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INEXACT MATRIX-VECTOR PRODUCTS IN KRYLOV METHODS FOR SOLVING LINEAR SYSTEMS: A RELAXATION STRATEGY*

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Abstract. Embedded iterative linear solvers are being used more and more often in linear algebra. An important issue is how to tune the level of accuracy of the inner solver to guarantee the convergence of the outer solver at the best global cost. As a first step towards the challenging goal of controlling embedded linear solvers, inexact Krylov methods are used as a model of inner-outer iterations with external Krylov scheme. This paper experimentally shows that Krylov methods for solving linear systems can still perform very well in the presence of carefully monitored inexact matrix-vector products. This surprising behavior of inexact Krylov methods, as opposed to Newton-like methods, is investigated in detail, and potentially important applications are mentioned. A new relaxation strategy for the inner accuracy is proposed for Krylov methods with inexact matrix-vector products; its efficiency is supported by a wide range of numerical experiments on different algorithms and contrasted against other potential approaches.

Key words. inner-outer iterations, Krylov method, inexact matrix-vector products, embedded iterative linear solvers.

AMS subject classifications. 65F10, 65F15, 15A06, 15A18

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1. About inner-outer iterations in linear algebra.

Iterative processes are widely used in linear algebra for treating large sets of data. It is becoming more and more common that one iterative solver has to be embedded in an outer one: this is the case, for instance, for solving eigenproblems with inverse iterations or with a Krylov method with invert. Each outer step (that is, each step of the eigensolver) requires the solution of a linear system which, if too large, must be solved in turn with an iterative method (inner steps). The question arises then: *What is the best strategy for stopping the inner iterations in order to ensure the convergence of the outer iterations while minimizing the global computational cost?* This question has been partially addressed by numerical experts since the eighties in the context of Newton-like and, more generally, fixed point methods [5, 7, 11]. It is generally concluded, as one could expect, that the accuracy of the inner iteration is a threshold for the convergence of the outer process: it cannot be weakened when the outer process comes closer to the solution. The proposed strategies for monitoring the inner iterations have so far been very problem- and method-dependent. More recently in the late nineties, the different behavior of embedded solvers involving a Krylov outer process has been emphasized [8, 12, 13, 19]. For instance, the strikingly different behaviors of inverse iterations and Krylov methods for the solution of eigenproblems with respect to inner iterations are mentioned in [13] for symmetric and in [3] for nonsymmetric matrices. It is observed, as for Newton-like methods, that inverse iterations require inner iterations

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to be more and more accurate while approaching the solution. But for Lanczos or Arnoldi methods, on the contrary, the first Krylov vectors need to be known with full accuracy, and this accuracy can be *relaxed* as the convergence proceeds. A strategy for monitoring the accuracy of inner iterations is proposed in the framework of symmetric eigenvalue problems with homogeneous linear constraints in [13].

In order to examine closely the seemingly counterintuitive behavior of inner-outer Krylov methods, we investigate in this paper the behavior of Krylov methods when information on the matrix may be partially unavailable, resulting in the use of inexact basis vectors. In order to focus on the root phenomenon, we set up this study in the context of linear systems (see [3] for a similar work on eigenproblems). We will show that, when the inaccuracy of the basis vectors is controlled by a carefully designed relaxation strategy, the Krylov method for solving linear systems can still perform with a remarkable efficiency. It is beyond the scope of this paper to provide a detailed comparison of the many possible relaxation strategies, although we will contrast a few of them in order to expose the reasons that motivated our choices. The inexact Krylov scheme serves here as a simple model for understanding more complex embedded iterative schemes where the outer iteration would be a Krylov method.

1.1. Some important applications. Understanding the effects of inexact matrix-vector products can have many applications. As such, inexact matrix-vector products are encountered in multipole methods, which have recently become popular in the numerical solution of large electromagnetism problems. The main feature of multipole methods is that the matrix-vector product is computed through an expansion whose order can be monitored [9]. In such a situation, the matrix is not formed explicitly and its application to a vector is computed within some level of accuracy only. The higher the order, the more expensive the product. Therefore, relaxation on the accuracy of the matrix-vector products would directly decrease the cost of the iterative method.

Moreover, embedded iterations involving an outer Krylov solver also fit within the scope of this study. This is the case, for instance, of the Arnoldi method with invert for computing the smallest eigenvalue of a large sparse matrix. Although the matrix A may be known exactly, the matrix A^{-1} is not: in order to compute an orthonormal basis for the Krylov space

$$\operatorname{span}\{v_1, A^{-1}v_1, A^{-2}v_1, \dots\}$$

one needs to solve a linear system $Az = v_k$ in order to get the next Krylov vector v_{k+1}. If one uses an approximate linear solver (such as an iterative method), the approximate solution $\hat{z}$ satisfies $(A + \Delta A_k)\hat{z} = v_k$. The backward error analysis viewpoint amounts to considering that the algorithm is applied to an approximation $(A + \Delta A_k)$ of A changing at each step. Again, it is possible to relax the accuracy on $\hat{z}$ as long as the outer process converges so that both the cost of the inner iterations and the global cost are reduced [3].

Another application of importance arises in the context of domain decomposition methods for partial differential equations (PDEs). For large problems, the local subproblems induced by the decomposition have to be solved by an iterative process which is embedded in the outer iterative process used to solve the Schur complement equation. The results from the present work readily apply. In [4], it is shown that, when the Schur complement equation is solved by the conjugate gradient (CG) method, a significant reduction of the computational cost can be obtained from a relaxation strategy on the inner iteration accuracy.

1.2. Outline. This paper is organized as follows. Section 2 defines the basic inexact Krylov scheme derived from the GMRES algorithm. A relaxation strategy, chosen for its good performance, is then described before its numerical behavior is illustrated in section 3 on a set of test matrices taken from the Harwell–Boeing collection and on various algorithms including CG (for short-recurrence algorithms), GMRES, and BiCGStab.

Then in section 4, we give the reasons that lead to the choice of the proposed relaxation strategy which we contrast against other possible relaxation schemes. We also discuss potential scaling issues and give some considerations on a practical implementations of such a strategy, based on our experience of real-world applications. The last section concluses this work by giving some hints and tracks to be investigated in order to progress towards a fully justified approach of inexact Krylov schemes.

2. Inner-outer iterations in Krylov methods.

2.1. The basic inexact Krylov scheme. We consider the GMRES method for solving the linear system $Ax = b$, where $A \in \mathbb{C}^{n\times n}$ and x and b are two vectors of $\mathbb{C}^n$. This method, detailed in Algorithm 1, is one of the simplest and, at the same time, one of the most widely used Krylov-type methods for solving a linear system [17].

Algorithm 1. GMRES.

$r_0 = b - Ax_0$; $\beta = \|r_0\|_2$
$v_1 = r_0/\beta$
for $k = 1, 2, \ldots,$ **do**
  $z = Av_k$
  for $i = 1$ `to` k **do**
    $h_{ik} = v_i^* z$
    $z = z - h_{ik} v_i$
  end for
  $h_{k+1k} = \|z\|$
  $v_{k+1} = z/h_{k+1k}$
  Solve the least-squares problem $\min \left\|\beta e_1 - \bar{H}_k y\right\|_2$ for y
  Set $x_k = x_0 + V_k y$
  Exit if satisfied
end for

Let x_0 be the initial guess and let $r_0 = b - Ax_0$ be the initial residual. We denote by e_k the kth canonical vector and by $\|\cdot\|$ the Euclidean norm. The GMRES method builds a basis $V_k = [v_1, \ldots, v_k]$ for the Krylov space

$$\mathcal{K}_k = \operatorname{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\},$$

and the Hessenberg matrix $H_k = V_k^* A V_k \in \mathbb{C}^{k\times k}$ is the orthogonal projection of A onto $\mathcal{K}_k$. Let $\bar{H}_k \in \mathbb{C}^{(k+1)\times k}$ be the H_k matrix augmented by the row vector $h_{k+1k}e_k^T$. The Krylov process can be viewed as the QR decomposition

$$[v_1 \; AV_k] = V_{k+1}[e_1 \; \bar{H}_k].$$

The outer iteration corresponds to the addition of a new Krylov vector in the basis $z = Av_k$. As such, the GMRES method does not show any inner iteration. To simulate the effects of an inner iteration, we perform inexact matrix-vector products

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Algorithm 2. GMRES with inexact matrix-vector products.

Set the initial guess $x_0 = 0$
$r_0 = b - Ax_0 = b$; $\beta = \|r_0\|_2$
$\hat{v}_1 = r_0 / \|r_0\|$;
for $k = 1, 2, \ldots,$ **do**
  $\hat{z} = (A + \Delta A_k)\hat{v}_k$
  for $i = 1$ `to` k **do**
    $\hat{h}_{ik} = \hat{v}_i^* \hat{z}$
    $\hat{z} = \hat{z} - \hat{h}_{ik}\hat{v}_i$
  end for
  $\hat{h}_{k+1k} = \|\hat{z}\|$
  $\hat{v}_{k+1} = \hat{z}/\hat{h}_{k+1k}$
  Solve the least-squares problem $\min \|\beta e_1 - \overline{\widehat{H}}_k y\|$ for y
  Set $x_k = x_0 + \widehat{V}_k y$ and $r_k = b - Ax_k$
  Exit if satisfied
end for

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in the computation of the Krylov vectors, as shown in Algorithm 2. More precisely, the vector $\hat{v}_{k+1}$ is obtained by computing

$$\hat{z} = (A + \Delta A_k)\hat{v}_k$$

and then orthonormalizing $\hat{z}$ against all the previous vectors $\hat{v}_i,\ i = 1, \ldots, k$. Although one could think of perturbing directly the result of the matrix-vector product Av_k, we think it is more realistic to apply the perturbation on the matrix A, thus modeling the effect of incomplete information available from the matrix itself (as would be the case in the multipole application, for instance) in addition to setting our analysis in a natural backward analysis framework. The matrix ΔA_k is a perturbation matrix satisfying some prescribed properties. A similar trick was used in [12] to simulate an inexact preconditioner for CG. Therefore, instead of working on the Krylov space $\mathcal{K}_k$, we use instead the space

$$\widehat{\mathcal{K}}_k = \text{span}\{\hat{v}_1, \hat{v}_2, \ldots, \hat{v}_k\},$$

where $\hat{z}$ is orthonormalized against $\widehat{V}_k = [\hat{v}_1, \ldots, \hat{v}_k]$ to produce $\widehat{V}_{k+1}$. We set $\hat{v}_1 = v_1 = r_0 / \|r_0\|$. The underlying QR decomposition is turned into

$$[\hat{v}_1 \ A\widehat{V}_k] + [0 \ \ \Delta A_1\hat{v}_1, \ldots, \Delta A_k\hat{v}_k] = \widehat{V}_{k+1}[e_1 \ \overline{\widehat{H}}_k \ ].$$

Therefore, the Hessenberg matrix $\overline{\widehat{H}}_k$ does not represent anymore the projection of A onto $\widehat{\mathcal{K}}_k$.

The aim of this work is to propose and experiment with a strategy which monitors the perturbations ΔA_i (in structure and in size) in such a way that the outer process still converges within only a few extra iterations (at most).

A preliminary remark is that if all the ΔA_i are equal to the same matrix E, then one solves in fact the linear system $(A+E)x = b$. The backward error for the computed solution $\tilde{x}$ with respect to the original system $Ax = b$ is $\|E\tilde{x}\|_2 / (\|A\|_2 \|\tilde{x}\|_2)$. It is bounded above by $\|E\|_2 / \|A\|_2$ and should not be much smaller unless $\tilde{x}$ specifically lies in the subspace associated with the smallest singular values of E. Similarly, numerical experiments show that if all the ΔA_i differ but stay equal in norm to $\eta \|A\|$, then in most of the cases the computed solution of the linear system is computed with a backward error of the order of η. This is not unexpected if one thinks of the GMRES process applied in finite precision: each matrix-vector product is indeed computed within a limited accuracy. It amounts to using a slightly perturbed matrix at each step, where the relative perturbation size is of the order of machine precision.

More surprisingly, this paper will show the remarkable fact that it is indeed possible to let the size of the perturbations ΔA_k grow significantly throughout the outer process. This fact is supported by a wide set of numerical experiments. An important feature of our approach is that it is set in the framework of the backward error analysis. We have chosen indeed to express the inexact matrix-vector product under the form $\hat{z} = (A + \Delta A_k)\hat{v}_k$. This is important for two reasons: first, because the backward error analysis is the tool of choice for understanding computational processes with inexact data; second, because this powerful framework naturally applies to inner-outer processes. With this modelization, we are then able to treat in a unified way inexact matrix-vector products (such as in the multipole methods for electromagnetism), or inner-outer methods with outer Krylov scheme (where the inaccuracy of the inner scheme can be interpreted if not monitored in terms of a backward error on the matrix).

In addition, we will be dealing with perturbations having a relative size always larger than machine precision, and often significantly larger: the observed phenomena are primarily due to the perturbations we apply and are not artifacts due to the finite precision of the computer arithmetic.

2.2. A relaxation strategy on the inner accuracy. Let us now define a strategy to increasingly perturb the matrix-vector product as long as the outer process converges. Let r_k be the residual $Ax_k - b$ at step k. Let η be the final tolerance required for the solution of the linear system. More precisely we aim at computing a solution $\tilde{x}$ with a backward error $\|A\tilde{x} - b\| / (\|A\| \, \|\tilde{x}\|)$ smaller than η.

The proposed strategy for performing the inexact matrix-vector products is the following. Let α_k be the scalar defined by

$$\alpha_k = \frac{1}{\min(\|r_{k-1}\|, 1)}.$$

Each matrix-vector product involved in the computation of the Krylov basis is replaced by

$$\hat{z} = (A + \Delta A_k)v_k,$$

where ΔA_k is a random matrix satisfying

$$\|\Delta A_k\| = \varepsilon_k \|A\|, \quad \varepsilon_k = \min(\alpha_k \eta, 1). \tag{2.1}$$

Therefore at each step the applied perturbation is always larger than or equal to the targeted tolerance η, and always smaller than or equal to 1, in a normwise relative sense:

$$\frac{\|\Delta A_k\|}{\|A\|} \in [\eta, 1]. \tag{2.2}$$

We have forced $\varepsilon_k \leq 1$ to avoid too large relative perturbations that would not retain information on A. We see that when r_k decreases, ε_k increases (or stays at 1). The first vectors of the Krylov basis are computed with a backward error of the order of the targeted tolerance η as long as the norm of the residual is larger than 1. On the contrary, the last vectors may correspond to relatively large perturbations of A. The accuracy of the matrix-vector products is therefore *relaxed* while the outer process converges.

It has to be noted that α_k is an absolute quantity because it involves the residual without normalization, whereas $\varepsilon_k = \|\Delta A_k\| / \|A\|$ is relative. As discussed in section 4, we have found this choice to be the best in our experimental practice.

We may impose additionally some structure on ΔA_k. We have performed tests with dense matrices ΔA_k and with matrices having the same sparsity pattern of A. Both approaches gave similar results. We report only the results obtained when preserving the sparsity structure (`sprand` from MATLAB).

3. Numerical experiments.

3.1. Test algorithms. The first algorithm we present is the GMRES method; its inexact version is described above in Algorithm 2. However, since the full GMRES does not always converge on our set of test matrices within a reasonably small projection size, we also use its restarted version, denoted GMRES(m). Let m be the value of the restart parameter, that is, the maximal size allowed for the projection. The restarted method with inexact matrix-vector products is detailed in Algorithm 3. The strategy for choosing ΔA_k for $k > 0$ is the same as for the full GMRES. Let $\Delta A_k^{(j)}$ be the perturbation introduced at step k of the jth restart; then

$$\|\Delta A_k^{(j)}\| = \varepsilon_k^{(j)} \, \|A\| \quad \text{with} \quad \varepsilon_k^{(j)} = \min(\alpha_k^{(j)}\eta, 1)$$

with

$$\begin{cases} \alpha_1^{(j)} = \dfrac{1}{\min(\|r_m^{(j-1)}\|, 1)}, \ \alpha_1^{(1)} = 1, \\ \alpha_k^{(j)} = \dfrac{1}{\min(\|r_{k-1}^{(j)}\|, 1)} \qquad \text{if } k > 1. \end{cases}$$

Therefore, the accuracy of $\hat{z}_1$ in Algorithm 3 is controlled by the reciprocal of the residual associated with the solution obtained at the end of the previous restart $(j-1)$.

However, the residual r_0 which initiates each restart is also computed inexactly at the targeted tolerance: $r_0 = b - (A + \Delta A_0)x_0$ with $\|\Delta A_0\| = \eta \, \|A\|$, as this is the only quantity in the algorithm that carries information about the right-hand side. In a context where the matrix A is accessed only via inexact matrix-vector products, it is important to be able to deal with an inexact r_0. But we observed that we could not allow perturbations of size larger than η on the computation of r_0.

However, this approach is quite different from the one chosen in [13], where the inner accuracy is increased at each restart while the projection size decreases.

To broaden our choice of algorithms, we have also implemented an inexact version of the following:

- CG, as a representative of short-term recurrence algorithms [14]. We would like to mention that we have also been able to combine successfully inexact CG with the inexact preconditioner proposed by Golub and Ye [12], which is an additional illustration of the remarkable robustness of Krylov methods.
- BiCGStab. We apply the same perturbation strategy as for GMRES. However, since one iteration of BiCGStab involves two matrix-vector products, we have chosen to use the same perturbation matrix for both products.

Algorithm 3. GMRES(m) with inexact matrix-vector products.

Set the initial guess $x_0 = 0$
for $j = 1, 2, \ldots,$ **do** {The subscript (j) is omitted}
  $r_0 = b - (A + \Delta A_0)x_0$; $\beta = \|r_0\|_2$
  $\hat{v}_1 = r_0 / \|r_0\|$
  for $k = 1, 2, \ldots, m$ **do**
    $\hat{z_k} = (A + \Delta A_k)\hat{v}_k$
    for $i = 1$ `to` k **do**
      $\hat{h}_{ik} = \hat{v}_i^* \hat{z_k}$
      $\hat{z_k} = \hat{z_k} - \hat{h}_{ik}\hat{v}_i$
    end for
    $\hat{h}_{k+1k} = \|\hat{z_k}\|$
    $\hat{v}_{k+1} = \hat{z_k} / \hat{h}_{k+1k}$
    Solve the least-squares problem $\min \|\beta e_1 - \widehat{H}_k(1:k+1, 1:k)y\|$ for y
    Set $x_k = x_0 + \widehat{V}_k y$ and $r_k = b - Ax_k$
    Exit if satisfied
  end for
  Set $x_0 = x_m$
end for

Finally, we may also need a preconditioner that we usually take as an incomplete LU factorization with some threshold t [16]. We denote it by ILU(t). The preconditioner is applied on the left after the inexact matrix-vector product.

We present a series of experiments done with MATLAB 5 on a set of matrices taken from the Harwell–Boeing collection [6]. The right-hand side has been computed so that the exact solution is the vector of all ones.

3.2. Convergence process under inexact matrix-vector products. A typical observed behavior is shown in Figure 3.1 for the matrix `e05r0400` of order 236. In this case we use GMRES(m) with a restart $m = 10$ and ILU(10^{-3}). The iteration number is shown on the horizontal axis and should be read in the following sense: iteration 25 $(= (3-1) \times m + 5)$ means the fifth step of the third restart. Each figure also bears the condition number and the norm of the matrix. The line with "$\circ$" is the convergence curve with exact matrix-vector products, and the line with "+" corresponds to inexact products. By convergence curve we mean the evolution of the normwise backward error associated with the current estimate of the solution. The line with "$\times$" represents the relative size $\varepsilon_k = \|\Delta A_k\| / \|A\|$ of the perturbation imposed on the matrix-vector product at each outer iteration. Finally the straight horizontal line represents the final targeted tolerance η.

We see in Figure 3.1 that the first 7 vectors of the first restart have been computed with a perturbation size equal to η: this is because the norm of the outer residual is still ≥ 1. As soon as the norm of the residual becomes less than 1, then $\varepsilon_k = \eta / \|r_k\| > \eta$ and the matrix-vector product is computed with less and less accuracy, as shown by the increasing line ($\times$). In this case, we see that the convergence curves with exact ($\circ$) and inexact (+) products cannot be distinguished (at the graphical level) before the targeted tolerance is reached. This amazing fact is observed in many experiments. When the backward error associated with the current iterate becomes of the order of η, the convergence curve corresponding to inexact products stalls at a value of the order of η, as expected. In this particular example, the linear system is solved

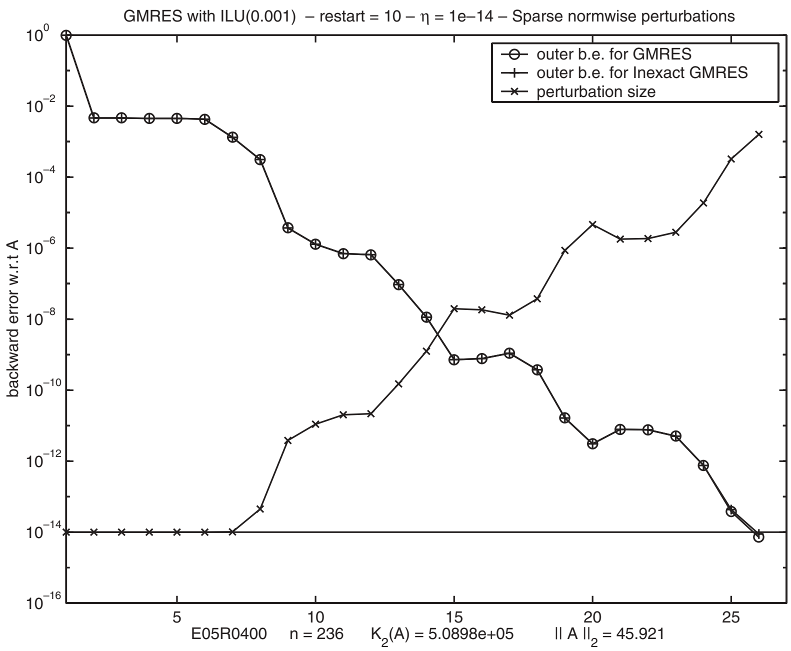

FIG. 3.1. *Exact* (○) *vs. inexact* (+) *matrix-vector products in GMRES*(m). $\eta = 10^{-14}$, $m = 10$.

in 25 steps (to reach a tolerance of 10^{-14}), whether the matrix-vector products are exact or perturbed. In practice, perturbing the matrix-vector products should result in an increase in the number of steps. It is remarkable to see that many (19 out of 26 in this example) of the Krylov vectors can be significantly perturbed (up to 10^{-3} in this example, to be compared to $\eta = 10^{-14}$) without altering the convergence process. Moreover, it was quite unexpected to see that all the Krylov vectors of the last restarts are computed with a high perturbation apart from the first vector $v_1 = r_0/\|r_0\|$, which is perturbed at the level of η.

3.3. Summary of the experiments. Let us now browse through a variety of matrices while testing several Krylov solvers. We first need to state more precisely the definition of convergence. Indeed, it may seem quite ambitious to expect the backward error to be of the order of η when each matrix-vector product is perturbed by at least the order of η. It is somehow like requiring a backward error to be less than machine precision in finite precision arithmetic. Therefore it is already very satisfactory to reach a final backward error of the order of 10η or even $10^2\eta$. To illustrate this point, we record the number of iterations N_1 (resp., N_{10} and N_{100}) necessary for the backward error to become smaller than η (resp., 10η and 100η) when possible. These numbers have to be compared with the number of iterations N_{ex} for the backward error to become smaller than η with exact products, to serve as a reference.

Table 3.1 (resp., Table 3.2) summarizes the experiments performed with GMRES (resp., GMRES(m)) according to Algorithm 2 (resp., Algorithm 3). Using a preconditioned restarted version of GMRES allows us to solve a wider range of linear systems (with or without a relaxation strategy), which is why Table 3.2 contains more test matrices than Table 3.1. Tables 3.3 and 3.4 are devoted to the results obtained with similar experiments on the CG and the BiCGStab methods, respectively. When an

Table 3.1
GMRES with inexact matrix-vector products.

Matrix	n	η	N_{ex}	Inexact products N_1	N_{10}	N_{100}	Figure
ARC130	130	10^{-14}	16	16	15	14	
	130	10^{-11}	12	12	5	5	
FS_183_6	183	10^{-12}	40	44	32	23	
	183	10^{-14}	44	47	44	42	
GRE115	115	10^{-14}	80	–	77	75	
	115	10^{-05}	51	–	46	30	
GRE185	185	10^{-12}	161	–	159	158	
	185	10^{-10}	158	–	156	154	Fig. A.1
WEST0132	132	10^{-10}	130	130	124	114	
	132	10^{-08}	114	111	91	16	

Table 3.2
GMRES(m) with inexact matrix-vector products.

Matrix	n	t	m	η	N_{ex}	Inexact products N_1	N_{10}	N_{100}	Figure
e05r0400	236	10^{-3}	10	10^{-14}	26	26	25	24	Fig. 3.1
e05r0000	236	10^{-2}	20	10^{-14}	95	110	93	76	
	236	10^{-2}	20	10^{-10}	59	69	57	55	
	236	10^{-2}	20	10^{-06}	36	63	34	30	
GRE115	115	10^{-1}	10	10^{-10}	18	18	17	15	
GRE185	185	10^{-2}	10	10^{-14}	91	–	80	73	
	185	10^{-2}	10	10^{-10}	59	166	53	43	
	185	10^{-2}	15	10^{-10}	29	155	39	27	Fig. A.3
GRE343	343	10^{-1}	10	10^{-10}	42	43	38	33	
CAVITY03	317	10^{-3}	10	10^{-10}	24	24	21	16	
PDE225	225	10^{-1}	10	10^{-14}	26	27	24	22	
	225	10^{-1}	10	10^{-13}	24	24	22	21	
	225	10^{-1}	10	10^{-10}	19	20	18	16	
SAYLR1	238	10^{-1}	10	10^{-13}	131	131	110	90	Fig. A.2
	238	10^{-1}	10	10^{-10}	81	91	66	51	
UTM300	300	10^{-3}	15	10^{-11}	56	–	–	46	
	300	10^{-3}	15	10^{-06}	30	–	28	16	
	300	10^{-3}	20	10^{-11}	34	–	28	21	
	300	10^{-3}	20	10^{-06}	18	–	17	16	
WEST0381	381	10^{-2}	10	10^{-10}	29	30	28	24	
	381	10^{-2}	10	10^{-06}	17	16	15	11	
BFW398A	398	10^{-1}	20	10^{-12}	148	–	138	116	
	398	10^{-1}	20	10^{-08}	93	–	73	62	

incomplete LU preconditioner with threshold is applied to the left of the system, the value t of the threshold is also reported in the tables. In the appendix, we present four figures of the same kind as Figure 3.1 selected from the experiments among those reported in the three tables. The interested reader is referred to [2] for the complete set of plots associated with Tables 3.1, 3.2, and 3.4.

In the experiments on GMRES and GMRES(m) with inexact products, we have always been able to obtain a backward error at least smaller than 100η with GMRES and GMRES(m). Even more, the cases where the backward error could not be lower than 10η are very seldom. It is also very interesting that the convergence with inexact products is achieved within a number of iterations which is of the order of the one obtained with exact products. Exceptionally, it may even happen that

Table 3.3
CG with inexact matrix-vector products.

					Inexact products			
Matrix	n	t	η	$N_{\rm ex}$	N_1	N_{10}	N_{100}	Figure
BCSSTK27	1224	10^{-2}	10^{-12}	50	52	48	45	
	1224	10^{-2}	10^{-14}	55	57	53	51	
BCSSTK14	1806	5.10^{-3}	10^{-12}	54	–	51	47	
	1806	5.10^{-3}	10^{-14}	60	–	58	55	
	1806	10^{-2}	10^{-12}	69	–	66	61	
BCSSTK15	3948	5.10^{-3}	10^{-12}	145	–	141	131	
	3948	10^{-1}	10^{-12}	221	–	224	210	
S1RMQ4M1	5489	10^{-2}	10^{-12}	135	147	129	116	
	5489	5.10^{-2}	10^{-12}	245	284	256	236	Fig. A.5
	5489	10^{-1}	10^{-08}	210	224	193	158	
	5489	10^{-1}	10^{-10}	246	260	232	213	
	5489	10^{-1}	10^{-12}	283	296	267	248	

Table 3.4
BiCGStab with inexact matrix-vector products.

					Inexact products			
Matrix	n	t	η	$N_{\rm ex}$	N_1	N_{10}	N_{100}	Figure
BFW398A	236	10^{-1}	10^{-12}	84	–	–	–	Fig. A.4
	236	10^{-3}	10^{-12}	11	–	10	10	
CAVITY03	317	10^{-3}	10^{-10}	23	–	–	18	
	317	10^{-3}	10^{-08}	16	–	–	13	
e05r0000	236	10^{-2}	10^{-10}	51	–	–	43	
	236	10^{-2}	10^{-06}	40	–	34	26	
e05r0400	236	10^{-3}	10^{-12}	20	–	–	17	
	236	10^{-3}	10^{-06}	10	–	10	2	
GRE115	115	10^{-1}	10^{-12}	24	27	24	24	
	115	10^{-1}	10^{-09}	21	–	20	18	
GRE185	185	10^{-2}	10^{-10}	34	–	–	–	
GRE343	343	10^{-1}	10^{-10}	38	–	36	32	
PDE225	225	10^{-1}	10^{-13}	25	25	22	21	
	225	10^{-1}	10^{-10}	20	20	18	16	
SAYLR1	238	10^{-1}	10^{-13}	44	–	44	39	
	238	10^{-1}	10^{-10}	32	43	37	36	

GMRES or GMRES(m) with perturbed matrix-vector products converge faster than their exact counterparts by a few iterations (see `WEST0132` in Table 3.1 and `WEST0381` in Table 3.2). In some cases, the convergence of the perturbed algorithm is achieved with many extra iterations: see, for instance, `GRE185` in Table 3.2. But usually in those cases convergence within 10η is always achieved with a number of iterations comparable to that for the exact algorithm. Therefore, the overhead in terms of iterations induced by the inexact matrix-vector products is quite low. This is all the more remarkable because the size of the perturbations allowed by the strategy described in (2.1) can grow fast and reach large values (see, for instance, Figure 3.1 or A.3). This shows that the Krylov process is robust to perturbations of the matrix-vector products provided that the first Krylov vectors are computed with the full targeted accuracy.

The results obtained for CG with inexact matrix-vector products (symmetry is not maintained) in Table 3.3 confirm that the observed robustness is inherent to Krylov processes and should be shared by other numerical Krylov schemes. The results, obtained on matrices of larger size than in the previous cases, show that decreasing the backward error below 10η was always achievable, and that the threshold of η was reached in more than half of the cases with a reasonable overhead in terms of additional steps. We refer the interested reader to [4] for a more detailed evaluation of the gain obtained with relaxation schemes for CG in the context of domain decomposition methods. The picture is slightly less clear with BiCGStab; if in most of the cases the backward error is smaller than 100η, we have also encountered a few examples where the backward error could not decrease significantly. Anyway, the possibility of applying a relaxation strategy still holds: the gain is just not as high.

3.4. Practical implementation. It has to be noted that the definition of ε_k in (2.1) relies upon information about the true residual $r_{k-1} = b - Ax_{k-1}$ at step $k-1$. However, in the context of avoiding exact matrix-vector products, $\|r_{k-1}\|$ needs to be replaced by a quantity directly available from the algorithm, such as the GMRES residual, which is a by-product of the QR factorization of the augmented Hessenberg matrix arising in the least-squares solution. However, whether this GMRES residual still gives information about the true residual when the Krylov space is perturbed has to be tested carefully. Experiments with embedded CG algorithms in domain decomposition techniques performed on realistic PDE problems are encouraging: a comparison of the true and the by-product residuals during the relaxation strategy can be found in [4] for CG, where it appears that the difference between both quantities is not particularly affected by the introduction of the relaxation scheme.

Note also that the quantities we have reported as the "true" or "exact" residual or any by-product quantity given by the algorithm were indeed computed in finite precision. However, we are dealing here with matrix perturbations of relatively large size (see (2.2)) so that effects of finite precision should not be dominant.

4. Variations on relaxation strategies.

4.1. Other relaxation schemes. The relaxation strategy proposed above basically varies as the reciprocal of the residual. One can legitimately wonder why, and whether other indexations such as those on the reciprocal of the square of the residual or its square root, for instance, would not be equally applicable.

A strategy indexed on the reciprocal of the square of the residual would generate larger inaccuracies, and our practice has shown us that not enough information would be retained to ensure the global convergence of the outer Krylov scheme in most of our attempts.

On the contrary, it is expected that a relaxation strategy based on the reciprocal of the square root of the residual would work in a larger number of cases than the strategy proposed above since the size of the perturbation would be smaller for a similar convergence pattern. This is observed on Tables 4.1 and 4.2, which offer the same test cases as in Tables 3.1 and 3.2 but with a relaxation scheme where α_k has been replaced by

$$\gamma_k = \frac{1}{\min(\sqrt{\|r_k\|}, 1)}.$$

It is clear that this more conservative strategy recovers the global convergence of GMRES (see `GRE115` and `GRE185`) or GMRES(m) (see `UTM300` and `BFW398A`) in most of the cases where the strategy indexed on the reciprocal of the residual would fail to ensure a final backward error smaller than η or would require a very high overhead

TABLE 4.1
GMRES with inexact matrix-vector products. Strategy indexed on $1/\sqrt{\|r_k\|}$.

Matrix	n	η	N_{ex}	Inexact products N_1	N_{10}	N_{100}
ARC130	130	10^{-14}	16	16	15	14
	130	10^{-11}	12	12	5	5
FS_183_6	183	10^{-12}	40	44	32	23
	183	10^{-14}	44	47	43	42
GRE115	115	10^{-14}	80	80	77	75
	115	10^{-05}	51	51	46	30
GRE185	185	10^{-12}	161	161	159	158
	185	10^{-10}	158	158	156	154
WEST0132	132	10^{-10}	130	130	124	114
	132	10^{-08}	114	111	91	16

TABLE 4.2
GMRES(m) with inexact matrix-vector products. Strategy indexed on $1/\sqrt{\|r_k\|}$.

Matrix	n	t	m	η	N_{ex}	Inexact products N_1	N_{10}	N_{100}
e05r0400	236	10^{-3}	10	10^{-14}	26	28	25	24
e05r0000	236	10^{-2}	20	10^{-14}	95	96	93	76
	236	10^{-2}	20	10^{-10}	59	72	57	55
	236	10^{-2}	20	10^{-06}	36	38	34	30
GRE115	115	10^{-1}	10	10^{-10}	18	18	17	15
GRE185	185	10^{-2}	10	10^{-14}	91	94	81	73
	185	10^{-2}	10	10^{-10}	59	61	54	43
	185	10^{-2}	15	10^{-10}	29	30	28	27
GRE343	343	10^{-1}	10	10^{-10}	42	43	38	33
CAVITY03	317	10^{-3}	10	10^{-10}	24	24	20	16
PDE225	225	10^{-1}	10	10^{-14}	26	27	24	22
	225	10^{-1}	10	10^{-13}	24	24	22	21
	225	10^{-1}	10	10^{-10}	19	20	18	16
SAYLR1	238	10^{-1}	10	10^{-13}	131	140	111	99
	238	10^{-1}	10	10^{-10}	81	91	66	51
UTM300	300	10^{-3}	15	10^{-10}	52	53	46	41
	300	10^{-3}	15	10^{-06}	30	–	61	19
	300	10^{-3}	20	10^{-11}	34	35	33	21
	300	10^{-3}	20	10^{-06}	18	–	17	17
WEST0381	381	10^{-2}	10	10^{-10}	29	29	28	26
	381	10^{-2}	10	10^{-06}	17	16	15	11
BFW398A	398	10^{-1}	20	10^{-12}	148	152	137	121
	398	10^{-1}	20	10^{-08}	93	82	62	62

of outer iterations to meet this criterion. In the cases where the strategy indexed on $1/\|r_k\|$ succeeds in ensuring the global convergence, the strategy with γ_k may require fewer outer iterations (see GMRES(m) on GRE185, for instance) but not always (see GMRES(m) on e05r0000). However, both strategies behave similarly when one considers obtaining a final backward error of the order of 10η as a satisfactory final goal. In order to achieve a final backward error of η on a given linear system, one may apply, for instance,

- a relaxation strategy indexed on the reciprocal of the square root of the residual (i.e., using γ_k) and η;
- a relaxation strategy indexed on the reciprocal of the residual and $\eta' = \eta/10$ with a stopping criterion chosen as $10\eta'$.

The quality of the computed solution would be the same, but the global computational cost may differ.

Indeed, many variants may be thought of as one starts playing with the parameters of the relaxation scheme, such as η, α_k, or the stopping criterion. It is particularly difficult to compare the different strategies on our model problem of inexact Krylov schemes because we do not have a good way to measure the performance of these strategies: the number of outer iterations itself is not a good criterion since it does not take into account the gain obtained from using inaccurate matrix-vector products. In practice, the choice of a good strategy will result from some trade-off between the cost of the inner iteration and the overhead on the outer iterations.

Therefore, so far we have been primarily interested in the achievable accuracy of the relaxation schemes. A general comparison of these schemes in terms of computational cost is beyond the scope of this paper. Such a study requires the knowledge of the inner process modeled here by a perturbation. We refer, for instance, to our work on domain decomposition methods with Giraud where the gain can be effectively measured in terms of a significant reduction of matrix-vector products [4].

The strategy which indexes the perturbation size on the reciprocal of the residual was therefore privileged because it is the one that allows the larger perturbations sizes while preserving the global convergence. If the inaccuracies allowed on the matrix-vector product translate into a significant gain in the computational cost, then the proposed strategy has a strong potential for reducing the global computational cost of the complete solution of the linear system.

4.2. Preconditioning. In the experiments proposed here, we have focused on the influence of perturbations of the matrix A (i.e., on inexact matrix-vector products) on the convergence of GMRES, regardless of the preconditioner. As a matter of fact, our strategy makes use of the residual of the original system $Ax = b$. However, in the case of left preconditioning, for instance, this residual may not be readily available: only the preconditioned residual would appear naturally in the algorithm. In such a case, it may be more appropriate to base the relaxation strategy on the preconditioned matrix, rather than on the original matrix.

4.3. Scaling issues. As mentioned in section 2.2, the relaxation strategy is based on the choice $\varepsilon_k = \min(\alpha_{k-1}\eta, 1)$, where $\alpha_{k-1} = 1/\min(\|r_{k-1}\|, 1)$ retains only an absolute information (the residual) from the outer process. Clearly this strategy suffers from the drawback of being scaling-dependent. Indeed, scaling the linear system $Ax = b$ by a constant will not change the convergence of GMRES but would definitely affect the relaxation strategy. It is therefore desirable to design a scaling-independent strategy. For instance, what would happen if one uses the backward error $\|r_{k-1}\|/(\|A\|\,\|x_{k-1}\|)$ instead of the residual $\|r_{k-1}\|$ alone? The corresponding strategy would be defined by

$$\varepsilon'_k = \min(\alpha'_{k-1}\eta, 1) \text{ with } \alpha'_{k-1} = \frac{1}{\min\left(\frac{\|r_{k-1}\|}{\|A\|\|x_{k-1}\|}, 1\right)}.$$

Surprisingly, this idea, which would seem natural a priori, does not lead to good results. Indeed, with such a choice, the convergence of the outer process is significantly delayed or even impeached (see Figures 4.1 and 4.2). Again, changing ε_k into ε'_k may be seen as another possible variant of the relaxation strategy if one also plays with the

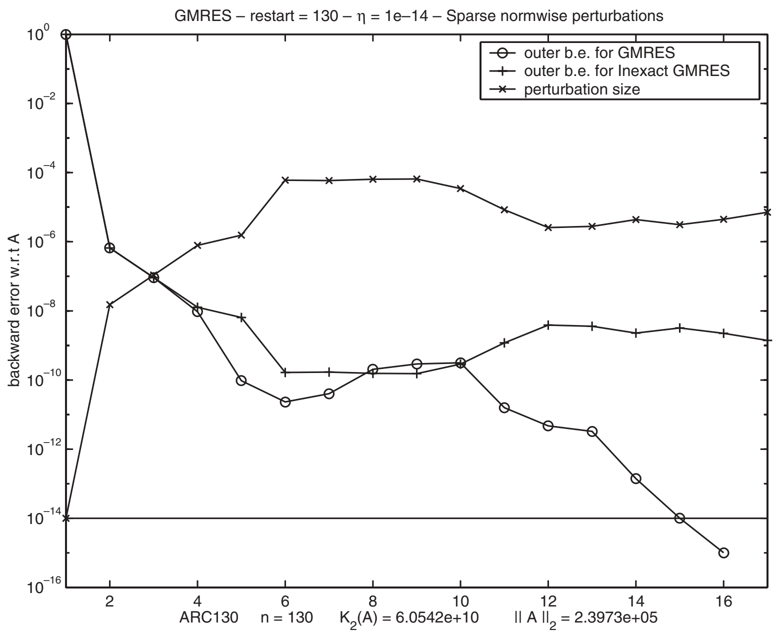

FIG. 4.1. *GMRES with inexact matrix-vector products.* ARC130. $\eta = 10^{-14}$. *Relaxation strategy with* ε'_k.

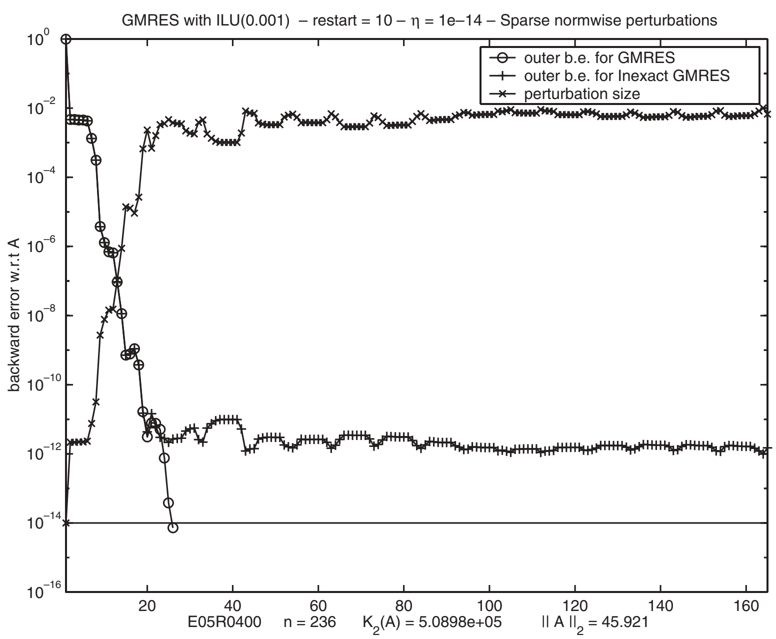

FIG. 4.2. *GMRES with inexact matrix-vector products.* E05R0400. $\eta = 10^{-14}$. *Relaxation strategy with* ε'_k.

choice of the parameter η, the targeted tolerance, and the stopping criterion, which can be any multiple of η. However, this means that further work remains to be done in order to obtain a deeper interpretation of the relaxation strategy, and why it seems to work so well.

4.4. Dependency on the starting vector. The dependency of the proposed relaxation strategy on the choice of the starting vector has also been explored. In practice we found that changing the initial vector, and thus the initial residual, would have no more effect on the global convergence than one would observe without using a relaxation scheme.

5. Conclusion and perspectives. Golub, Zhang, and Zha have been among the first to expose the robustness of Krylov schemes to variable inaccuracies in their work on inner-outer Lanczos processes in [13]. The inner process solves a linear least-squares problem with a tolerance τ_j which varies at each outer step j of the Lanczos algorithm. The authors discuss a way to deduce the sequence $\{\tau_j\}$ from the eigenvector associated with the smallest eigenvalue of the Lanczos tridiagonal matrix. It is noted that the sequence $\{\tau_j\}$ can grow (implying a lesser inner accuracy) and yet the outer process converges and the overall computation is cheaper.

Similarly, our experiments clearly demonstrate that Krylov methods are robust to inexact matrix-vector products, provided an appropriate strategy (of type (2.1), for example) is applied. In particular, the first vectors of the Krylov space need to be computed with full accuracy, while this constraint can be relaxed further on. It is remarkable that the Krylov process still converges while the Krylov vectors are significantly perturbed. In the case of linear systems, we have proposed a practical way (chosen amongst possible others for its large scope of good performance) to control the inner accuracy: the relaxation strategy indexes the accuracy of the kth Krylov vector (in terms of its backward error) on the reciprocal of the residual of the current iterate. Since inexact matrix-vector products induce an overhead in terms of outer iterations, it is crucial to see whether this overhead is compensated at the global level by the reduction of the cost of the inner level. Only then will a complete comparison of different relaxation schemes be possible.

This paper sets up a framework, inspired by the backward error analysis, which seems extremely promising for future investigations on the robustness of Krylov methods. Although essentially experimental, this work and the applications performed on eigenproblems [3] and on domain decomposition techniques with Giraud [4] seem to have captured the interest of engineers and researchers since the first time it was presented [1]. Among the practical uses of this relaxation scheme, we wish to cite the work of [21] and [15]. More recently, a few papers have shown significant progress in building the basis for a more theoretical explanation of the phenomena explored here: [10, 18, 20] show sufficient conditions for convergence of Krylov schemes under a relaxation scheme indexed on the reciprocal of the residual. Not surprisingly, these sufficient conditions on the perturbation size involve factors such as the condition number of the computed Hessenberg matrix or the matrix itself. Further work should be performed in order to check whether these conditions provide the full explanation for the robustness of Krylov methods observed in practice. Once their estimation using quantities readily available in the inner-outer schemes has been worked out carefully, these promising results may lead to more refined and more efficient relaxation strategies.

Appendix. Some convergence plots for inexact Krylov methods.

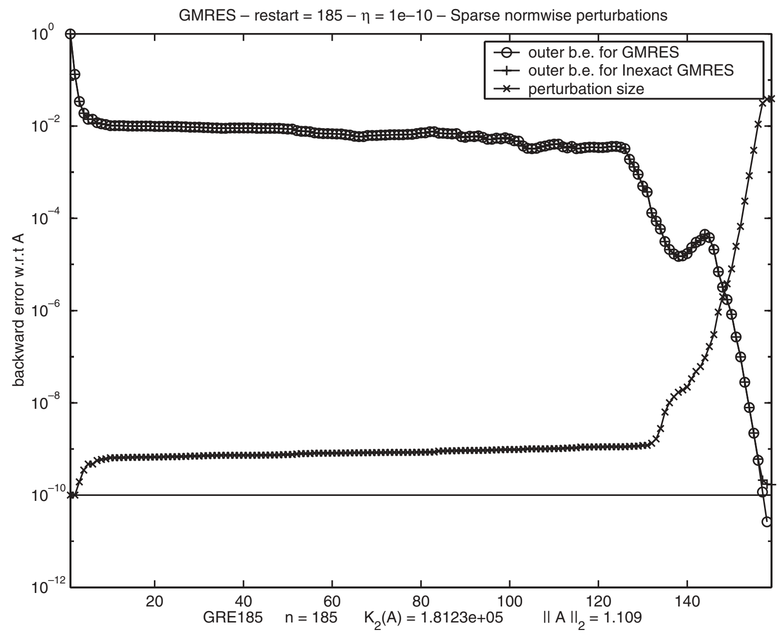

FIG. A.1. *GMRES with inexact matrix-vector products.* `GRE185`. $\eta = 10^{-10}$.

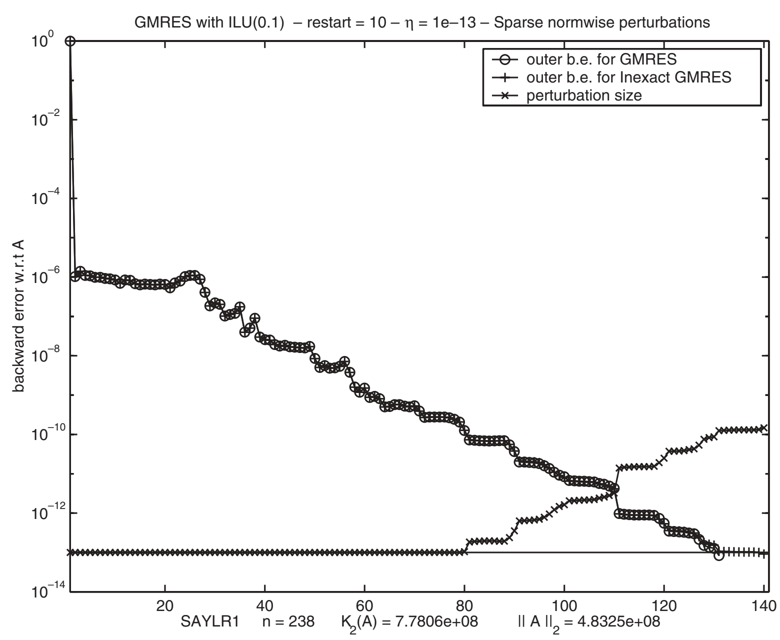

FIG. A.2. *GMRES*(m) *with inexact matrix-vector products.* `SAYLR1`. $\eta = 10^{-13}$, $m = 10$.

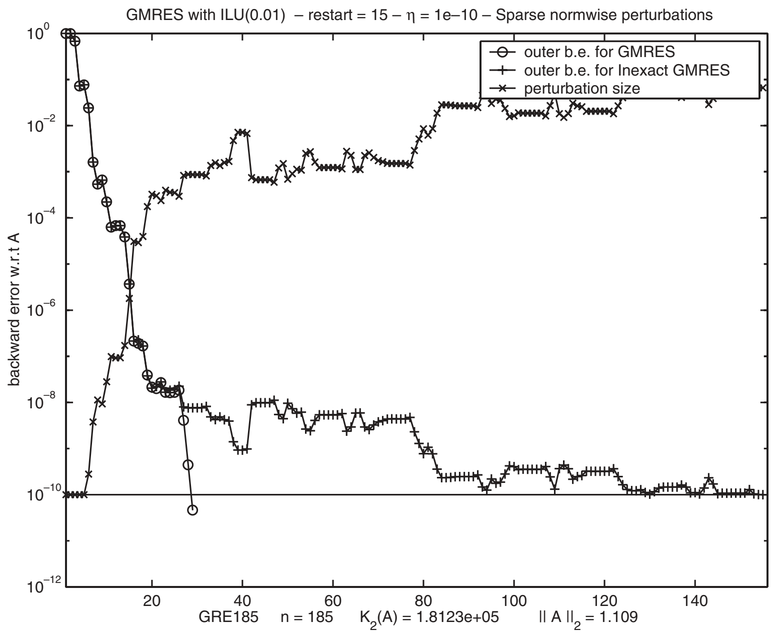

FIG. A.3. *GMRES*(m) *with inexact matrix-vector products.* `GRE185`. $\eta = 10^{-10},\ m = 15$.

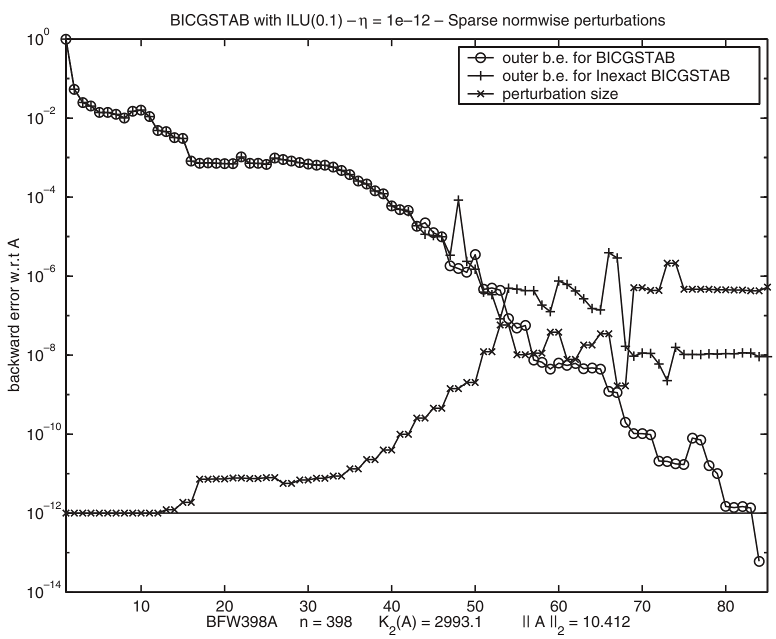

FIG. A.4. *BiCGStab with inexact matrix-vector products.* `BFW398A`. $\eta = 10^{-12}$.

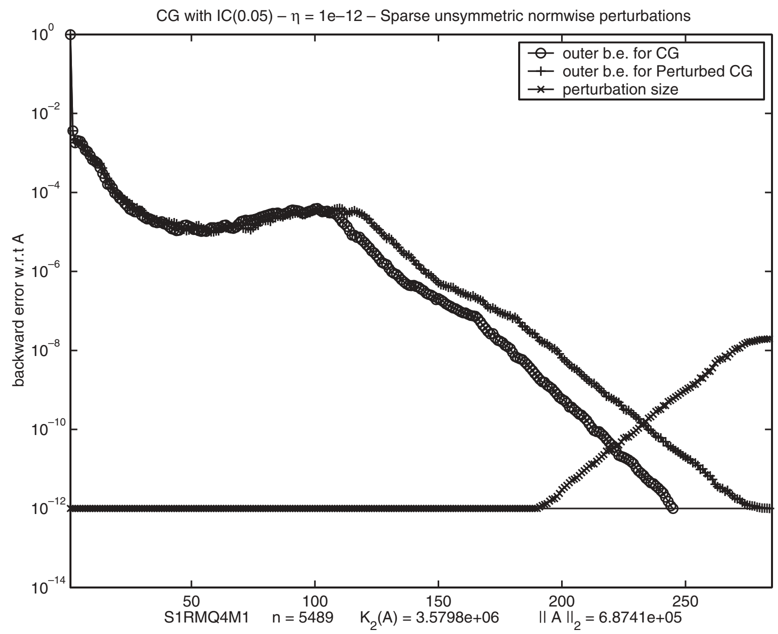

FIG. A.5. *CG with inexact matrix-vector products.* S1RMQ4M1. $\eta = 10^{-12}$.

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