CONVERGENCE BOUNDS FOR PRECONDITIONED GMRES USING ELEMENT-BY-ELEMENT ESTIMATES OF THE FIELD OF VALUES

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Abstract. By combining element-by-element estimates for the field of values of a preconditioned matrix with GMRES-convergence estimates it is possible to derive an easily computable upper bound on the GMRES-residual norm. This method can be applied to general finite element systems, but the preconditioner has to be Hermitian and positive definite. The resulting upper bound for the GMRES-residual norm can be used to analyse a given preconditioner, or to optimize a parameter dependent preconditioner. In this paper we will apply this approach to derive a suitable shift for a so-called shifted Laplace preconditioner for the damped Helmholtz equation. Numerical experiments show that the shift that is derived in this way is close to optimal.

1 Introduction

Preconditioned GMRES1 is among the most popular methods for solving nonsymmetric linear systems of equations. To analyse the convergence of GMRES several upper bounds on the residual norm have been proposed. A class of such bounds is based on the field of values of the (preconditioned) matrix2,3,4,5,6. These bounds are quite useful in the analysis of preconditioners, for example to establish mesh-independence or to determine an optimal value for a tuning parameter.

To apply these bounds knowledge of the field of values is necessary. In a recent paper by Loghin et al.7 bounds on the field of values of a preconditioned global Finite Element matrix are derived based on the fields of values of the element matrices. These bounds are easy to compute and are applicable to general matrices that are preconditioned with a Hermitian positive definite preconditioning matrix.

The GMRES-convergence estimates and bounds for the field of values can be combined to analyse and improve the performance of a preconditioner. To illustrate this we will discuss two problems. For the damped Helmholtz equation that is preconditioned with a shifted Laplacian8 we will show how a quasi optimal (real) shift
can be determined. We will also show that for a wide class of convection-diffusion-reaction problems the number of iterations is mesh-independent if the matrix is preconditioned with the symmetric part of the operator.

2 An elementwise computable upper bound on the GMRES-residual norm

2.1 GMRES

GMRES is an iterative method for solving nonsymmetric linear systems of equations

\[ Ax = b. \tag{1} \]

Given an initial guess \( x_0 \) the method computes an approximate solution \( x_{m-1} \) in the Krylov-subspace \( K_m(A, r_0) \), which is defined by

\[ K_m(A, r_0) = \text{span}\{r_0, Ar_0, A^2r_0, \ldots, A^{m-1}r_0\}, \tag{2} \]

such that the norm of the residual \( r_{m-1} = b - Ax_{m-1} \) is minimized. To compute this optimal approximation \( x_{m-1} \) a set of \( m - 1 \) orthogonal basis vectors has to be computed and stored and this set has to be expanded with one new basis vector in every iteration. In practice the computation and storage of a new basis vector may become prohibitively expensive if \( m \) becomes large. The usual way to overcome this problem is to restart GMRES if \( m \) exceeds a threshold. The price that one has to pay for restarting is that GMRES looses its optimality property, and convergence may slow down considerably.

2.2 Field of values

In order to predict and analyse the convergence of GMRES a number of upper bounds on the GMRES-residual norm has been proposed that make use of the field of values of the system matrix \( A \). The field of values of a matrix \( A \) is defined by

\[ \text{FOV}(A) = \left\{ \frac{x^H A x}{x^H x}, x \in \mathbb{C}^n, x \neq 0 \right\}. \tag{3} \]

Let \( \Re(A) \) and \( \Im(A) \) be defined as

\[ \Re(A) = \frac{1}{2}(A + A^H) \quad \text{and} \quad \Im(A) = \frac{1}{2i}(A - A^H). \tag{4} \]

We then have for the field of values of \( A \)

\[ \text{FOV}(A) = \text{FOV}(\Re(A) + i\Im(A)). \tag{5} \]

Since the field of values of a Hermitian matrix is real we have the following projection property\(^9\) for the real and imaginary parts of the field of values of a non-Hermitian matrix

\[ \Re(\text{FOV}(A)) = \text{FOV}(\Re(A)) \quad \text{and} \quad \Im(\text{FOV}(A)) = \text{FOV}(\Im(A)). \tag{6} \]

Hence, bounds on \( \text{FOV}(\Re(A)) \) and on \( \text{FOV}(\Im(A)) \) amount to a bounding box in the complex plane for \( \text{FOV}(A) \).
2.3 Bounds on the GMRES-residual norm based on the field of values.

The classical bound that uses $\text{FOV}(A)$ was proposed by Elman\(^2\). This bound can be summarised as follows. If $A$ is real and $\Re(A)$ positive definite the GMRES-residual norm after $k$ iterations satisfies
\[
\frac{\|r^k\|}{\|r^0\|} \leq (1 - \frac{\lambda_{\min}^{\Re(A)^2}}{\|A\|^2})^{k/2}.
\] (7)

This bound has been generalised for complex matrices by Eiermann and Ernst\(^5\).

A second bound is given in the book of Greenbaum\(^3\), page 56. This bound states that if $\text{FOV}(A)$ is contained in a disk $D = \{z \in \mathbb{C} : |z-c| \leq s\}$ which does not contain the origin, then the GMRES-residual norm after $k$ iterations satisfies
\[
\frac{\|r^k\|}{\|r^0\|} \leq 2 \left( \frac{s}{|c|} \right)^k.
\] (8)

The third bound we mention can be found in the book of Elman, Silvester and Wathen\(^4\), page 171, and also in a paper of Joubert\(^6\). Let $\Re(A)$ be positive definite. Then the GMRES-residual norm after $k$ iterations satisfies
\[
\frac{\|r^k\|}{\|r^0\|} \leq (1 - \frac{\lambda_{\min}^{\Re(A)^2}}{\lambda_{\min}^{\Re(A)} \lambda_{\max}^{\Re(A)} + \lambda_{\max}^{\Im(A)^2}})^{k/2}.
\] (9)

All three upper bounds are also valid for restarted GMRES, including GMRES(1). Consequently, the upper bounds can be quite pessimistic, in particular for unrestarted GMRES. Nevertheless, the bounds are quite useful for the performance prediction of GMRES, in particular to analyse how the rate of convergence is influenced if GMRES is applied with a preconditioner.

2.4 Generalisation of the GMRES-convergence bounds for preconditioned systems.

In practice, GMRES is always applied with a suitably chosen preconditioner to speed-up the rate of convergence. Preconditioning means that GMRES is applied to one of the following equivalent systems
\[
P^{-1}Ax = P^{-1}b \quad \text{left preconditioning},
\] (10)
\[
AP^{-1}y = b, \; x = P^{-1}y \quad \text{right preconditioning},
\] (11)
\[
L^{-1}AU^{-1}y = L^{-1}b, \; x = U^{-1}y \; P = LU \quad \text{symmetric preconditioning}.
\] (12)

The preconditioner $P$ is chosen such that $P \approx A$ and operations with the inverse of $P$ are relatively easy to perform.

The bounds on the GMRES-residual norm can in principle still be applied, with the system matrix $A$ being replaced by the preconditioned matrix $P^{-1}A$, $AP^{-1}$, or $L^{-1}AU^{-1}$. In practice, however, it can be difficult to split the preconditioned matrix into its real and imaginary part if both $P$ and $A$ are non-Hermitian. If that is the case the projection property (6) can not be used to derive bounds on the field of values. However, if the preconditioner is Hermitian positive definite,
the field of values of the symmetrically preconditioned matrix can still be bounded using a projection property. If $P$ is Hermitian positive definite it can be written as $P = CC^H$, and symmetric preconditioning gives $C^{-1}AC^{-H}$ as system matrix. For the field of values we get

$$FOV(C^{-1}AC^{-H}) = \left\{ \frac{x^H C^{-1}AC^{-H} x}{x^H x}, x \in \mathbb{C}^n, x \neq 0 \right\} = \left\{ \frac{y^H Ay}{y^H Py}, y \in \mathbb{C}^n, y \neq 0 \right\}. \tag{13}$$

If we define the field of values of the matrix pair $(A, B)$ as

$$FOV(A, P) = \left\{ \frac{x^H Ax}{x^H Px}, x \in \mathbb{C}^n, x \neq 0 \right\}, \tag{14}$$

we get the following projection property:

$$\Re(FOV(A, P)) = FOV(\Re(A), P) \quad \text{and} \quad \Im(FOV(A, P)) = FOV(\Im(A), P). \tag{15}$$

### 2.5 Element-by-element bounds on the field of values of the preconditioned matrix.

Loghin et al.\(^7\) have formulated element-by-element bounds on the field of value $FOV(A, P)$ and on the numerical radius $r(A, P)$ of the matrix pair $(A, P)$. These bounds are based on the fields of values of the element matrices and hence are easy to compute. They are derived by using the projection property (15), and by applying the element-by-element bounds of Fried\(^10\) to $\Re(A)$ and $\Im(A)$. The bounds are valid for $A$ general, and $P$ Hermitian positive definite.

The element-by-element bound on the field of values $FOV(A, P)$ is summarised as follows. Let $A^e, e = 1, \cdots, n_e$ be (possibly non-Hermitian) element matrices and $P^e, e = 1, \cdots, n_e$ be Hermitian positive definite element matrices and let $A$ and $P$ be the global matrices that are assembled from these element matrices. Then the following bounds hold for $z \in FOV(A, P)$:

$$\min_e \lambda_{\min}^{\Re(A^e), P^e} \leq \Re(z) \leq \max_e \lambda_{\max}^{\Re(A^e), P^e}$$

$$\min_e \lambda_{\min}^{\Im(A^e), P^e} \leq \Im(z) \leq \max_e \lambda_{\max}^{\Im(A^e), P^e}. \tag{16}$$

Here $\Re(A^e) = \frac{1}{2}(A^e + A^e H)$ and $\Im(A^e) = \frac{1}{2i}(A^e - A^e H)$. $\lambda^{\Re(A^e), P^e}$ and $\lambda^{\Im(A^e), P^e}$ are eigenvalues of the generalised element eigenproblems $\Re(A^e)x^e = \lambda^{\Re(A^e), P^e} P^e x^e$, and $\Im(A^e)x^e = \lambda^{\Im(A^e), P^e} P^e x^e$, respectively.

The numerical radius $r(A, P)$ can be bounded from above as follows. Let $A^e, e = 1, \cdots, n_e$ be (possibly non-Hermitian) element matrices and $P^e, e = 1, \cdots, n_e$ be Hermitian positive definite element matrices and let $A$ and $P$ be the global matrices that are assembled from these element matrices. Let $\nu$ be defined by

$$\nu = \max \left\{ |z| : z \in \bigcup_{e=1}^{n_e} FOV(A^e, P^e) \right\}, \tag{18}$$

then

$$r(A, P) \leq \nu. \tag{19}$$
By making use of the well known inequality

\[ r(A) \leq \| A \| \leq 2r(A) \]  \hspace{1cm} (20)

an element-by-element estimate for the norm of the preconditioned matrix \( \| C^{-1}AC^{-H} \| \) is given by

\[ \| C^{-1}AC^{-H} \| \leq 2 \nu . \]  \hspace{1cm} (21)

### 3 Numerical examples

In this section we will combine the element-by-element bounds on the field of values with the field-of-values bounds on the GMRES residual norm in order to analyse and improve a preconditioner.

#### 3.1 Damped Helmholtz equation

As a first example we consider the damped Helmholtz equation

\[ -\Delta u - (k^2 - i\gamma k)u = f . \]

on the unit square with Neumann boundary conditions. In this equation, \( \gamma \) represents the damping parameter and \( k \) the wave number. Discretisation on a uniform mesh with mesh-size \( h \), using linear triangular elements yields element matrices \( A^e \) of the form

\[ A^e = L^e - (k^2 - i\gamma k)M^e \]  \hspace{1cm} (22)

with

\[ L^e = \frac{1}{2} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \quad M^e = \frac{h^2}{6} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \]  \hspace{1cm} (23)

As a preconditioner we take the discretisation of a shifted Laplace operator

\[ -\Delta + s^2, \]  \hspace{1cm}

in which \( s^2 \) is a positive shift. The element preconditioning matrices are then given by

\[ P^e = L^e + s^2M^e . \]  \hspace{1cm} (24)

The question is how to chose \( s \) for optimal performance.

To answer this question we will make use of the bound (9). We first compute a box in the complex plane that encloses \( FOV(A, P) \) using the element-by-element estimates described in the previous section. To this end we have to solve the following two element-eigenvalue problems:

\[ (L^e - k^2M^e)x^e = \lambda^{R(A^e), P^e}(L^e + s^2M^e)x^e , \]  \hspace{1cm} (25)

and

\[ \gamma kM^e x^e = \lambda^{\Im(A^e), P^e}(L^e + s^2M^e)x^e . \]  \hspace{1cm} (26)

Equation (25) gives that

\[ \lambda^{\Re(A^e), P^e}_{\text{max}} = \frac{9}{4\pi^2} - \frac{k^2}{s^2}, \quad \lambda^{\Re(A^e), P^e}_{\text{min}} = -\frac{k^2}{s^2}. \]  \hspace{1cm} (27)
and equation (26) gives
\[
\lambda_{\text{max}}^{3(A^e),P^e} = \frac{k\gamma}{s^2} \quad \lambda_{\text{min}}^{3(A^e),P^e} = \frac{k\gamma}{\gamma^2 + s^2}
\] (28)

Figure 1, left picture, gives an example of a bounding box and spectrum of a pre-conditioned system matrix. As is obvious form this picture, \( \Re(A) \) is not positive definite. In order to overcome this problem we can multiply the system with a complex number \( z = e^{i\phi} \), which rotates the spectrum but does not change the norm of the residual. Since for this problem the spectrum is on a straight line, it is even possible to align the spectrum with the imaginary axis. It is easy to check that the complex number that has to be used to achieve this is
\[
z = e^{i\phi} \quad \phi = \arctan \left( \frac{\lambda_{\text{max}}^{3(A^e),P^e} - \lambda_{\text{min}}^{3(A^e),P^e}}{\lambda_{\text{max}}^{3(A^e),P^e} - \lambda_{\text{min}}} \right)
\] (29)

The result is shown in figure 1, right picture.

We test our procedure with an example with meshsize \( h = 0.05 \), which yields 20 x 20 x 2 linear triangular elements, with wavenumber \( k = 10 \), and for three different values of the damping parameter \( \gamma: 5, 10 \) and 20. We compute for values of \( s \) ranging from 1 to 25 (with stepsize 0.1) an upper bound on the number of GMRES-iterations by combining (9) with the element-by-element estimates for the rotated field of values. The result is plotted in figure 2, right picture. We also determine the actual number of GMRES-iterations needed to solving the systems with GMRES(1) for shifts \( s \) ranging again from 1 to 25, with stepsize 1. The results of this are plotted in figure 2, left picture. As can be seen, there is a good qualitative correspondence between the upper bounds and the actual number of iterations. More importantly, the optimal value for \( s \) is accurately predicted. To underline this we have tabulated in Table 1 the experimentally determined optimal value for \( s \) with the corresponding number of iterations, and the predicted optimal value for \( s \) with the corresponding upper bound on the number of iterations.
The above example is quite structured. It contains only one type of element. However, the same procedure can be followed for more general problems. The steps that have to be made are:

- Make a bounding box around the field of values using the element-by-element bounds.
- Multiply the matrix with a complex number $z = e^{i\phi}$ to make $\Re(A)$ positive definite. Note that it is always possible to find such a number as long as 0 is not included in the bounding box around the field of values.
- Apply the element-by-element bounds to the rotated matrix and combine the bounds on the field of values of the rotated matrix with (9) or one of the other bounds on the GMRES-residual norm.

The procedure can be repeated for different values of $s$ and the one yielding the most favorable upperbound can be selected for solving the actual Helmholtz problem. Note that the above procedure can also be applied on irregular meshes, and for problems with a non-constant wavenumber $k$.

### 3.2 Convection-diffusion-reaction equation

This example is discussed in detail in Loghin et al.\textsuperscript{7}. Here we give a short summary of the results.

Consider the following family of convection-diffusion-reaction equations

$$-\varepsilon \Delta u + \mu u + \beta_x \frac{\partial u}{\partial x} + \beta_y \frac{\partial u}{\partial y} = f.$$  

(30)
with homogeneous Neumann boundary conditions. We assume that the parameters \( \epsilon \) (diffusion), \( \mu \) (reaction), and \( \beta_x \) and \( \beta_y \) (convection) are constant, and that \( \epsilon > 0 \) and \( \mu \geq 0 \). Discretisation of equation (30) using linear triangular elements on a uniform mesh with mesh-size \( h \) yields a global matrix \( A \). As a preconditioner we take the matrix \( P \) that corresponds to the symmetric part of the partial differential operator, i.e., to \(-\epsilon \Delta + \mu \).

To derive an upper bound on the number of GMRES iterations we use (8). Since \( FOV(A, P) = 1 - FOV(A - P, P) \), \( FOV(A, P) \) is enclosed by a circle centered at 1 and with radius \( r(A - P, P) \). An upper bound for \( r(A, P) \) can be derived using (19). It can be shown that the numerical radius of the element matrices is given by

\[
\nu = r(A^e - P^e, P^e) = \frac{1}{2} \sqrt{\frac{(\beta_x - \beta_y)^2}{2\epsilon \mu + \frac{2}{3}h^2 \mu^2} + \frac{(\beta_x + \beta_y)^2}{2\epsilon \mu + \frac{2}{9}h^2 \mu^2}}.
\]

Since \( \lim_{h \to 0} \gamma = \frac{\|b\|}{2\sqrt{\epsilon \mu}} \) we have derived an upper bound on the GMRES-residual norm that is independent of the mesh-size \( h \). This is also confirmed by extensive numerical experiments.

4 Concluding remarks

We have discussed two examples for which the combination of element-by-element bounds on the field of values and bounds on the GMRES-residual norm provides a useful approach to analyse a given preconditioner. This approach works well for problems where the preconditioner is Hermitian positive definite and where the fields of values of the element matrices do not include the origin. Further research aims to generalise our approach to problems with singular element preconditioning matrices following the approach of Haase et al.\(^{11}\).

REFERENCES


