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A comparison of abstract versions of deflation, balancing and additive coarse grid correction preconditioners

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SUMMARY

In this paper we consider various preconditioners for the conjugate gradient (CG) method to solve large linear systems of equations with symmetric positive definite system matrix. We continue the comparison between abstract versions of the deflation, balancing and additive coarse grid correction preconditioning techniques started in (*SIAM J. Numer. Anal.* 2004; **42**:1631–1647; *SIAM J. Sci. Comput.* 2006; **27**:1742–1759). There the deflation method is compared with the abstract additive coarse grid correction preconditioner and the abstract balancing preconditioner. Here, we close the triangle between these three methods. First of all, we show that a theoretical comparison of the condition numbers of the abstract additive coarse grid correction and the condition number of the system preconditioned by the abstract balancing preconditioner is not possible. We present a counter example, for which the condition number of the abstract additive coarse grid correction preconditioned system is below the condition number of the system preconditioned with the abstract balancing preconditioner. However, if the CG method is preconditioned by the abstract balancing preconditioner and is started with a special starting vector, the asymptotic convergence behavior of the CG method can be described by the so-called effective condition number with respect to the starting vector. We prove that this effective condition number of the system preconditioned by the abstract balancing preconditioner is less than or equal to the condition number of the system preconditioned by the abstract additive coarse grid correction method. We also provide a short proof of the relationship between the effective condition number and the convergence of CG. Moreover, we compare the A-norm of the errors of the iterates given by the different preconditioners and establish the orthogonal invariants of all three types of preconditioners. Copyright © 2008 John Wiley & Sons, Ltd.

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1. INTRODUCTION

In 1952, Hestenes and Stiefel [1] introduced the conjugate gradient (CG) method to solve large linear systems of equations

$$Ax = b$$

whose coefficient matrices A are sparse and symmetric positive definite. The convergence rate of the CG method is bounded as a function of the condition number of the system matrix to which it is applied. If the condition number of A is large, it is advisable to solve, instead, a preconditioned system $M^{-1}Ax = M^{-1}b$, where the symmetric positive definite preconditioner M is chosen such that $M^{-1}A$ has a more clustered spectrum or a smaller condition number than that of A. Furthermore, systems $Mz = r$ must be cheap to solve relative to the improvement it provides in convergence rate.

Today, the design and analysis of preconditioners for the CG method are in the main focus whenever a linear system with symmetric positive definite coefficient matrix needs to be solved. Even fast solvers, such as multigrid or domain decomposition method, are used as preconditioners. However, there are just a few theoretical comparisons of different preconditioners.

Here, we consider three different preconditioning techniques: the additive coarse grid correction, the balancing and the deflation preconditioner. These preconditioners differ a lot in practice. However, we consider these techniques from an abstract point of view. This abstract point of view allows us to derive comparisons between these preconditioners.

In [2, 3] the authors theoretically compared the abstract deflation method with the abstract additive coarse grid correction preconditioner and the abstract balancing preconditioner. It is proved in [2, 3] that the condition number of the system matrix preconditioned by the deflation method is always below the condition number of the system matrix preconditioned by the additive coarse grid correction. Moreover, the authors showed that the spectrum of the system matrix preconditioned by the deflation method and the spectrum of the system matrix preconditioned by the abstract balancing preconditioner are similar. The only difference is that in the spectrum of the deflated system matrix some eigenvalues of the original matrix have been shifted to zero, while the abstract balancing preconditioner shifts the same eigenvalues to one. This implies that the condition number of the deflated system is always below or equal to the condition number of the system preconditioned by the abstract balancing preconditioner.

Here we close the triangle between these three methods. We compare the abstract additive coarse grid correction preconditioner with the abstract balancing preconditioner.

It is suggested, e.g. in [4, 5] that the balancing preconditioner always yields a smaller condition number than the additive coarse grid correction preconditioner. However, it is worth to have a closer look at the abstract versions of these preconditioners. First of all, we show that a theoretical comparison of the condition numbers of the abstract additive coarse grid correction and the condition number of the system preconditioned by the abstract balancing preconditioner is in general not possible. We present a 2×2 counter example, for which the condition number of the abstract additive coarse grid correction preconditioned system is below the condition number of the system preconditioned with the abstract balancing preconditioner.

However, if the CG method is preconditioned by the abstract balancing preconditioner and is started with a special starting vector, a theoretical comparison can be established. In this case, the asymptotic convergence behavior of the CG method can be described by the so-called effective condition number with respect to the starting vector. We provide a short proof of the relationship

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between the effective condition number with respect to the starting vector and the convergence of CG.

We then prove that this effective condition number of the system preconditioned by the abstract balancing preconditioner is less than or equal to the condition number of the system preconditioned by the abstract additive coarse grid correction method.

Moreover, we compare the A-norm of the errors of the iterates given by the different preconditioners. It was shown in [3] that the A-norm of the error of the iterates given by the deflation preconditioner is below the error of the iterates given by the abstract balancing preconditioner. Such general results do not hold between the other preconditioners. However, we prove here that the error of the iterates given by the deflation method is below the error of the iterates given by the additive coarse grid correction if eigenvectors are used as projection vectors.

Finally, we established the orthogonal invariance of all the preconditioners mentioned above.

We should mention that the convergence of Krylov subspace methods depends not only on the condition number of the system matrix. The clustering of the spectrum, the right-hand side, and also implementation issues have a major influence on the practical speed of convergence. A numerical comparison of the above-mentioned methods is given in [6]. Here we try to complete the collection of theoretical comparisons of the abstract versions of these preconditioners.

This paper is organized as follows. Section 2 describes the preconditioners. In Section 3 the comparison of balancing and the coarse grid correction is given. In Section 4 we compare the A-norm of the deflation and coarse grid correction errors. In Section 5 it is shown that the preconditioners are invariant under orthogonal transformations. Section 6 contains some numerical results.

2. THE PRECONDITIONER

The balancing and additive coarse grid correction preconditioners are used mainly in domain decomposition methods [5]. The additive coarse grid correction is introduced by Bramble *et al.* [7], Dryja and Widlund [8] and Dryja [9]. An abstract analysis of this preconditioner is given by Padiy *et al.* [10]. The balancing preconditioner is proposed by Mandel [4, 11] and Mandel and Brezina [12] and further analyzed by Dryja and Widlund [13], Pavarino and Widlund [14] and Toselli and Widlund [5].

Here, we consider these preconditioners from an abstract point of view. We use an algebraic formulation to describe these preconditioners. This approach leads to abstract versions of these methods. Hence, we call these methods abstract additive coarse grid correction and abstract balancing preconditioners.

In our notation, the abstract balancing, the abstract additive coarse grid and the deflation preconditioners are given in the following form.

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric positive definite matrix. With a rectangular but full rank matrix $Z \in \mathbb{R}^{n\times r}$, the matrix $E = Z^{\mathrm{T}}AZ$ and an arbitrary symmetric positive definite matrix M, the abstract balancing preconditioner is given by

$$P_B = (I - ZE^{-1}Z^{\mathrm{T}}A)M^{-1}(I - AZE^{-1}Z^{\mathrm{T}}) + ZE^{-1}Z^{\mathrm{T}} \tag{1}$$

Note that P_B is symmetric and positive definite.

In the original balancing preconditioner, M^{-1} contains the additive Schwarz preconditioner and some scaling.

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The abstract additive coarse grid correction can be expressed as

$$P_{CM} = M^{-1} + \sigma Z E^{-1} Z^{\mathrm{T}} \tag{2}$$

where in most applications $\sigma = 1$.

As for the balancing method, the additive Schwarz preconditioner is used as M^{-1} in the original version of the additive coarse grid correction.

From our algebraic point of view, Z is an arbitrary rectangular matrix with full rank. Moreover, M is an arbitrary symmetric positive definite matrix. In practice, the particular choices of Z and M in the coarse grid correction preconditioner and the balancing preconditioner can be different. More details about the balancing and the additive coarse grid correction preconditioners are given in [5, 15, 16].

The deflation technique has been exploited by several authors. Among them are Nicolaides [17], Morgan [18], Kolotilina [19] and Saad *et al.* [20]. There are also many different ways to describe the deflation technique. We prefer the following one.

We define the projection P_D by

$$P_D = I - AZ(Z^{\mathrm{T}}AZ)^{-1}Z^{\mathrm{T}}, \quad Z \in \mathbb{R}^{n\times r} \tag{3}$$

where the column space of Z is the deflation subspace, i.e. the space to be projected out of the residual, and I is the identity matrix of appropriate size.

We assume that $r \ll n$ and that Z has rank r. Under this assumption, $E \equiv Z^{\mathrm{T}}AZ$ may be easily computed and factored and is symmetric positive definite. Since $x = (I - P_D^{\mathrm{T}})x + P_D^{\mathrm{T}}x$ and

$$(I - P_D^{\mathrm{T}})x = Z(Z^{\mathrm{T}}AZ)^{-1}Z^{\mathrm{T}}Ax = ZE^{-1}Z^{\mathrm{T}}b \tag{4}$$

can be immediately computed, we need to compute only $P_D^{\mathrm{T}}x$. In light of the identity $AP_D^{\mathrm{T}} = P_D A$, we can solve the deflated system

$$P_D A\tilde{x} = P_D b \tag{5}$$

for $\tilde{x}$ using the CG method, premultiply this by P_D^{T} and add it to (4).

Obviously (5) is singular. However, a positive semidefinite system can be solved by the CG method as long as the right-hand side is consistent (i.e. as long as $b = Ax$ for some x) [21]. This is certainly true for (5), where the same projection is applied to both sides of the nonsingular system.

The deflated system can also be solved by using a symmetric positive definite preconditioner M^{-1}:

$$M^{-1}P_D A\tilde{x} = M^{-1}P_D b \tag{6}$$

3. COMPARISON OF ABSTRACT BALANCING AND THE ABSTRACT COARSE GRID CORRECTION

There are some results known in the literature which compare the balancing preconditioner with the additive coarse grid correction preconditioner. However, it is worth to have a closer look at these comparisons and to derive a comparison of the abstract versions.

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It is suggested in [4, 5] that the balancing preconditioner always yields a better condition number than the additive coarse grid correction preconditioner. In Mandel [4], the original versions of the balancing or hybrid preconditioner and the additive coarse grid preconditioner are compared, i.e. the additive Schwarz preconditioner is used as M^{-1} such that $M^{-1}A$ is a sum of projections. In the comparison of [5], the additive Schwarz preconditioner is also used. Moreover, not the full balancing operator is used as a preconditioner in the CG run. We discuss in detail the result stated in [5] at the end of this section.

However, a comparison of the abstract versions of these preconditioners is not possible. Example 3.1 shows that the additive coarse grid correction preconditioner can lead to a smaller condition number.

Example 3.1
We take the following matrix A:

$$A = \begin{pmatrix} 100 & 0 \\ 0 & 101 \end{pmatrix} \tag{7}$$

Further we choose matrix $M = I$ and matrix Z as

$$Z = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{8}$$

It appears that $Z^{\mathrm{T}}AZ = 100$ and

$$P_D = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad P_B = \begin{pmatrix} 0.01 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } P_{CM} = \begin{pmatrix} 1.01 & 0 \\ 0 & 1 \end{pmatrix} \tag{9}$$

Computing the condition numbers give

$$\kappa(A) = 1.01$$
$$\kappa(P_{CM}A) = 1$$
$$\kappa(P_B A) = 101$$

which clearly shows that $\kappa(P_B A)$ can be larger than $\kappa(P_{CM}A)$.

Of course, the eigenvalue 1 in the spectrum of $P_B A$ is responsible for the large condition number of $P_B A$. Note that the corresponding eigenvalue of $P_D A$ is 0. Example 3.1 shows that Lemma 3.2 in [4] is not valid for the abstract preconditioner. Even if the additive Schwarz preconditioner is used as M^{-1}, this lemma has to be modified [22] by accounting for the possibility of an eigenvalue equal to 1.

Nevertheless, one can prove a comparison if the CG method, preconditioned by the abstract balancing preconditioner, is started with a specific starting vector. The asymptotic convergence behavior of the CG method can then be described by the so-called effective condition number with respect to the starting vector. We will describe this concept in the following.

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In [23–25], the convergence of the CG method is related to the condition number $\kappa(A)$ of A. In [26], these papers are cited to relate the convergence of the CG method to the effective condition number with respect to a specific starting vector; however, as far as we know the theorem is neither explicitly stated nor proved. For this reason we give this theorem here, together with a short proof.

Definition 3.2
Let A be symmetric positive definite and (λ_i, y_i) be the eigenpairs of A, i.e. $Ay_i = \lambda_i y_i$ and $y_i^{\mathrm{T}} y_j = \delta_{ij}$. For $x_0 \in \mathbb{R}^n$ let

$$x - x_0 = \sum_{j=1}^{n} \gamma_j y_j$$

Define

$$\alpha := \min\{\lambda_j | \gamma_j \neq 0\}$$

$$\beta := \max\{\lambda_j | \gamma_j \neq 0\}$$

$$\kappa(A, x - x_0) := \frac{\beta}{\alpha}$$

where $\kappa(A, x - x_0)$ is called the effective condition number of A with respect to x and x_0.

Theorem 3.3
If the CG method is applied to solve $Ax = b$ with starting vector x_0, the ith iterate satisfies

$$\|x - x_i\|_A \leqslant 2 \left\{ \frac{\sqrt{\kappa(A, x - x_0)} - 1}{\sqrt{\kappa(A, x - x_0)} + 1} \right\}^i \|x - x_0\|_A$$

Proof
To prove this result, we define j_α and j_β such that $\alpha = \lambda_{j_\alpha}$ and $\beta = \lambda_{j_\beta}$. For the CG errors, it is well known [27, p. 586] that there exists a polynomial $p_i \in \Pi_i^1$, which is of degree i and $p_i(0) = 1$, such that

$$\|x - x_i\|_A^2 = \sum_{j=1}^{n} \lambda_j (p_i(\lambda_j))^2 \gamma_j^2 \leqslant \sum_{j=1}^{n} \lambda_j (q_i(\lambda_j))^2 \gamma_j^2 = \sum_{j=j_\alpha}^{j_\beta} \lambda_j (q_i(\lambda_j))^2 \gamma_j^2 \tag{10}$$

for all $q_i \in \Pi_i^1$. Take q_i equal to the following shifted and scaled Chebyshev polynomial of degree i:

$$\hat{T}_i(t) = \frac{T_i\left(\dfrac{\beta+\alpha}{\beta-\alpha} - \dfrac{2t}{\beta-\alpha}\right)}{T_i\left(\dfrac{\beta+\alpha}{\beta-\alpha}\right)} \tag{11}$$

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It now follows that

$$\|x-x_i\|_A^2 \leqslant \sum_{j=j_\alpha}^{j_\beta} \lambda_j (\hat{T}_i(\lambda_j))^2 \gamma_j^2 \leqslant 4 \left\{ \frac{\sqrt{\dfrac{\beta}{\alpha}}-1}{\sqrt{\dfrac{\beta}{\alpha}}+1} \right\}^{2i} \sum_{j=j_\alpha}^{j_\beta} \lambda_j \gamma_j^2$$

$$= 4 \left\{ \frac{\sqrt{\kappa(A, x-x_0)}-1}{\sqrt{\kappa(A, x-x_0)}+1} \right\}^{2i} \|x-x_0\|_A^2$$

where we have used that γ_j^2 and λ_j are positive, together with the inequality:

$$|\hat{T}_i(\lambda_j)| \leqslant 2 \left\{ \frac{\sqrt{\dfrac{\beta}{\alpha}}-1}{\sqrt{\dfrac{\beta}{\alpha}}+1} \right\}^{i} \quad \text{for } j_\alpha \leqslant j \leqslant j_\beta$$ □

In the following we wish to apply the above theorem to the preconditioned CG (PCG) method with a symmetric positive definite preconditioner M and a special starting vector x_0. Therefore, we point out that PCG for $Ax=b$ with starting vector x_0 is equivalent to the CG method applied to $M^{1/2}AM^{1/2}\tilde{x}=M^{1/2}b$ and starting vector $\tilde{x}_0=M^{-1/2}x_0$. The CG method will return $\tilde{x}$ that satisfies $\tilde{x}=M^{-1/2}x$ or $M^{1/2}\tilde{x}=x$. Hence, the next corollary follows from Theorem 3.3 immediately.

Corollary 3.4
Let A and M be symmetric positive definite. Let $(\tilde{\lambda}_i, \tilde{y}_i)$ be the eigenpairs of $M^{1/2}AM^{1/2}$. For $x_0 \in \mathbb{R}^n$ let

$$M^{-1/2}x - M^{-1/2}x_0 = \sum_{j=1}^{n} \tilde{\gamma}_j \tilde{y}_j$$

Define

$$\tilde{\alpha} := \min\{\tilde{\lambda}_j \,|\, \tilde{\gamma}_j \neq 0\}$$

$$\tilde{\beta} := \max\{\tilde{\lambda}_j \,|\, \tilde{\gamma}_j \neq 0\}$$

$$\kappa(MA, x-x_0) := \frac{\tilde{\beta}}{\tilde{\alpha}}$$

If the PCG method is applied to solve $Ax=b$ with starting vector x_0 and preconditioner M, the ith iterate satisfies

$$\|x-x_i\|_A \leqslant 2 \left\{ \frac{\sqrt{\kappa(MA, x-x_0)}-1}{\sqrt{\kappa(MA, x-x_0)}+1} \right\}^{i} \|x-x_0\|_A$$

As shown in Example 3.1, for general starting vectors there is no ordering possible between $\kappa(P_B A)$ and $\kappa(P_{CM} A)$. Starting with the starting vector $x_{0,B} = ZE^{-1}Z^{\mathrm{T}}b$, it is possible to compare the effective condition number of $P_B A$ and the condition number of $P_{CM} A$.

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Theorem 3.5
Let A be symmetric positive definite. Let the preconditioners P_B and P_{CM} be defined as in (1) and (2). With $x_{0,B}=ZE^{-1}Z^{\mathrm{T}}b$, we obtain

$$\kappa(P_B A, x-x_{0,B})\leqslant\kappa(P_{CM}A)$$

Proof
First of all, we consider the deflation operator P_D defined in (3) and $M^{-1}P_D A$.

Suppose that the spectrum of $M^{-1}P_D A$ is given by

$$\text{spectrum}(M^{-1}P_D A)=\{0,\ldots,0,\mu_{r+1},\ldots,\mu_n\}$$

with the corresponding eigenvectors $\{z_1,\ldots,z_r\}$ and $\{v_{r+1},\ldots,v_n\}$ satisfying

$$M^{-1}P_D A z_i=0 \quad \text{and} \quad M^{-1}P_D A v_j=\mu_j v_j$$

Note that $\mu_j\neq 0$, for $j=r+1,\ldots,n$, because A and M are non-singular and P_D has rank $n-r$.

From the proof of Theorem 2.8 in [3], we know that

$$P_B A z_i=z_i \quad \text{and} \quad P_B A(P_D^{\mathrm{T}}v_j)=\mu_j P_D^{\mathrm{T}}v_j$$

Now we consider the eigenpairs of $P_B^{1/2}AP_B^{1/2}$. Obviously

$$P_B^{1/2}AP_B^{1/2}(P_B^{-1/2}z_i)=(P_B^{-1/2}z_i)$$

$$P_B^{1/2}AP_B^{1/2}(P_B^{-1/2}P_D^{\mathrm{T}}v_j)=\mu_j(P_B^{-1/2}P_D^{\mathrm{T}}v_j)$$

Moreover, we obtain for $\tilde{r}:=P_B^{1/2}AP_B^{1/2}(P_B^{-1/2}(x-x_{0,B}))$

$$\begin{aligned}\tilde{r}=P_B^{1/2}AP_B^{1/2}(P_B^{-1/2}(x-x_{0,B}))&=P_B^{1/2}b-P_B^{1/2}AP_B^{1/2}P_B^{-1/2}ZE^{-1}Z^{\mathrm{T}}b\\&=P_B^{1/2}b-P_B^{1/2}AZE^{-1}Z^{\mathrm{T}}b\end{aligned}$$

We can decompose $\tilde{r}$ as

$$\tilde{r}=\sum_{i=1}^{r}\gamma_i(P_B^{-1/2}z_i)+\sum_{i=r+1}^{n}\gamma_i(P_B^{-1/2}P_D^{\mathrm{T}}v_i)$$

Next we establish that $\gamma_i=0$ for $i=1,\ldots,r$. Since

$$P_B^{-1/2}z_1,\ldots,P_B^{-1/2}z_r,\quad P_B^{-1/2}P_D^{\mathrm{T}}v_{r+1},\ldots,P_B^{-1/2}P_D^{\mathrm{T}}v_n$$

are the eigenvectors of $P_B^{1/2}AP_B^{1/2}$, which can be chosen as an orthonormal set, it suffices to prove that $(P_B^{-1/2}Z)^{\mathrm{T}}\tilde{r}=0$.

We obtain

$$\begin{aligned}(P_B^{-1/2}Z)^{\mathrm{T}}\tilde{r}&=Z^{\mathrm{T}}P_B^{-1/2}(P_B^{1/2}b-P_B^{1/2}AZE^{-1}Z^{\mathrm{T}}b)\\&=Z^{\mathrm{T}}b-Z^{\mathrm{T}}AZE^{-1}Z^{\mathrm{T}}b\\&=Z^{\mathrm{T}}b-Z^{\mathrm{T}}b\\&=0\end{aligned}$$

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Hence,

$$P_B^{1/2} A P_B^{1/2} (P_B^{-1/2}(x - x_{0,B})) = \tilde{r} = \sum_{i=r+1}^{n} \gamma_i (P_B^{-1/2} P_D^{\mathrm{T}} v_i)$$

Thus,

$$P_B^{-1/2} x - P_B^{-1/2} x_{0,B} = \sum_{i=r+1}^{n} \frac{\gamma_i}{\mu_i} (P_B^{-1/2} P_D^{\mathrm{T}} v_i)$$

With Corollary 3.4, we obtain

$$\kappa(P_B A, x - x_{0,B}) = \kappa(P_D A, x - x_{0,D}) \leqslant \frac{\mu_n}{\mu_{r+1}}$$

Using Theorem 2.11 of [2] together with $\mu_n/\mu_{r+1} = \kappa_{\mathrm{eff}}(M^{-1} P_D A)$, we finally obtain

$$\kappa(P_B A, x - x_{0,B}) \leqslant \frac{\mu_n}{\mu_{r+1}} \leqslant \kappa(P_{CM} A) \qquad \square$$

From Theorem 3.5, we conclude that the abstract balancing preconditioner with starting vector $x_{0,B} = ZE^{-1} Z^{\mathrm{T}} b$ is asymptotically a better preconditioner than the coarse grid correction preconditioner. Hence, we expect a faster convergence of the PCG method if the abstract balancing preconditioner is used.

As shown in Example 3.1, for general starting vectors there is no ordering possible between $\kappa(P_B A)$ and $\kappa(P_{CM} A)$.

In [5, Lemma 2.15] it is proved that

$$\kappa(P_D^{\mathrm{T}} M^{-1} P_D A) \leqslant \kappa(P_{CM} A) \tag{12}$$

However, note that

$$P_B = P_D^{\mathrm{T}} M^{-1} P_D + Z E^{-1} Z^{\mathrm{T}} \tag{13}$$

From (12) it is deduced that the balancing preconditioner with starting vector $x_{0,B} = ZE^{-1} Z^{\mathrm{T}} b$ is asymptotically a better preconditioner than the coarse grid correction preconditioner. However, to derive this statement, some properties of the balancing preconditioner have to be proved in detail earlier, namely, that starting with $x_{0,B} = ZE^{-1} Z^{\mathrm{T}} b$ implies that the balancing approximations stay in the range(P_D), and that starting with $x_{0,B} = ZE^{-1} Z^{\mathrm{T}} b$ implies that the term $ZE^{-1} Z^{\mathrm{T}}$ in (13) can be neglected. Thus, the balancing preconditioner can be implemented only with the use of $P_D^{\mathrm{T}} A P_D$.

Moreover, the systems $P_D^{\mathrm{T}} M^{-1} P_D A$ and $P_D^{\mathrm{T}} M^{-1} A$ are singular and it is not clear at all which condition number describes the convergence behavior of the CG method started with $x_{0,B} = ZE^{-1} Z^{\mathrm{T}} b$. Note that $\kappa(P_B A)$ can be larger than $\kappa(P_{CM} A)$.

The effective condition number with respect to a starting vector, however, gives a complete description of the convergence behavior of the CG method. Thus, Theorem 3.5 provides a complete comparison of the abstract balancing method with the abstract additive coarse grid correction method. Furthermore, the proof is self-contained.

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4. COMPARING THE A-NORM OF THE DEFLATION AND COARSE GRID CORRECTION ERRORS

It appears that the effective condition number of a preconditioned matrix combined with a deflation operator is always less than the condition number of the matrix preconditioned with a coarse grid correction operator [2, Theorem 2.11]. However, instead of comparing condition numbers, it is more valuable to compare the errors of different preconditioners measured in some norm. However, such a kind of comparison results is hard to find. In [3] such a comparison of the norm of the errors is given for the deflation and the balancing preconditioners. Of course, the similar spectrum of both preconditioned systems influenced such a comparison.

Definition 4.1
The eigenvalues of A are denoted by λ_k, and the eigenvectors y_k of A are chosen such that $y_k^{\mathrm{T}} y_j = \delta_{kj}$. Define $Z = [y_1 \dots y_r]$.

In this section we assume that the eigenvalues are arbitrarily ordered.

From [2, Theorem 2.5], we know for this choice of projection vectors that the spectra of $P_D A$ and $P_C A$ are

$$\text{spectrum}(P_D A) = \{0, \dots, 0, \lambda_{r+1}, \dots, \lambda_n\}$$

and

$$\text{spectrum}(P_C A) = \{\sigma + \lambda_1, \dots, \sigma + \lambda_r, \lambda_{r+1}, \dots, \lambda_n\}$$

As in Section 3 of [3] we note that

$$x_{k,D} = x_0 + Z E^{-1} Z^{\mathrm{T}} r_0 + P_D^{\mathrm{T}} \tilde{x}_{k,D} \tag{14}$$

where $\tilde{x}_{k,D}$ is the kth iterate of CG applied to the singular deflated system $P_D A x = P_D r_0$. We take $\tilde{x}_{0,D} = 0$ as the starting solution. The coarse grid correction method is started with $x_{0,C} = x_0$.

Definition 4.2
The initial error vector can be expressed as a linear combination of the eigenvectors:

$$x - x_0 = \sum_{j=1}^{n} \gamma_j y_j$$

We first investigate $x - x_{0,D}$.

Lemma 4.3
Using (14) and Definition 4.2, it appears that

$$x - x_{0,D} = \sum_{j=r+1}^{n} \gamma_j y_j \tag{15}$$

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Proof
It is easy to show that $E=Z^{\mathrm{T}}AZ=\mathrm{diag}(\lambda_1,\ldots,\lambda_r)$. This together with (14) is used to derive the following expressions:

$$
\begin{aligned}
x-x_{0,D} &= x-x_0-ZE^{-1}Z^{\mathrm{T}}(b-Ax_0)\\
&= x-x_0-[y_1\ldots y_r]\mathrm{diag}\left(\frac{1}{\lambda_1},\ldots,\frac{1}{\lambda_r}\right)[y_1\ldots y_r]^{\mathrm{T}}\sum_{j=1}^{n}\gamma_j\lambda_j y_j\\
&= \sum_{j=1}^{n}\gamma_j y_j-\sum_{j=1}^{r}\gamma_j y_j=\sum_{j=r+1}^{n}\gamma_j y_j
\end{aligned}
$$

Now we are able to prove the following comparison result. □

Theorem 4.4
Using Z as in Definition 4.1, $\tilde{x}_{0,D}=0$ and $x_{0,C}=x_0$, it appears that

$$\|x-x_{k,D}\|_A\leqslant\|x-x_{k,C}\|_A \tag{16}$$

Proof
The exact solution x can be expressed as

$$x=x_0+(I-P_D^{\mathrm{T}})(x-x_0)+P_D^{\mathrm{T}}(x-x_0)=x_0+ZE^{-1}Z^{\mathrm{T}}r_0+P_D^{\mathrm{T}}(x-x_0)$$

Combination with (14) shows that

$$x-x_{k,D}=P_D^{\mathrm{T}}(x-x_0-\tilde{x}_{k,D}) \tag{17}$$

Note that

$$\tilde{x}_{k,D}=s_k(P_DA)P_Dr_0=s_k(P_DA)P_DA(x-x_0)$$

where s_k is a polynomial of degree $k-1$. Substituting this into (17) yields

$$P_D^{\mathrm{T}}(x-x_0-\tilde{x}_{k,D})=P_D^{\mathrm{T}}p_{k,D}(P_DA)(x-x_0)\quad\text{with } p_{k,D}\in\Pi_k^1 \tag{18}$$

Since Z consists of eigenvectors, we know that $P_D=I-ZZ^{\mathrm{T}}=P_D^{\mathrm{T}}$. Together with $P_DA=AP_D$ this implies that

$$P_D^{\mathrm{T}}p_{k,D}(P_DA)=p_{k,D}(P_DA)P_D$$

With Definition 4.2 and (18), we obtain

$$
\begin{aligned}
P_D^{\mathrm{T}}(x-x_0-\tilde{x}_{k,D}) &= p_{k,D}(P_DA)P_D(x-x_0)=p_{k,D}(P_DA)(I-ZZ^{\mathrm{T}})\sum_{j=1}^{n}\gamma_j y_j\\
&= p_{k,D}(P_DA)\sum_{j=r+1}^{n}\gamma_j y_j=\sum_{j=r+1}^{n}p_{k,D}(\lambda_j)\gamma_j y_j
\end{aligned}
$$

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Using the optimality property of the CG method, we observe that

$$\|x-x_{k,D}\|_A^2 = \left\| \sum_{j=r+1}^{n} p_{k,D}(\lambda_j)\gamma_j y_j \right\|_A^2 = \sum_{j=r+1}^{n} \lambda_j (p_{k,D}(\lambda_j))^2 \gamma_j^2$$
$$\leqslant \sum_{j=r+1}^{n} \lambda_j (q_k(\lambda_j))^2 \gamma_j^2 \tag{19}$$

where q_k is an arbitrary polynomial in the set Π_k^1. Using the polynomial property of the CG method again, we note that there is a $p_{k,C} \in \Pi_k^1$ such that

$$\|x-x_{k,C}\|_A^2 = \sum_{j=1}^{r} \lambda_j (p_{k,C}(\sigma+\lambda_j))^2 \gamma_j^2 + \sum_{j=r+1}^{n} \lambda_j (p_{k,C}(\lambda_j))^2 \gamma_j^2 \tag{20}$$

Combination of (19) and (20) leads to

$$\|x-x_{k,D}\|_A^2 \leqslant \sum_{j=r+1}^{n} \lambda_j (p_{k,C}(\lambda_j))^2 \gamma_j^2$$
$$\leqslant \sum_{j=1}^{r} \lambda_j (p_{k,C}(\sigma+\lambda_j))^2 \gamma_j^2 + \sum_{j=r+1}^{n} \lambda_j (p_{k,C}(\lambda_j))^2 \gamma_j^2$$
$$= \|x-x_{k,C}\|_A^2$$

which proves the theorem. □

The A-norm inequality as given in Theorem 4.4 is not valid if the projection vectors are general vectors. This is illustrated by the example given below.

Example 4.5
Applying deflation and coarse grid correction to problem with

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}, \quad b = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad \text{with } Z = \begin{pmatrix} 1 \\ -10 \\ 0 \end{pmatrix} \text{ and } x_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \tag{21}$$

one obtains the results as given in Table I. Note that the A-norm of the deflation error is larger than the A-norm of the coarse grid correction error in the first iterate.

Table I. The error for deflation and coarse grid correction.

Iteration	$\|x-x_{k,D}\|_A$	$\|x-x_{k,C}\|_A$
0	2.4495	2.4495
1	0.7138	0.6899
2	0	0.0018

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Table II. The error for deflation, coarse grid correction and balancing.

Iteration	$\|x-x_{k,D}\|_A$	$\|x-x_{k,C}\|_A$	$\|x-x_{k,B}\|_A$
0	2.4495	2.4495	2.4495
1	0.414	0.4804	0.7454
2	0	0	0.2689

We end and conclude this section with some remarks concerning error norm comparisons.

Remark 4.6

- It is possible to prove an equivalent comparison result as in Theorem 4.4 if an additional symmetric positive definite preconditioner M is used.
- Using Theorem 3.7 of [3], it appears that for the balancing iterate $x_{k,B}$ the inequality

$$\|x-x_{k,B}\|_A \leqslant \|x-x_{k,C}\|_A$$

  also holds if the CG method is started with $x_{0,B}=ZE^{-1}Z^{\mathrm{T}}r_0$ and Z is chosen as in Definition 4.1.
- If $x_{0,B}\neq ZE^{-1}Z^{\mathrm{T}}r_0$, but Z is chosen as in Definition 4.1, the inequality is not valid. To show this we again use Example 4.5, but now the projection vector is chosen to be equal to the first eigenvector; hence,

$$Z=\begin{pmatrix}1\\0\\0\end{pmatrix}$$

  The results are given in Table II. Note that the A-norm of the balancing error is larger than the A-norm of the coarse grid correction error in the first iterate.
- Repeating Theorem 3.4 of [3], we know that

$$\|x-x_{k,D}\|_A \leqslant \|x-x_{k,B}\|_A$$

  for all choices of Z and x_0.

5. ORTHOGONAL TRANSFORMATIONS

It is well known that Krylov subspace methods are invariant to orthogonal transformations. Suppose that Q is an orthogonal matrix ($Q^{\mathrm{T}}Q=QQ^{\mathrm{T}}=I$). Consider a change of basis from $e_1,\dots e_n$ to $q_1,\dots q_n$, the columns of Q. The linear system $Ax=b$ in the Euclidean basis is equivalent to the transformed system

$$\hat{A}\hat{x}=\hat{b} \tag{22}$$

in the new basis, where $\hat{x}=Q^{\mathrm{T}}x$, $\hat{b}=Q^{\mathrm{T}}b$ and $\hat{A}=Q^{\mathrm{T}}AQ$. The fact that the CG method applied to $Ax=b$ is equivalent to the CG method applied to $\hat{A}\hat{x}=\hat{b}$ can be proved by expressing the formulas

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of the CG method algorithm or by analyzing the optimization properties of the CG method. Note that if the columns of Q are equal to the normalized and orthogonal eigenvectors of A, the transformed matrix $\hat{A}$ is a diagonal matrix. This implies that theorems proved for a diagonal matrix can be generalized to the same results for an arbitrary symmetric matrix, and numerical experiments can also be restricted to diagonal matrices (except the rounding error behavior, which can be different).

In this section we show that the deflation, coarse grid correction and balancing Neumann–Neumann operators are all invariant with respect to orthogonal coordinate transformations.

Theorem 5.1
It appears that

$$\hat{P}_D = Q^{\mathrm{T}} P_D Q \tag{23}$$

$$\hat{P}_{CM} = Q^{\mathrm{T}} P_{CM} Q \text{ provided that } \hat{\sigma} = \sigma \tag{24}$$

$$\hat{P}_B = Q^{\mathrm{T}} P_B Q \tag{25}$$

Proof
We start to prove (23). Since we have a change of basis, the projection vectors are changed as follows: $\hat{Z} = Q^{\mathrm{T}} Z$. From the definition of $\hat{P}_D$ it follows that

$$\begin{aligned}\hat{P}_D &= I - \hat{A}\hat{Z}(\hat{Z}^{\mathrm{T}}\hat{A}\hat{Z})^{-1}\hat{Z}^{\mathrm{T}}\\ &= I - Q^{\mathrm{T}}AQQ^{\mathrm{T}}Z(Z^{\mathrm{T}}QQ^{\mathrm{T}}AQQ^{\mathrm{T}}Z)^{-1}Z^{\mathrm{T}}Q\\ &= Q^{\mathrm{T}}(I - AZ(Z^{\mathrm{T}}AZ)^{-1}Z^{\mathrm{T}})Q = Q^{\mathrm{T}}P_D Q\end{aligned}$$

In the same way, we can prove (24) where we use $\hat{\sigma} = \sigma$:

$$\begin{aligned}\hat{P}_{CM} &= \hat{M}^{-1} + \hat{\sigma}\hat{Z}(\hat{Z}^{\mathrm{T}}\hat{A}\hat{Z})^{-1}\hat{Z}^{\mathrm{T}}\\ &= Q^{\mathrm{T}}M^{-1}Q + \sigma Q^{\mathrm{T}}Z(Z^{\mathrm{T}}AZ)^{-1}Z^{\mathrm{T}}Q\\ &= Q^{\mathrm{T}}(M^{-1} + \sigma Z(Z^{\mathrm{T}}AZ)^{-1}Z^{\mathrm{T}})Q = Q^{\mathrm{T}}P_{CM}Q\end{aligned}$$

Finally to prove (25), we note that

$$\begin{aligned}\hat{P}_B &= \hat{P}_D^{\mathrm{T}}\hat{M}^{-1}\hat{P}_D + \hat{Z}(\hat{Z}^{\mathrm{T}}\hat{A}\hat{Z})^{-1}\hat{Z}^{\mathrm{T}}\\ &= Q^{\mathrm{T}}P_D^{\mathrm{T}}QQ^{\mathrm{T}}M^{-1}QQ^{\mathrm{T}}P_DQ + Q^{\mathrm{T}}Z(Z^{\mathrm{T}}AZ)^{-1}Z^{\mathrm{T}}Q\\ &= Q^{\mathrm{T}}(P_D^{\mathrm{T}}M^{-1}P_D + Z(Z^{\mathrm{T}}AZ)^{-1}Z^{\mathrm{T}})Q = Q^{\mathrm{T}}P_BQ\end{aligned}$$ □

This theorem implies that if one is able to compare the various methods for a diagonal matrix, the comparison is also valid for a general symmetric matrix.

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6. NUMERICAL EXPERIMENTS

In all our numerical experiments, the multiplication $y = E^{-1}b$ is done by solving y from $Ey = b$, where E is decomposed into a product of its Cholesky factors. The choice of the boundary conditions is such that all problems have the vector with components equal to 1 as the exact solution. To make the convergence behavior representative for general problems, we chose a random vector as starting solution, instead of the zero start vector.

We apply both methods (balancing and additive coarse grid correction) to the Poisson equation. To investigate the scaling properties of the methods, we use the scaled linear system:

$$\gamma Ax = \gamma b$$

In all our examples, the balancing preconditioner performs better than the additive coarse grid preconditioner as indicated by the theoretical results if $x_0 = ZE^{-1}Z^{\mathrm{T}}r_0$. We observe from Figures 1 and 2 that both methods are not scaling invariant. In exact arithmetic, the balancing preconditioner with $x_0 = ZE^{-1}Z^{\mathrm{T}}r_0$ is scaling invariant. This implies that the rounding errors spoil the invariance properties in practice. It is clear that the additive coarse grid preconditioner is more sensitive to scaling. This can be explained as follows: for the balancing preconditioner r eigenvalues of the original matrix are changed into 1 by the preconditioner. Hence, if the scaling is bad, there is only one outlier in the spectrum. Owing to the superlinear convergence, this has only a limited effect on the convergence. Using the additive coarse grid preconditioner r eigenvalues are shifted. For a bad scaling, the spectrum has r outliers, which are worse than one outlier for the convergence of the method.

Finally, from Figure 3, we conclude that in general the balancing preconditioner converges faster than the additive coarse grid preconditioner, also for arbitrary starting vectors. However, the A-norm inequality is not always valid. Initially, the additive coarse grid preconditioner converges faster than the balancing preconditioner.

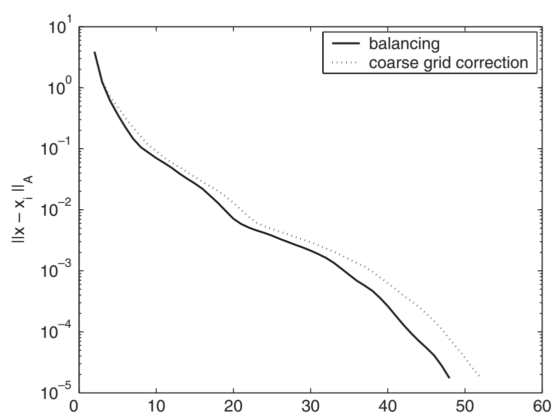

Figure 1. Convergence of the balancing and additive coarse grid correction preconditioners with $\gamma = 1$ and $x_0 = ZE^{-1}Z^{\mathrm{T}}r_0$.

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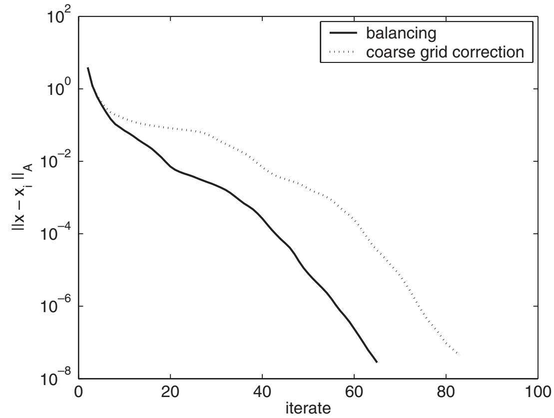

Figure 2. Convergence of the balancing and additive coarse grid correction preconditioners with $\gamma = 500$ and $x_0 = ZE^{-1}Z^{\mathrm{T}}r_0$.

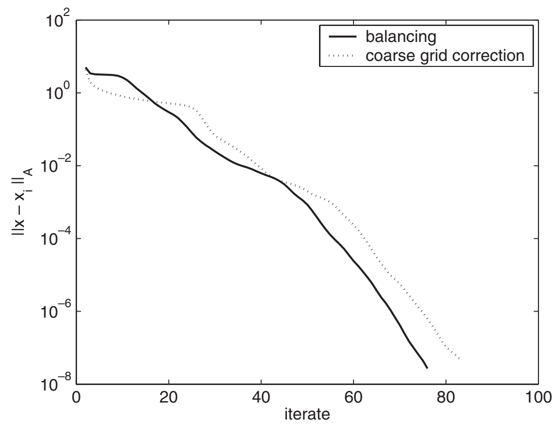

Figure 3. Convergence of the balancing and additive coarse grid correction preconditioners with $\gamma = 500$. In this example a random starting vector is used.

7. CONCLUSIONS

We considered various preconditioners for the CG method, namely the deflation, the abstract balancing and the abstract additive coarse grid correction preconditioners. In [2, 3] the deflation method is compared with the abstract additive coarse grid correction preconditioner and the abstract balancing preconditioner. Here we established a direct comparison between the condition numbers of the abstract coarse grid correction preconditioner and the abstract balancing preconditioner. We showed that the effective condition number with respect to a specific starting vector of the system preconditioned by the abstract balancing preconditioner is less than or equal to the condition number of the system preconditioned by the additive coarse grid correction method.

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Moreover, we compared the A-norm of the errors of the iterates given by the different preconditioners and established the orthogonal invariance of all three types of preconditioners.

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