HOW TO OPTIMIZE PRECONDITIONERS FOR THE CONJUGATE
GRADIENT METHOD: A STOCHASTIC APPROACH∗

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Abstract.
The conjugate gradient method (CG) is usually used with a preconditioner which improves efficiency and
robustness of the method. Many preconditioners include parameters and a proper choice of a preconditioner
and its parameters is often not a trivial task. Although many convergence estimates exist which can be used
for optimizing preconditioners, these estimates typically hold for all initial guess vectors, in other words, they
reflect the worst convergence rate. To account for the mean convergence rate instead, in this paper, we follow a
simple stochastic approach. It is based on trial runs with random initial guess vectors and leads to a functional
which can be used to monitor convergence and to optimize preconditioner parameters in CG. Presented numerical
experiments show that optimization of this new functional with respect to preconditioner parameters usually
yields a better parameter value than optimization of the functional based on the spectral condition number.

Key words. linear system solution, conjugate gradient method, preconditioners, condition number, eigen-
value clustering, relaxed incomplete Cholesky preconditioner

AMS subject classifications. 65F08; 65F10

1. Introduction. Preconditioning is an important tool for improving convergence while
solving linear systems iteratively [3, 24, 29]. Efficient preconditioners typically do not (only)
improve the condition number of the system matrix (as the name suggests) but, more impor-
tantly, often lead to clustering of its eigenvalues. In nonstationary methods, like the conjugate
gradient method (CG) [13, 15] or the generalized minimal residual method (GMRES) [24, 25],
this improved clustering usually manifests in superlinear convergence [27, 30].

Many preconditioners include parameters and, although major preconditioner classes have
been extensively analyzed [3, 24, 29], a practical choice of their parameters is often not a trivial
task. To optimize preconditioners (or their parameters) in practice different target functionals
can be used [6], such as the spectral radius [31], Ritz values [12, Chapter 8.4] of the preconditioned
matrix, the so-called K-condition number [18, 17], a suitable norm of the iteration matrix [8, 9],
closeness in the Frobenius norm of the preconditioned matrix to the identity matrix [6], and the
trace of the preconditioned matrix [7]. All these functionals reflect the convergence behavior of
preconditioned iterations and have one common feature: they are based on certain convergence
estimates, which hold for all possible initial guess vectors. In this sense, they represent a worst-
case scenario and, hence, a question arises whether these functionals are adequate for choosing
preconditioner parameters in practice. Would, for example, monitoring the mean convergence
rate be a better option rather than the worst-case rate?

This paper presents an attempt to answer this question. A simple convergence analysis shows
that a faster convergence is observed for an nonempty open set of initial guess vectors. This
suggests that the mean convergence rate can indeed be a more adequate convergence measure
than the worst-case rate. Furthermore, we present a stochastic optimization approach based on
trial runs with random initial guess vectors. This leads to an optimization functional which can
be used to monitor convergence and to optimize preconditioner parameters in CG. We show in
numerical experiments that optimization of this new functional with respect to preconditioner
parameters usually gives a better parameter value than optimization of the functional based

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on the condition number. We emphasize that the suggested approach is currently of restricted practical value if just a single linear system has to be solved. This is because the proposed optimization procedure is based on trial runs with many random initial guess vectors and implies significant computational costs. However, there are situations where many linear systems with the same system matrix have to be solved (as, e.g., in implicit time integration of large dynamical systems) and the preconditioner optimization can lead to a significant convergence improvement. In such cases our approach can be practically useful.

We note that solving many linear systems with the same system matrix has been an active research direction (for some recent work see [2, 5]). The contribution of our stochastic optimization approach here is that it can be used in combination with these techniques, leading to further savings of computational costs by an appropriate choice of preconditioner parameters.

Throughout this paper, we assume that a linear system

\[ Ax = b \]  

has to be solved for a given symmetric positive definite matrix \( A \in \mathbb{R}^{m \times m} \) and many different right hand side vectors \( b \in \mathbb{R}^m \). The rest of the paper is organized as follows. In Section 2 a stochastic convergence measure (a convergence functional) is considered for stationary linear iterative methods, i.e., for iterations of the form

\[ Mx_{k+1} = Nx_k + b, \]

with \( M - N = A \) and nonsingular \( M \). In the same section, we also introduce a similar convergence functional for nonstationary nonlinear iterations such as CG. A question whether the proposed convergence functional provides a convergence measure different than a classical convergence estimate is discussed in Section 3. There we show that an open set of initial guess vectors exists for which CG converges faster than predicted by the classical estimate. This supports our proposed convergence functional. Numerical experiments are presented in Section 5, where we apply our technique to optimize the relaxation parameter \( \alpha \) in the well-known relaxed incomplete Cholesky preconditioner without fill in, which we denote by \( \text{RIC}_\alpha(0) \) [4, 29, 20]. Conclusions are drawn in Section 6.

2. Mean convergence rate. Iterative solvers for linear systems are well studied [3, 13, 14, 21, 24, 29] and many classical convergence estimates are available. A convergence estimate typically has the form

\[ \|x^* - x_k\|_* \leq C q_A^k \|x^* - x_0\|_*, \]  

where \( x^* \) is the exact solution vector of (1.1), \( x_k \) is the \( k \)-th iterand of the method, \( \| \cdot \|_* \) is some vector norm, \( C > 0 \) is a constant and \( q_A > 0 \) is a constant depending on the matrix \( A \). The estimate (2.1) is a worst-case estimate among all initial guess vectors \( x_0 \), whereas it is quite natural to study mean convergence rate of a given iterative method instead. In this paper we want to study this approach which, as far as we know, has not been explored in this way. We consider initial error vector \( x^* - x_0 \) to be a random vector with independent and identically distributed (i.i.d.) entries with a mean of 0 and a standard deviation of 1, i.e., in \( N(0,1) \). Then the error \( x^* - x_k \) is also the random vector, and we can define its expectation \( e_k \) by

\[ e_k^2 = \mathbb{E}(\|x^* - x_k\|_*^2). \]

A question arises whether an estimate of the form

\[ e_k \sim C \mu_A k \]
can be obtained, where $\mu_A > 0$ is a constant which depends on $A$ and determines the convergence rate. We should be careful while giving a meaning to the asymptotic behavior in (2.2), since for some methods (e.g., CG) in exact arithmetic we have convergence after $m$ iterations. Nevertheless, for large $m$ the estimates of the form (2.2) are of interest and provide useful information about convergence.

First, the important special case is the stationary linear iterative method (1.2),

$$x_{*} - x_{k+1} = G(x_{*} - x_{k}), \quad G = M^{-1}N,$$

where $G$ is the iteration matrix and $M - N = A$. Then, using the classical Hutchinson result on stochastic trace estimator [16] and denoting $d_k = x_{*} - x_{k}, \ k \geq 0$, we obtain in the 2-norm

$$e_k^2 = E \left( G^k d_0, G^k d_0 \right) = E \left( (G^k)^T G^k d_0, d_0 \right) = \text{Tr}(G^k G^k) = \|G^k\|_F^2,$$

where $\|\cdot\|_F$ is the Frobenius matrix norm and Tr denotes the trace of a matrix. Due to Gelfand’s formula

$$\lim_{k \to \infty} \|G^k\|_1^{1/k} = \rho(G),$$

where $\|\cdot\|_*$ is any norm\(^1\) and $\rho(G)$ denotes the spectral radius of $G$, we have

\begin{equation}
(2.4) \quad e_k \sim \rho(G)^k,
\end{equation}

i.e., in this case the worst-case rate is also the mean rate [19].

For nonlinear nonstationary iterative methods, such as CG or MINRES, similar analysis appears to be quite complicated and is left beyond the scope of this paper. However, we find experimentally, by Monte-Carlo simulations and fitting estimated convergence rates, that the situation is completely different, i.e., the worst-case rates are significantly larger than the estimated mean convergence rates. Since analytical expressions for the mean convergence rate are not available, we can follow practical approach and try to derive a computable measure of convergence similar to (2.4). As $k$ iterations of a stationary linear method (1.2) are carried out through $k$ matrix-vector multiplication with the iteration matrix $G$, similarly, $k$ iterations of a nonstationary method can be seen an action of some nonlinear mapping (defining the method) $k$ times\(^2\). Hence, abusing to some extend the notation, we can write

\begin{equation}
(2.5) \quad x_{*} - x_k = G[x_{*} - x_{k-1}] = G^k[x_{*} - x_0],
\end{equation}

where $G$ is the mapping of the nonlinear method and $G^k$ denotes the mapping applied $k$ times. Then, a straightforward, practical way to monitor convergence of the method is to perform $k$ iterations for a number of random initial guess vectors $x_0^{(i)}$. Indeed, let us define a stochastic convergence functional

\begin{equation}
(2.6) \quad F_s \equiv \frac{1}{n} \sum_{i=1}^{n} \|x_{*} - x_k^{(i)}\|_*,
\end{equation}

where $n$ is the number of random initial guess vectors and $x_k^{(i)}$ is the $k$-th iterand of the method started at initial guess vector $x_0^{(i)}$. Although for CG the functional $F_s$ is computable if the

\(^1\)The norm does not have to be an operator norm (i.e., induced by a vector norm) but if so the limit is approached from above.

\(^2\)For CG, which is a three-term recurrence method, this mapping $G$ depends on the last two iterands $x_k$ and $x_{k-1}$ and the two corresponding $A$-conjugate search directions $p_k$ and $p_{k-1}$.
A-norm is used, in practice one may just set \( x^\ast \) to zero, which means that a linear system with the right hand side \( b = 0 \) is solved. In this paper in all cases \( F_s \) is computed for \( x^\ast = 0 \) and the 2-norm. Note that, analogously to (2.2), we can write

\[
F_s = \frac{1}{n} \sum_{i=1}^{n} \| x^\ast - x_k^{(i)} \|_2 = \frac{1}{n} \sum_{i=1}^{n} \| G[x^\ast - x_0] \|_2 \approx E_{x_0} \| G[x^\ast - x_0] \|_2.
\]

A possible application of this approach explored in this paper is optimization of the preconditioner parameters in preconditioned CG method to get faster convergence. Evidently, such an optimization process based on many trial runs is expensive (one trial run means carrying out \( k \cdot n \) iterations of the method). These costs are only paid off if the optimized preconditioner is to be used in many iterations, for example, if many linear systems with the same matrix and different right hand sides have to be solved. This is why we make this assumption while introducing (1.1).

Since for stationary iterations the stochastic convergence functional appears to be identical to a classical convergence measure (i.e., the spectral radius of the iteration matrix), a question arises whether our stochastic convergence functional \( F_s \) does not coincide with the some known convergence measure for nonstationary iterations. In the next section we study this question for the CG method. A well-known classical convergence estimate for CG (see e.g., [3, 13, 21, 24, 29]), is based on the condition number \( \kappa \) of the system matrix \( A \):

\[
(2.7) \quad \| x^\ast - x_k \|_A \leq 2 \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k \| x^\ast - x_0 \|_A.
\]

Although this estimate can in general be pessimistic, as it does not reflect the often observed superlinear convergence of CG [27, 4], it can still be used for monitoring the convergence rate of CG. Hence, together with (2.6), we consider the corresponding classical convergence functional, i.e.,

\[
(2.8) \quad F_c \equiv \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^k.
\]

Note that (2.7) can be improved if a clustering of the eigenvalues is assumed [4, 24, 27]. In the next section we show that even if no assumptions on eigenvalue clustering are made, there is an open set of initial guess vectors for which CG exhibits a faster convergence than predicted by the classical estimate (2.7). This implies that our stochastic functional (2.6) is essentially different than the classical convergence functional (2.8).

3. Initial guess vectors and convergence of CG. Analysis in this section is inspired by results of [27]. Let \( A \) be a symmetric positive definite \( m \times m \) matrix, \( z_1, \ldots, z_m \) be orthonormal eigenvectors of \( A \), and \( 0 < \lambda_1 \leq \cdots \leq \lambda_m \) be the corresponding eigenvalues. For simplicity of notation throughout this section we omit the subscript \( \ast \), in the exact solution vector \( x^\ast \). For the CG iterands \( x_j, \ j = 1, 2, \ldots \), the optimality property reads

\[
(3.1) \quad \| x - x_j \|_A = \min_{q \in \mathcal{H}_j^{\ast 1}} \| q(A)(x - x_0) \|_A,
\]

where \( \mathcal{H}_j^{\ast 1} \) denotes the set of all polynomials of degree at most \( j \) with the constant term 1. Let \( q \) be the CG residual polynomial (i.e., the polynomial at which the minimum in (3.1) is attained), and let

\[
x - x_0 = \sum_{i=1}^{m} \gamma_i z_i,
\]
It is easy to check that the optimality property (3.1) can be rewritten as

\[(3.2) \quad \|x - x_j\|_A^2 = \sum_{i=1}^{m} \lambda_i (\gamma_i q(\lambda_i))^2 \leq \sum_{i=1}^{m} \lambda_i (\bar{\gamma}_i q(\lambda_i))^2, \quad \forall \bar{\gamma} \in \Pi_{j+1}. \]

Moreover, we have

\[(3.3) \quad q(t) = \frac{(\theta_1 - t) \ldots (\theta_j - t)}{\theta_1 \ldots \theta_j}, \]

where the roots \(\theta_1, \ldots, \theta_j\) of \(q(t)\) are the Ritz values of the CG process.

Furthermore, consider \(\bar{x}_0\) chosen such that

\[(3.4) \quad x - \bar{x}_0 = \sum_{i=2}^{m} \gamma_i z_i, \]

and denote by \(\tilde{q}(t)\) the CG residual polynomial of the CG iterations with \(\bar{x}_0\) taken as the initial guess. Similarly to (3.3), it holds

\[\tilde{q}(t) = \frac{(\bar{\theta}_1 - t) \ldots (\bar{\theta}_j - t)}{\bar{\theta}_1 \ldots \bar{\theta}_j}, \]

with \(\bar{\theta}_1, \ldots, \bar{\theta}_j\) being the Ritz values of the CG process started at \(\bar{x}_0\). Note that by taking in (3.2) the polynomial \(\tilde{q}(t)\) as the Chebyshev minimax polynomial on the interval \([\lambda_1, \lambda_m]\), we obtain the classical convergence estimate:

\[\|x - x_j\|_A^2 \leq \sum_{i=1}^{m} \lambda_i (\gamma_i \tilde{q}(\lambda_i))^2 \leq \max \tilde{q}(\lambda_i)^2 \sum_{i=1}^{m} \lambda_i \gamma_i^2 \leq \max_{\lambda \in [\lambda_1, \lambda_m]} \tilde{q}(\lambda)^2 \sum_{i=1}^{m} \lambda_i \gamma_i^2 \]

\[= \max_{\lambda \in [\lambda_1, \lambda_m]} \tilde{q}(\lambda)^2 \cdot \|x - x_0\|_A^2 = 4C_1^2 \delta, \quad \|x - x_0\|_A^2 = 4C_1^2 \delta, \quad \|x - x_0\|_A^2 = 4C_2^2 \delta, \quad \|x - x_0\|_A^2 = 4C_2^2 \delta, \]

where

\[C_1 = \frac{\sqrt{\kappa_1} - 1}{\sqrt{\kappa_1} + 1}, \quad \kappa_1 = \frac{\lambda_m}{\lambda_1}. \]

For the CG process started at \(\bar{x}_0\) the corresponding convergence estimate reads

\[(3.6) \quad \|x - x_j\|_A^2 \leq 4C_2^2 \delta, \quad \|x - x_0\|_A^2 \leq 4C_2^2 \delta, \quad \|x - x_0\|_A^2 \leq 4C_2^2 \delta, \quad \|x - x_0\|_A^2 \leq 4C_2^2 \delta, \]

THEOREM 3.1. Let the initial guess vector \(x_0\) in the CG process be chosen such that the first component \(\gamma_1\) of the initial error \(x - x_0\) is small with respect to the other components; more precisely, let there exist a constant \(\delta > 0\) such that

\[(3.7) \quad \sum_{i=1}^{m} \lambda_i \gamma_i^2 \|x - x_0\|_A^2 \leq 4C_2^2 \delta, \quad \kappa_2 = \frac{\lambda_m}{\lambda_2}. \]

where \(x_0\) is defined in (3.4). Then convergence of the CG process in the first \(J\) iterations is determined by the constant \(C_2\) rather than by \(C_1\) (cf. (3.5),(3.6)) in the sense that

\[(3.8) \quad \|x - x_j\|_A^2 \leq 4(1 + \delta)C_2^2 \delta, \quad \|x - x_0\|_A^2 \leq 4(1 + \delta)C_2^2 \delta, \quad \|x - x_0\|_A^2 \leq 4(1 + \delta)C_2^2 \delta, \quad \|x - x_0\|_A^2 \leq 4(1 + \delta)C_2^2 \delta. \]
Proof. Choosing in (3.2) polynomial $\tilde{q}(t)$ as the residual polynomial $\bar{q}(t)$ of the CG process started at $\bar{x}_0$, we have

\[
\|x - x_j\|_A^2 = \sum_{i=1}^{m} \lambda_i (\gamma_i \bar{q}(\lambda_i))^2 \leq \sum_{i=1}^{m} \lambda_i (\gamma_i \tilde{q}(\lambda_i))^2 = \lambda_1 (\gamma_1 \tilde{q}(\lambda_1))^2 + \sum_{i=2}^{m} \lambda_i (\gamma_i \tilde{q}(\lambda_i))^2 \leq \lambda_1 (\gamma_1 \tilde{q}(\lambda_1))^2 + 4C_2^2 \|x - \bar{x}_0\|_A^2 \leq \lambda_1 \gamma_1^2 + 4C_2^2 \|x - \bar{x}_0\|_A^2,
\]

where the last inequality holds because

\[0 \leq \tilde{q}(t) \leq 1,\]

which is true since $\tilde{q}(t)$ is monotonically non-increasing on the interval $[0, \lambda_2]$ and $\tilde{q}(0) = 1$. Finally, we use assumption (3.7) and obtain

\[
\|x - x_j\|_A^2 \leq \lambda_1 \gamma_1^2 + 4C_2^2 \|x - \bar{x}_0\|_A^2 \leq 4C_2^2 \|x - \bar{x}_0\|_A^2 + 4(1 + \delta)C_2^2 \|x - x_0\|_A^2.
\]

This ends the proof. \(\square\)

It is not difficult to see that the last theorem can be generalized for the case where several first components of the initial error are small with respect to the other error components. Indeed, denote

\[
C_s = \kappa_s \frac{\sqrt{\kappa_s + 1}}{\sqrt{\kappa_s - 1}}, \quad \kappa_s = \frac{\lambda_m}{\lambda_s}.
\]

Then the following result holds.

**Theorem 3.2.** Let the initial guess vector $x_0$ in the CG process be chosen such that the first $s - 1$ components $\gamma_1, \ldots, \gamma_{s-1}$ of the initial error $x - x_0$ are small with respect to the other components; more precisely, let there exist a constant $\delta > 0$ such that

\[
\sum_{i=1}^{s-1} \lambda_i \gamma_i^2 \leq \lambda_1 \gamma_1^2 + 4C_2^j \|x - \bar{x}_0\|_A^2, \quad \text{for } j = 1, \ldots, J,
\]

where

\[
\sum_{i=s}^{m} \lambda_i \gamma_i^2 / \|x - \bar{x}_0\|_A^2 \leq 4C_2^2 \delta, \quad \text{for } j = 1, \ldots, J.
\]

Then convergence of the CG process in the first $J$ iterations is determined by the constant $C_s$ rather than by $C_1$ (cf. (3.5)) in the sense that

\[
\|x - x_j\|_A^2 \leq 4(1 + \delta)C_2^2 \|x - x_0\|_A^2, \quad \text{for } j = 1, \ldots, J.
\]
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Fig. 1: CG convergence for the initial guess vectors with $\gamma_1 = 0.05$ (top) and $\gamma_1 = 5$ (bottom): the error norm $\|x - x_j\|_A$ (the $\times$ curve), estimate $2C_j^2$ (the $\circ$ line), estimate $2C_j^2$ (the $\triangle$ line), and the values $\gamma_1 q(\lambda_1)$ and $\gamma_1 \bar{q}(\lambda_1)$ (the $*$ and $\diamond$ curves, respectively).

Proof. The proof is analogous to the proof of Theorem 3.1. We take in (3.2) polynomial $\tilde{q}(t)$ as the residual polynomial $\bar{q}(t)$ of the CG process started at $\bar{x}_0$ defined in (3.11). Using the convergence estimate

$$\|x - \bar{x}_j\|_A^2 \leq 4C_j^2 \|x - \bar{x}_0\|_A^2,$$

which holds for this CG process, and the assumption (3.10), we arrive at (3.12).

Theorems 3.1, 3.2 can be illustrated by the following numerical test. Let $A$ be a diagonal
matrix of dimension \( m = 1000 \), with the diagonal entries
\[ 1, 2, 3, \ldots, 1000. \]

Let, furthermore, the right hand side vector \( b \) be taken such that the exact solution vector has all its components one. The initial guess vector \( x_0 \) is chosen such all the components of \( x - x_0 \) except the first one are i.i.d. and in \( N(0, 1) \) (independent normally distributed random values with zero mean and variance one). The first entry of \( x - x_0 \) is set to \( \gamma_1 \).

In Figure 1 the CG error convergence is plotted, together with the Chebyshev bounds (3.5), (3.6) and the values \( \gamma_1 q(\lambda_1), \gamma_1 \bar{q}(\lambda_1) \). As we see, at first iterations (approximately until iteration 75 for \( \gamma_1 = 0.05 \) and iteration 25 for \( \gamma_1 = 5 \)) the values \( \gamma_1 q(\lambda_1) \) and \( \gamma_1 \bar{q}(\lambda_1) \) are practically equal and stay almost constant. This means that the CG converges just as if the first error component were absent. As clearly seen in the first plot of Figure 1, upto iteration 75, the slope of the error \( A \)-norm (the \( \times \) curve) is determined by the improved Chebyshev estimate (the \( \triangle \) line), which confirms the estimate (3.8). The first error component is ignored by the CG iterations until it becomes comparable in magnitude with the total error norm (until the \( \times \) curve crosses the \( * \) curve). Starting from this point, \( \gamma_1 \bar{q}(\lambda_1) \) starts to decrease, thus damping the first error component. The value of \( \gamma_1 q(\lambda_1) \) keeps on staying almost unchanged and exceeds the error norm. It is interesting to note that at the cross point of the \( \times \) line and the \( * \) curve (corresponding to iteration 75 for \( \gamma_1 = 0.05 \) and iteration 25 for \( \gamma_1 = 5 \)) the estimate (3.7) holds for approximately the same values of \( \delta \), namely for \( \delta < 10^{-3} \). Thus, this value can be seen as a “threshold” value for what CG process “considers” as small.

Results of a similar test are presented in Figure 2. The parameters of test runs are the same, except that the first three components of the initial error \( \gamma_1, \gamma_2, \gamma_3 \) are now given the same specific value (namely, either 0.05 or 2). Accordingly, the comparison CG process with the polynomial \( q(t) \) (plot by the \( \diamond \) curve) is now started at \( x_0 \), as defined in (3.11) with \( s = 4 \).

Remark 3.3. We note that our convergence results can be seen as a complement to the classical convergence estimates of Van der Sluis and Van der Vorst [27] in the following sense. Our results specify possible convergence behavior of CG at the initial stage, i.e., before the certain components in the error are damped and CG exhibits its well known superlinear convergence (this “superlinear” convergence phase is seen in the \( \times \) curves in Figures 1 and 2 after they cross the \( \diamond \) curves).

4. Costs of the optimization procedure. To optimize preconditioner parameters with respect to the stochastic convergence functional \( F_c \), we use Brent’s method [10]. This optimization method, which is a combination of the golden search and inverse quadratic interpolation, requires a single evaluation of the functional per optimization step. Hence, the total costs of the optimization procedure can approximately be expressed as \( Kn_8 \) preconditioned matrix–vector products (matvecs), where \( K \) is the number of the preconditioned iterations (its choice is discussed below in Section 5.2), \( n \) is the number of random initial guess vectors, \( s \) is the number of optimization steps needed to find the optimal value to an acceptable accuracy.

Thus, our optimization procedure is more efficient than a simple trial-and-error search provided that the number of optimization steps \( s \) is smaller than the number of trial-and-error runs. In our case, we restrict the search to the interval \( \alpha \in [0.9, 1] \) which is known to contain the optimal value for the RIC\(_c(0)\) preconditioner, see, e.g., [28], [29], Section 13.2.1]. In numerical experiments we typically observe that up to \( s = 25 \) optimization steps suffice, whereas to find the optimal value by trial-and-error runs usually approximately 100 are needed.

The same optimization procedure with Brent’s method is used in numerical tests of Section 5 to optimize the classical condition number functional \( F_c \). To compute the condition number in \( F_c \) we use a standard sparse eigenvalue solver of Python numerical library (this eigenvalue solver
Fig. 2: CG convergence for the initial guess vectors with $\gamma_1 = \gamma_2 = \gamma_3 = 0.05$ (top) and $\gamma_1 = \gamma_2 = \gamma_3 = 2$ (bottom): the error norm $\|x - x_j\|_A$ (the $\times$ curve), estimate $2C_j^1$ (the $\circ$ line), estimate $2C_j^2$ (the $\triangle$ line), and the values $\gamma_1 q_1$ and $\gamma_1 \bar{q}_1$ (the $*$ and $\text{⋄}$ curves, respectively).

is similar to the \texttt{eigs} command in Octave and Matlab and based on the ARPACK software [1]). We note that using eigensolvers for evaluating $F_c$ may be prohibitively expensive in practice and is done only to compare parameter optimization based on $F_s$ and on $F_c$.

5. Numerical experiments. In this section we present comparison of the classical functional and the proposed one for choosing an optimal parameter in the RIC\textsubscript{$\alpha$}(0) preconditioner [4]. We start with describing the test problem.
5.1. Test problem. In the tests we use linear systems obtained by the standard second order central finite difference approximation of the following Dirichlet boundary value problem for unknown $u(x,y)$:

\begin{align}
- (D_1 u_x)_x - (D_2 u_y)_y = g(x,y), \quad (x,y) \in \Omega = [0, 1] \times [0, 1], \\
u(x,y)|_{\partial \Omega} = 0,
\end{align}

where the subscripts $\cdot_x, \cdot_y$ denote the partial derivatives with respect to $x$ and $y$. We consider two cases: in the first case the coefficients $D_{1,2}$ are taken to be identically one in the whole domain $\Omega$. In the second case the coefficients $D_{1,2}$ are discontinuous:

\begin{align*}
D_1 &= \begin{cases} 
1000, & (x,y) \in [\frac{1}{4}, \frac{3}{4}] \times [\frac{1}{4}, \frac{3}{4}], \\
1, & \text{otherwise},
\end{cases} \\
D_2 &= \frac{1}{2} D_1.
\end{align*}

The right hand side function $g(x,y)$ is taken such that values of the function $u(x,y) = \sin(\pi x) \sin(\pi y)$ on the finite difference mesh are the entries of the exact solution of the discretized problem.

5.2. Comparison of the two functionals. To perform comparison of the proposed functional (2.6) and the classical one (2.8) four particular test linear systems are considered. These linear systems are obtained from test problem (5.1) with the right hand side (5.2) and the following four sets of parameters:

1. $m = 2500$ (mesh $52 \times 52$), constant coefficients $D_{1,2}$;
2. $m = 2500$ (mesh $52 \times 52$), discontinuous coefficients $D_{1,2}$;
3. $m = 10000$ (mesh $102 \times 102$), constant coefficients $D_{1,2}$;
4. $m = 10000$ (mesh $102 \times 102$), discontinuous coefficients $D_{1,2}$.

In the experiments the 2-norm is used to compute $F_s$. Also, we use $n = 50$ initial guess vectors, which, taking into account stochastic convergence, appears to be a reasonable value (see also Section 5.3).

The optimal $\alpha$ value for the RIC$_\alpha(0)$ preconditioner is sought for in the interval $[0.9, 1]$, known to contain the optimal value [28], [29, Section 13.2.1]. The number of iterations $K$ (used in the convergence functionals $F_s$ and $F_r$) is determined such that a required tolerance is achieved for a reasonable (not yet optimized) value of $\alpha$. In the experiments below we set the required tolerance for the residual norm reduction $\|r_k\|/\|r_0\|$ to $10^{-7}$ (where the residual is defined as $r_k = b - A x_k$). This tolerance value yields the values of $K$ given in Table 1. To find the optimal parameters $\alpha_s^*$ and $\alpha_r^*$ (corresponding to the classical and to the stochastic convergence functionals, respectively), Brent’s optimization solver is applied. The accuracy of the optimization procedure is set to $10^{-5}$ which is sufficient for our purposes. The computed optimal values $\alpha_s^*$ and $\alpha_r^*$ are given in Table 1. Here insignificant (taking into account optimization accuracy) digits are shown in brackets.

Figures 3–6 show dependence of the both functionals on the preconditioner parameter $\alpha$ (see plots (a) for stochastic functional and plots (c) for the classical one). As can be seen in the plots, the stochastic functional $F_s$ tends, more often than $F_r$, to have a minimum close to one, rather than exactly at one. To investigate this difference, we plot eigenvalue distribution of the preconditioned matrices corresponding to $\alpha_s^*$ and $\alpha_r^*$ and compare eigenvalue clustering. Figures 3b, 4b, 5b and 6b show the spectra of the preconditioned matrices corresponding to $\alpha_s^*$. The similar plots for $\alpha_r^*$ are given in Figures 3d, 4d, 5d and 6d. Spectrum distribution plots demonstrate that $\alpha_s^*$ yields spectra better clustered around small eigenvalues than $\alpha_r^*$. Consequently, convergence of the preconditioned CG for $\alpha_s^*$ is faster than for $\alpha_r^*$, see Figure 3e, 4e, 5e and 6e.
Table 1: Number of iterations $K$ used in the convergence functionals $F_s$ and $F_c$ (for the tolerance is $10^{-7}$) and corresponding optimal parameters $\alpha^*_s$ and $\alpha^*_c$.

| Test case                        | $K$ | $\alpha^*_s$    | $\alpha^*_c$    |
|----------------------------------|-----|----------------|----------------|
| $m = 2500$, constant $D_{1,2}$   | 20  | 0.98257(07)    | 0.99618(02)    |
| $m = 2500$, discontinuous $D_{1,2}$ | 30  | 0.97671(44)    | 0.99999(47)    |
| $m = 10000$, constant $D_{1,2}$  | 35  | 0.99245(52)    | 0.99900(93)    |
| $m = 10000$, discontinuous $D_{1,2}$ | 45  | 0.99451(65)    | 0.99999(33)    |

5.3. The number of random initial guess vectors $n$. The costs of optimization procedure depend heavily on the choice of the number of initial guess vectors $n$ (see Section 4). As mentioned above, we use $n = 50$ in all the experiments presented above. In this section we test how sensitive the obtained results are to the choice of $n$. It appears that similar results can be obtained with smaller values of $n$. We consider the test case with $m = 2500$ and constant coefficients $D_{1,2}$. According to Table 1, number of iterations $K$ for this test case is set to 20. For this experiment setting, the dependence of the proposed stochastic convergence functional $F_s$ on the preconditioner parameter $\alpha$ for several values of $n$ is plot in Figure 7. As we see in the plots, the larger $n$, the smoother the dependence line and already $n = 10$ is enough for an adequate representation of the considered dependence. In Figure 8 the confidence interval is plot for $F_s$.

6. Conclusion. In this paper, a stochastic approach to estimate convergence rate of iterative linear system solvers is presented. Our estimate (which we call a stochastic convergence functional) is essentially based on monitoring the mean convergence rate for a number of random initial guess vectors. For linear stationary iterative methods it is shown that the stochastic convergence functional coincides with the classical convergence estimate based on the spectral radius of the iteration matrix. For the CG method, which is a nonlinear nonstationary method, both analysis and experiments suggest that the stochastic convergence functional provides a sharper convergence measure than the classical estimate based on the spectral condition number of the system matrix. We also show that the new stochastic convergence functional can be used for optimizing parameters in preconditioners for the CG method. Numerical tests for the CG method preconditioned by the $\text{RIC}_{\alpha}(0)$ preconditioner (relaxed incomplete Cholesky factorization with no fill in) are presented. The tests demonstrate that the new stochastic functional provides a better means for optimizing the relaxation parameter in $\text{RIC}_{\alpha}(0)$ than minimizing the spectral condition number.

Simple convergence analysis presented here shows that the classical convergence estimate based on the spectral condition number can be improved for some initial guess vectors. An interesting open question remains whether other convergence estimates, in particular, which demonstrate superlinear convergence, can be improved for some initial guess vectors. We believe that this is true and leave this proving for a future work.

Another interesting extension of this work would be preconditioner optimization with respect to different parameters. This is relevant, for instance, for circulant preconditioners [11, 23, 26]. In this case some gradient optimization methods in combination with automatic differentiation tools (such as Autograd, Pytorch, etc.) can be successfully used (see our recent work [19]).

Finally, a relevant question is whether our stochastic optimization procedure can be combined with solving multiple linear systems by Krylov subspace recycling [2, 5, 22]. One could, for example, carry out optimization based on the given (rather than on random) right hand vectors, starting off with unoptimized preconditioner and carrying out optimization “on the fly”. We
Fig. 3: Test case $m = 2500$, discontinuous coefficients $D_{1,2}$. Plots (a),(c): dependence of the functionals $F_s$, $F_c$ on the preconditioner parameter $\alpha$ for different iteration number $K$. Plots (b),(d): eigenvalues of the preconditioned matrix for the optimal $\alpha^*_s$ (based on $F_s$, plot (b)) and $\alpha^*_c$ (based on $F_c$ (plot (d)). Plot (e): Residual norm convergence of CG preconditioned by RIC$\alpha(0)$ for $\alpha^*_s$ and $\alpha^*_c$.

hope to explore this in a future work.
Fig. 4: Test case $m = 2500$, constant coefficients $D_{1,2}$. Plots (a),(c): dependence of the functionals $F_s, F_c$ on the preconditioner parameter $\alpha$ for different iteration number $K$. Plots (b),(d): eigenvalues of the preconditioned matrix for the optimal $\alpha^*_s$ (based on $F_s$, plot (b)) and $\alpha^*_c$ (based on $F_c$ (plot (d)). Plot (e): Residual norm convergence of CG preconditioned by RIC$_\alpha(0)$ for $\alpha^*_s$ and $\alpha^*_c$. 

REFERENCES
Preconditioner parameter, $\alpha$

Stochastic functional, $F_s$

(a)

Plots (a),(c): dependence of the functionals $F_s$, $F_c$ on the preconditioner parameter $\alpha$ for different iteration number $K$.

Plots (b),(d): eigenvalues of the preconditioned matrix for the optimal $\alpha_s^*$ (based on $F_s$, plot (b)) and $\alpha_c^*$ (based on $F_c$ (plot (d)).

Plot (e): Residual norm convergence of CG preconditioned by $\text{RIC}_\alpha(0)$ for $\alpha_s^*$ and $\alpha_c^*$.

Fig. 5: Test case $m = 10000$, discontinuous coefficients $D_{1, 2}$. Plots (a),(c): dependence of the functionals $F_s$, $F_c$ on the preconditioner parameter $\alpha$ for different iteration number $K$.

[1] ARPACK: a collection of subroutines designed to solve large scale eigenvalue problems. http://www.caam.
Fig. 6: Test case $m = 10000$, constant coefficients $D_{1,2}$. Plots (a),(c): dependence of the functionals $F_s, F_c$ on the preconditioner parameter $\alpha$ for different iteration number $K$. Plots (b),(d): eigenvalues of the preconditioned matrix for the optimal $\alpha^*_s$ (based on $F_s$, plot (b)) and $\alpha^*_c$ (based on $F_c$ (plot (d)). Plot (e): Residual norm convergence of CG preconditioned by RIC$_\alpha(0)$ for $\alpha^*_s$ and $\alpha^*_c$.

rice.edu/software/ARPACK/.
Fig. 7: Dependence of the stochastic convergence functional \( F_s \) on the preconditioner parameter \( \alpha \) for \( K = 20 \) and different values of initial guess vectors \( n \). The test case is \( m = 2500 \), constant coefficients \( D_{1,2} \). The value \( n = 50 \) used in the experiments results in a plot indistinguishable from the plot for \( n = 25 \).

Fig. 8: Confidence interval (the gray area) of the stochastic convergence functional \( F_s \) for \( \alpha \in [0.9, 1] \) (left) and \( \alpha \in [0.5, 1] \) (right). The test case is \( m = 2500 \), constant coefficients \( D_{1,2} \).

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