha w$
11. $\tilde{x} \leftarrow \tilde{x} + \beta \tilde{w}$
12. end for
13. return $\frac{1}{2}(x + \tilde{x})$.

The Mutual-Step Algorithm requires two different starting vectors; if we start with the same vector, the initial error gauge would be zero, causing the step sizes to come out zero. Consequently, the algorithm would exit immediately. Furthermore, according to [6] the starting vector should lie in the row space of $A$. Our approach is simply to use a single down-sweep and up-sweep starting from the zero vector. These vectors are different and lie in the correct space.

4.3. Computational cost. We now turn to the computational cost of the Mutual-Step Method. At this point, it is convenient to introduce a work unit: a certain number of operations so that we can easily compare the cost of the various methods. The most convenient work unit in our context is a single Kaczmarz sweep. For X-ray tomography problems, the average number of nonzero elements in a row of $A$ is $\sqrt{n}$ for a 2D problem and $3\sqrt{n}$ for a 3D problem. Carefully going through the operations reveals that there are $4m\sqrt{n}$ or $4m\sqrt{\frac{n}{m}}$ operations in a sweep. We omit constant numbers of operations as they will be negligible. Note that the cost of one matrix-vector multiplication is half a work unit.
For each method, we examine the total cost and express it in terms of work units in Table 1. The Twin Method requires two Kaczmarz sweeps together with determination of the difference between the two iterates. The Mutual-Step Method requires two Kaczmarz sweeps and the solution of the system (4.3). All the stopping rules (see Section 5 for details) require a trace estimate which means that, per iteration, the additional amount of work is one Kaczmarz sweep, the determination of the residual and its norm, and an inner product. There are a small number of additional operations which we ignore here.

Naturally, as $m$ and $n$ grow, the cost of each method becomes dominated by the cost of the Kaczmarz sweeps and the determination of the residual, if needed. The cost of inner products are evidently negligible in the larger scheme of things. Our proposed methods do not require the residual, so that their asymptotic cost is 2 work units per iteration. The stopping rules have an asymptotic cost of $\frac{5}{2}$ work units per iteration. Our methods are therefore slightly cheaper for large systems. As an example, for a small $128 \times 128$ image we have a system size of $n = 128^2 = 16384$ and $m \approx 1.2 n$. We should remark that this choice of $m$ is entirely arbitrary. In practice, a whole range of $m$ is used, from vastly underdetermined systems to extremely overdetermined. This amounts to a cost of about 2.005 work units per iteration for the Twin Method and 2.02 work units per iteration for the Mutual-Step Method.

4.4. Summing up. To recap our principal idea: we use Kaczmarz’s method in tandem with its twin, the reverse-ordered version. The difference between the two iterates is subsequently used as an error gauge. The reasoning is fairly simple: when the linear system is consistent, the two approximations converge at the same speed to the same solution, but along different paths, so that their difference is a gauge of the true error. When the system is inconsistent, as long as the two approximations are converging they are also getting closer to the noise-free solution. Only when the noise error starts to dominate do they diverge from each other.

This approach has some major advantages over the standard stopping rules such as UPRE, GCV and variants of the discrepancy principle. First, our method is independent of the type of noise while, e.g., UPRE and GCV need to be specifically derived for each type of noise. Second, we do not require an a priori noise estimate as required by UPRE and the discrepancy principle. Our methods, like GCV, can be used to provide a noise estimate a posteriori, after a good reconstruction has been found.

We emphasize that our two new methods do not depend on any statistical assumption about the noise. The standard Kaczmarz method equipped with a statistical stopping rule depends, by its very nature, on such assumptions. Our methods simply takes the empirical data and “adapts” to the particular instance of the noise by producing a locally optimal reconstruction as the final result; cf. Corollary 4.2.

Another point is that the proposed error gauge approximates the forward error, i.e., the error with respect to the noise-free solution $\|x_k - x^*\|$. Most other stopping rules, as far as the authors are aware, are based on the prediction error, i.e., the residual norm of the original noise-free system $\|b - Ax_k\|$. These two error metrics can give quite different results for ill-posed inverse problems, even if we use the best possible iterate. We actually seek a regularized solution of the problem, and so we should aim to stop as close as possible to the noise-free solution, rather than minimizing the residual. Up till now, this was a prohibitively impractical proposition.

5. Numerical experiments. To conduct our numerical experiments, we use the AIR TOOLS II package for MATLAB which contains various codes for the creation
and solution of tomographic problems [13]. The package also contains a function `phantomgallery` that creates various phantoms with different features. We use the parallel beam set-up with $128 \times 128$ phantoms, projection angles $0^\circ, 1.5^\circ, 3^\circ, \ldots, 178.5^\circ$ and $\text{round}(\sqrt{2} \cdot 128) = 181$ rays per projection. Furthermore, as a tolerance for the Mutual-Step Algorithm we use $\text{tol} = 10^{-4}$. Finally, we will always use $x_0 = 0$ as an initial guess.

**Key Point 5.** We will use $x_0 = 0$ throughout this work, unless mentioned otherwise. This choice simplifies the expressions somewhat, but more importantly it serves as a good initial guess for noisy inverse problems.

To simulate noise, we add white Gaussian noise $\delta b \sim \mathcal{N}(0, \sigma^2 I_m)$ scaled such that we can specify the expected relative noise level to be $\eta$, i.e.,

$$
\eta^2 = \frac{\mathbb{E}(\|\delta b\|^2)}{\|b^*\|^2} = \frac{m \sigma^2}{\|b^*\|^2}.
$$

To demonstrate the effect of noise on the reconstruction, Figure 2 shows error histories of the relative error $\|x_k - x^*\| / \|x^*\|$ for various noise levels. Our phantom of choice is the grains phantom, which simulates the polycrystalline structure found in many metals, rocks, and bones. We used the standard Kaczmars (down-sweep) method with $\omega = 1$. We see that as $\eta$ increases the whole curve moves up and the minimum becomes less flat.

For the lowest noise level, $\eta = 10^{-3}$, any iteration between $k = 70$ and 100 gives almost the same relative error. However, for the highest noise level it is more critical to find the right number of iterations. The general trend is clear: for higher noise levels the stopping rule needs to be more accurate.

**5.1. Casing the competition.** As the closest competitors of our proposed algorithms, we consider the standard Kaczmarz algorithm with either of the three statistical stopping rules from Section 2.2: UPRE, GCV, and CDP. Our experience is that the performance of these stopping rules for Kaczmarz’s algorithm is generally quite poor, especially for high noise levels, and to demonstrate this we show a representative error history for the grains phantom in Figure 3.

It is clear that all three statistical stopping rules overshoot the mark by quite a margin. GCV and UPRE overshoot by roughly 100 iterations, while CDP did not
stop for $\text{maxits} = 300$. As already mentioned in Section 1, this may not matter very much for the simultaneous iterative methods where the minimum is very flat. For Kaczmarz’s algorithm, on the other hand, there is a significant difference. For the current example, our error gauge stops within two iterations of the minimum and produces an image that is roughly 60% better compared to the statistical stopping rules.

A careful reader might observe that the output of the Twin Algorithm is not on the exact error curve in Figure 3. The outputs of GCV and UPRE are in fact on the curve, and so would CDP be if it had stopped within $\text{maxits}$ iterations. The difference is that the Twin Algorithm is not employed as a pure stopping rule. Indeed, the output of the Twin Algorithm is the average of the up- and down-sweeps, which evidently produces a better reconstruction. As we will demonstrate below, the Mutual-Step Algorithm produces even better results. Instead of comparing the proposed algorithms with statistical stopping rules, we therefore from now on compare with the exact minimum.

We will suppose that we have an oracle\(^3\) that can tell you the exact error of a reconstruction, but importantly, not anything else. Having access to the exact error allows one to pick out the absolute best iteration from the sequence of reconstructions generated by an iterative method. This is what we will compare our algorithms with.

5.2. Haunted house: a selection of phantoms. From now on, we use the relative noise level $\eta = 8 \cdot 10^{-3}$ in our experiments, as this may be seen as realistic; it is also the second-largest noise level from Figure 2. To illustrate the point of the previous subsection visually, we plot the results of the various algorithms under consideration for two phantoms from phantomgallery, namely, the already-mentioned grains phantom and shepplogan which implements the Shepp–Logan phantom. The corresponding reconstructions are shown in Figure 4. Both phantoms have pixel values between 0 and 1. When we compute the relative error with respect to each phantom we use the solutions as produced by the algorithms, with some negative pixel and some pixels greater than one. The figures, on the other hand, show the

\(^3\)The oracle is a concept borrowed from computational complexity theory [19]: oracle machines “are machines that are given access to an “oracle” that can magically solve the decision problem for some language”. Here, we will take the oracle to magically provide the exact error of a reconstruction.
reconstructions with the pixel values limited to the range $[0, 1]$. For both phantoms the Mutual-Step Algorithm produces the best reconstruction.

First consider the results for the shepplogan phantom. The Mutual-Step Algorithm produces the best reconstruction, and by visual inspection one would probably pick this as the best as well. It is the least grainy picture, while the small details can be clearly distinguished. Both GCV and UPRE produce a very grainy image and the smallest details are hard to make out.

The results for the grains phantom are slightly more interesting to examine. This phantom consists of a collection of piecewise constant regions (which are Voronoi regions belonging to a random collection of points). The relative performance of the algorithms can be visually evaluated by looking especially at the contrast, e.g., between two neighbouring regions that have close intensity values. Whether or not
one can distinguish two such regions is a matter of opinion, but generally speaking it does appear that the Mutual-Step Algorithm produces the best results as well as the least grainy picture. GCV and UPRE perform particularly badly, it seems, where neighbouring regions are sometimes very hard, if not impossible, to discern.

To demonstrate that the observed behavior is not an oddity or statistical fluke, we run the reconstructions of the grains phantom 500 times and keep track of the relative errors. From this point on, we compare our algorithms to the Kaczmarz algorithm with the oracle stopping rule, as the statistical stopping rules can never do better. We refer to this algorithm as “Kaczmarz+Oracle” or KO for short.

The results are shown in the histograms in Figure 5. The histograms show several interesting features. First off, the Mutual-Step Algorithm is overall best, with the lowest average error and the smallest spread. It is in fact so much better that any outcome from this algorithm is better than any outcome from the other methods. The Twin Algorithm gives a slightly better average performance than the Kaczmarz+Oracle, though their histograms overlap completely. The Kaczmarz+Oracle has the largest spread, and is on average slightly worse than the Twin Algorithm. At first, it may seem odd that the Twin Algorithm produces a better result on average than the Kaczmarz+Oracle. Yet, we should recall that the output of the Twin Algorithm is the average of the up-sweeps and down-sweep iterates, while the Kaczmarz+Oracle algorithm is associated with the down-sweep iterates only. Evidently the averaging often gives a better result than a down-sweep or up-sweep algorithm separately.

To provide further support for the quality of our methods, we ran the proposed algorithms 100 times on each of the seven phantoms available from phantomgallery. For each run, we assign points based on which method produces the best result. Our point system assigns a score of 1 point to the method with the best reconstruction, half a point for the second best, and no point for the worst. Hence, a score of 100 means the algorithm produced the best result each time, while a score of 0 means it produced the worst result each time. This allows us to see roughly how well the methods behave relative to each other. The final tally is contained in Table 2.

The Mutual-Step Algorithm is certainly the best algorithm under consideration when it comes to producing a high-quality image. For four phantoms this algorithm gets the full marks of 100 points and for two phantoms the score is slightly less than 100, while for the binary phantom the algorithm performs somewhat poorly. While we cannot prove that our new algorithms are always better than, or at least as good as,
Table 2

| Phantom   | Relative errors | Work units | Score |
|-----------|-----------------|------------|-------|
|           | TA  | MSA | KO | TA  | MSA | KO | TA  | MSA | KO |
| shepplogan| 0.18 | 0.17 | 0.19 | 45.8 | 10.5 | 19.0 | 39 | 98 | 13 |
| smooth    | 0.29 | 0.14 | 0.25 | 34.1 | 11.6 | 19.8 | 6 | 100 | 44 |
| binary    | 0.22 | 0.22 | 0.23 | 37.1 | 14.5 | 12.0 | 91.5 | 33 | 25.5 |
| threephases| 0.17 | 0.14 | 0.20 | 47.2 | 18.4 | 12.4 | 45.5 | 100 | 5.5 |
| threephasessmooth | 0.16 | 0.12 | 0.19 | 42.7 | 20.9 | 10.1 | 47.5 | 100 | 2.5 |
| fourphases | 0.20 | 0.20 | 0.22 | 47.4 | 14.3 | 15.0 | 53 | 90.5 | 6.5 |
| grains    | 0.17 | 0.11 | 0.21 | 46.1 | 20.5 | 13.1 | 45.5 | 100 | 4.5 |
| Average   | 0.20 | 0.16 | 0.21 | 42.9 | 15.8 | 14.5 | 46.7 | 88.8 | 14.5 |

Kaczmarz+Oracle we see that they both perform really well and that the Mutual-Step Algorithm is definitely the winner in terms of producing the smallest error.

To provide more insight, we also display the average errors for each particular phantom and the total average error in the first three columns of Table 2. Here we see another remarkable aspect of the proposed algorithms that was also observed in Figure 5: both are on average better than Kaczmarz+Oracle. The Mutual-Step Algorithm produces the best results on average for every phantom, while Kaczmarz+Oracle sometimes gives a better reconstruction than the Twin Algorithm. Whereas the Twin Algorithm is on average only slightly better than Kaczmarz+Oracle, the Mutual-Step Algorithm does quite a lot better: the average error is reduced with roughly 25% compared to Kaczmarz+Oracle.

Finally, in the middle three columns of Table 2 we also compare the methods when it comes to computing cost expressed in our work units (recall that one work unit is the work required to complete one sweep of Kaczmarz’s method). We should point out that Kaczmarz+Oracle has a very low work load, which is due to the fact that consulting the oracle is assumed to be free. The corresponding workload should therefore be read as a lower bound on the work required. Interestingly, the Mutual-Step Algorithm is not too far off on average, sometimes requiring less work than the oracle and sometimes more. The Twin Algorithm usually requires much more work than the oracle, which is to be expected of course. If the Twin Algorithm would stop at the same point as the oracle, it would have done roughly twice the work plus the slack.

6. Conclusion and future work. We presented a new approach to using Kaczmarz’s method, with applications to tomography problems in mind. The regularizing property of this method is due to its semi-convergence where the iteration number is used as the regularization parameter. The problem of choosing the regularization parameter takes the form of a stopping rule, typically based on a statistical analysis of the noise and the error.

Our key idea is to combine two Kaczmarz iterations with different row orderings and the same convergence rate, which allows us to compute an error gauge, i.e., an estimate of the reconstruction error. We then stop the iterations when the error gauge is minimum, providing an alternative to the standard stopping rules and avoiding assumptions about the noise statistics.

We argued that our error gauge roughly displays the same behavior as the forward
error (the reconstruction error). When the original linear system (1.1) is consistent, we can prove this fact rigorously. For noisy systems we argued that the error gauge represents semi-convergence with a reasonable fidelity. We provided first a heuristic argument of why this is the case, which we then expanded with a formal argument.

We suggested two algorithms that utilize the error gauge: the Twin Algorithm and the Mutual-Step Algorithm. The former uses the error gauge directly as a stopping rule, stopping when the error gauge is minimal. The latter uses the error gauge to determine approximately optimal step sizes for every iteration. We showed that the Mutual-Step Algorithm converges monotonically to a locally optimal pair of approximations. It therefore converges to a good approximation of the semi-convergence point, precluding the need for a stopping rule.

Using several numerical experiments from parallel-beam X-ray CT, we demonstrated that the proposed algorithms perform very well indeed. As a reference, we used an oracle for the standard Kaczmarz algorithm that provides the exact error, which is therefore able to pick the best possible reconstruction from the sequence of iterates. Our proposed algorithms perform on average better than Kaczmarz’s method equipped with the oracle; in fact, the Mutual-Step Algorithm performs much better and uses a comparable amount of computational work, on average.

For four out of the seven phantoms that we considered, the Mutual-Step Algorithm produced the best image every time over 100 runs. For two other phantoms, the algorithm reaches close to that number. Only for a single phantom does the algorithm not produce the best reconstruction in the majority of the cases.

This work focused on a twin algorithm that simultaneously performs a down-sweep and an up-sweep. For future work, we plan to investigate the effect of using alternative twin algorithms. Preliminary results (not reported here) show that our error gauge is robust with respect to the row-ordering of the twins. This opens the door to extending our methods to randomized orderings, block methods, variable relaxation parameters, etc. In particular, the popular randomized orderings seem interesting to consider. Moreover, block methods are probably the best option for high-performance computing implementations, so that any proposed method must allow such a version.

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