Stability of the Krylov bases and subspaces

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Abstract: The problems of numerical analysis with large sparse matrices involve often a projection of this matrix onto a Krylov subspace to obtain a smaller matrix which is used to solve the initial problem. The subspace depends on the matrix and on an arbritary vector. We consider, in this paper, a method to study the stability of the Krylov subspace through a matrix perturbation. This method includes a definition of the condition numbers for the computation of the Krylov basis and the Krylov subspace. A practical method for estimating these numbers is provided. It is based on the solution of a large triangular system.

Key-words: Krylov basis and subspace, Condition number, Stability.

(Résumé : tsvp)

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Stabilité des bases et des sous-espaces de Krylov

Résumé : Les problèmes d'analyse numérique avec des grandes matrices creuses requièrent souvent une projection de cette matrice sur un sous-espace de Krylov pour obtenir une matrice plus petite utilisée pour résoudre le problème initial. Le sous-espace dépend de la matrice et d'un vecteur arbitraire. On se propose ici d'étudier la stabilité des bases et sous-espaces de Krylov lorsqu'on perturbe la matrice. Cette méthode inclut une définition du conditionnement des bases et sous-espaces de Krylov. On fournit un algorithme de calcul de ces conditionnements, basé sur la solution d'un grand système triangulaire.

Mots-clé : Base et sous-espace de Krylov, Conditionnement, Stabilité.

1 Introduction

Using a computer to solve a numerical problem, we have to ensure the accuracy of the result by computing the condition number of the problem, i.e. to give a measure of the sensitivity of the result to a data perturbation. It is with this aim that we deal, in this paper, with a method studying the condition number of Krylov basis and subspace. The Krylov subspaces [3], built from a matrix $A \in \mathbb{R}^{n \times n}$ and an arbitrary vector $f \in \mathbb{R}^n$, are often used in numerical analysis with large sparse matrices [1, 4]. Indeed, in these problems, we need to project the large matrix onto a subspace to obtain a smaller matrix which is used to solve the initial problem. We give here a method to measure the sensitivity of the Krylov basis and subspace to a matrix perturbation. This method is proposed by S.K. Godunov.

First, in section 2, we give the definitions of the distance between two bases and two subspaces, the definition of the Krylov basis and subspace and the condition number of them. At the end of this section, we show that only the case of a matrix perturbation on an Hessenberg matrix with the vector $f = (1, 0, \ldots, 0)^T$ has to be taken into account. In section 3, we give the method for the computation of the condition numbers : we study the sensitivity, at the first order, of the Krylov basis F of dimension k construted from A and f, to a matrix perturbation Δ, i.e. we search X such that $(I + X)F$ is a Krylov basis of $A + \Delta$. Then, we show that X is solution of a Sylvester equation ; S.V. Kuznetsov proved that X could be found from the solution of a linear system involving a large triangular matrix $B^{(A,k)}$ constructed from the elements of A. We prove then that the condition number for the computation of the Krylov basis and subspace are deduced from the 2-norm of the inverse of $B^{(A,k)}$. In section 5, J-F. Carpraux implements the algorithm for the computation of the condition number and gives some bounds to ensure the quality of the result. Finally, in section 6, we illustrate this method by computing some condition numbers for several matrices and vectors.

2 Definitions and preliminaries

2.1 Distance between two bases and subspaces

Let $\mathcal{F}$ and $\mathcal{G}$ be two subspaces of $\mathbb{R}^n$ of dimension k, and let F and G be two orthonormal bases of $\mathcal{F}$ and $\mathcal{G}$ respectively. Then, there exists some matrix $W \in \mathbb{R}^{n \times n}$, such that $W^*W = I$ and $G = WF$. Let $\mathcal{W}$ be the set of such matrices, then $\forall W \in \mathcal{W}$, there exists some unitary matrices $U \in \mathbb{R}^{n\times n}$ such that

$$W = U^* \begin{pmatrix} \cos\omega_1 & -\sin\omega_1 & & & & & & & \\ \sin\omega_1 & \cos\omega_1 & & & & & & & \\ & & \ddots & & & \mathbf{0} & & & \\ & & & \cos\omega_j & -\sin\omega_j & & & & \\ & & & \sin\omega_j & \cos\omega_j & & & & \\ & & & & & 1 & & & \\ & & \mathbf{0} & & & & \ddots & & \\ & & & & & & & 1 & \\ & & & & & & & & \pm 1 \end{pmatrix} U$$

Definition 1

The distance between F *and* G *is given by* $d(F,G) = \min_{W\in\mathcal{W}} \sqrt{\sum_{i=1}^{j} \omega_i^2}$ *where* $\mathcal{W} = \{W \in \mathbb{R}^{n\times n}$ *such that* $G = WF$ *and* $W^*W = I\}$.

The distance between $\mathcal{F}$ *and* $\mathcal{G}$ *is given by* $d(\mathcal{F},\mathcal{G}) = \min_{F,G} d(F,G)$ *where* F *and* G *are respectively two orthonormal bases of* $\mathcal{F}$ *and* $\mathcal{G}$.

If F and G are close from each other, then $G = WF$ with $W = I + X + O(\|X\|^2)$ where $\|X\| \ll 1$ and $X^* = -X$. Let $\mathcal{X}$ be the set of all these matrices X. Then $\forall X \in \mathcal{X}$,

$$X = U^* \begin{pmatrix} 0 & -\omega_1 & & & & \\ \omega_1 & \ddots & \ddots & & \mathbf{0} & \\ & \ddots & \ddots & -\omega_j & & \\ & & \omega_j & 0 & & \\ & \mathbf{0} & & & \ddots & \\ & & & & & 0 \end{pmatrix} U.$$

Since $\|X\|_F = \sqrt{2\sum_{i=1}^{j} \omega_i^2}$, we get the following:

Lemma 1 *At the first order in $\|X\|$, $d(F,G) = \min_{X\in\mathcal{X}} \frac{1}{\sqrt{2}}\|X\|_F$, where $\mathcal{X} = \{X$ such that $\|X\| \ll 1, X^* = -X$*

2.2 Krylov subspace and basis

Let $A \in \mathbb{R}^{n\times n}$ and $f \in \mathbb{R}^n$, $\|f\|_2 = 1$. The Krylov subspaces are, for $1 \leq k \leq n$, the subspaces $\mathcal{K}_k(A,f) = span[f, Af, A^2f, \ldots, A^{k-1}f]$ of dimension $\leq k$.

Let l be the dimension of $\mathcal{K}_n(A,f) = span[f, Af, \ldots, A^{n-1}f]$: in fact, we have $\mathcal{K}_n(A,f) = span[f, Af, \ldots, A^{l-1}f]$.

Definition 2 *For $1 \leq k \leq l$, the natural orthonormal Krylov basis of $\mathcal{K}_k(A,f)$ is an orthonormal basis $F_k = \{f_1, f_2, \ldots, f_k\}$ such that for $1 \leq j \leq k$, F_j is the Krylov basis of $\mathcal{K}_j(A,f)$. F_k is unique up to the sign.*

Remark *F_k can be constructed by the Arnoldi process for example.*

Let V be an orthonormal basis of $\mathbb{R}^n$ such that $V = (F_l, F')$, where F' is an orthonormal basis of $\mathcal{K}_l^{\perp}(A,f)$, and such that, in this basis, $f = (1, 0, \ldots, 0)^T$ and A is an Hessenberg matrix, where $a_{l+1,l} = 0$ and $a_{i+1,i} \neq 0$ for $1 \leq i < l$.

Remark *If $l < n-1$ then V is not unique.*

2.3 Condition number of Krylov subspace and basis

We give here the definitions of the condition numbers of the Krylov subspace $\mathcal{K}_k(A,f)$ and of its natural orthonormal Krylov basis through a matrix perturbation Δ. These condition numbers are denoted respectively by $\mu\{\mathcal{K}_k(A,f)\}$ and $\mu_b\{\mathcal{K}_k(A,f)\}$.

For $1 \leq k \leq l$, let

- $\mathcal{K} = \mathcal{K}_k(A,f)$, and F its natural orthonormal Krylov basis. Since $k \leq l$, F is of dimension k.
- $\tilde{\mathcal{K}} = \mathcal{K}_k(A+\Delta, f)$, and $\tilde{F}$ its natural orthonormal Krylov basis.

We assume that $\|\Delta\|$ is small enough to ensure that $\tilde{F}$ is also of dimension k. We apply the usual definition of condition number [6] where the metric in the set of subspaces is defined in Definition 1 and we choose the Frobenius norm in the space of matrices.

Definition 3 *For* $1 \leq k \leq l$*,*

$$\mu\{\mathcal{K}_k(A,f)\} = \inf_{\epsilon>0}\left\{\sup_{\|\Delta\|_F\leq\epsilon}\left(\frac{d(\mathcal{K},\tilde{\mathcal{K}})}{\|\Delta\|_F}\|A\|_F\right)\right\}$$

and

$$\mu_b\{\mathcal{K}_k(A,f)\} = \inf_{\epsilon>0}\left\{\sup_{\|\Delta\|_F\leq\epsilon}\left(\frac{d(F,\tilde{F})}{\|\Delta\|_F}\|A\|_F\right)\right\}$$

For $l < k \leq n$*,*

$$\mu\{\mathcal{K}_k(A,f)\} = \mu_b\{\mathcal{K}_k(A,f)\} = \infty$$

Remarks

- *It is easy to see that* $\mu\{\mathcal{K}_1(A,f)\} = \mu_b\{\mathcal{K}_1(A,f)\} = 0$.
- *If* $l = n$*, then* $\mu\{\mathcal{K}_n(A,f)\} = 0$ *and* $\mu_b\{\mathcal{K}_n(A,f)\} = \mu_b\{\mathcal{K}_{n-1}(A,f)\}$ *because in this case, the last vector is uniquely defined up to the sign.*

2.4 Simplification of the problem

We saw in subsection 2.2 that there exists some orthonormal bases V of $\mathbb{R}^n$, such that $H = V^*AV$ is an Hessenberg matrix, and $V^*f = (1,0,\ldots,0)^T = e_1$. We prove in the following theorem that the condition number does not depend on the basis in which A and f are expressed.

Theorem 1 *For* $1 \leq k \leq l$*,*

$$\mu\{\mathcal{K}_k(H,e_1)\} = \mu\{\mathcal{K}_k(A,f)\} \quad \textit{and} \quad \mu_b\{\mathcal{K}_k(H,e_1)\} = \mu_b\{\mathcal{K}_k(A,f)\}$$

Remarks *Let* U *be an orthonormal basis of* $\mathbb{R}^n$*,*

- *Let* $X \in \mathbb{R}^{n\times n}$*, then* $\|U^*XU\|_F = \|X\|_F$.
- *Let* G *be an orthonormal basis of* $\mathcal{K}_k(A,f)$*, then* UG *is an orthonormal basis of* $U\mathcal{K}_k(A,f)$.

Proof of the theorem

$$\begin{aligned}\mathcal{K}_k(H,e_1) &= \mathcal{K}_k(V^*AV,V^*f)\\ &= span[V^*f,V^*Af,V^*A^2f,\ldots,V^*A^{k-1}f]\\ &= V^*\mathcal{K}_k(A,f)\end{aligned}$$

Let F and $\tilde{F}$ be the orthonormal basis of $\mathcal{K}_k(A,f)$ and $\mathcal{K}_k(A+\Delta,f)$, then V^*F and $V^*\tilde{F}$ are the orthonormal basis of $V^*\mathcal{K}_k(A,f)$ and $V^*\mathcal{K}_k(A+\Delta,f)=\mathcal{K}_k(H+V^*\Delta V,e_1)=\mathcal{K}_k(H+\Delta',e_1)$ where $\|\Delta'\|_F=\|\Delta\|_F$.

$$d(V^*F,V^*\tilde{F})=\min_{Y\in\mathcal{Y}}\frac{1}{\sqrt{2}}\|Y\|_F, \text{ where}$$

$$\begin{aligned}\mathcal{Y} &= \left\{Y \text{ s.t. } \|Y\|_F\ll 1, Y^*=-Y \text{ and } V^*\tilde{F}=\left(I+Y+O(\|Y\|_F^2)\right)V^*F\right\}\\ &= \left\{Y \text{ s.t. } \|Y\|_F\ll 1, Y^*=-Y \text{ and } \tilde{F}=\left(I+VYV^*+O(\|Y\|_F^2)\right)F\right\}\\ &= \left\{Y \text{ s.t. } \|Y\|_F\ll 1, Y^*=-Y \text{ and } \tilde{F}=\left(I+Y+O(\|Y\|_F^2)\right)F\right\}\end{aligned}$$

$\Longrightarrow \quad d(V^*F,V^*\tilde{F})=d(F,\tilde{F})$. Hence $\mu_b\{\mathcal{K}_k(H,e_1)\}=\mu_b\{\mathcal{K}_k(A,f)\}$

$$\begin{aligned}d(\mathcal{K}_k(H,e_1),\mathcal{K}_k(H+\Delta',e_1)) &= d(V^*\mathcal{K}_k(A,f),V^*\mathcal{K}_k(A+\Delta,f)\\ &= \min_{F,\tilde{F}} d(V^*F,V^*\tilde{F})\\ &= \min_{F,\tilde{F}} d(F,\tilde{F})\\ &= d(\mathcal{K}_k(A,f),\mathcal{K}_k(A+\Delta,f)\end{aligned}$$

Therefore $\mu\{\mathcal{K}_k(H,e_1)\}=\mu\{\mathcal{K}_k(A,f)\}$.

□

3 Method to compute the condition numbers of Krylov subspace and basis

We want here to give a method to compute the condition number of the Krylov subspace $\mathcal{K}_k(A,f)$ and of its natural orthonormal basis.

We saw in subsection 2.4 that we can suppose that A is an Hessenberg matrix and that $f = (1, 0, \ldots, 0)^T$. Let us suppose now that $\boxed{2 \le k \le \min(l, n-1)}$

Remark *l is such that $a_{l+1,l}$ is the first zero of the subdiagonal of A, therefore l is the dimension of $\mathcal{K}_n(A, f)$.*

Let $F = [f_1, \ldots, f_k]$ be the natural orthonormal basis of $\mathcal{K}_k(A, f)$ where $f_1 = f = (1, 0, \ldots, 0)^T$, and let $\tilde{F} = [\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_k]$ be the natural orthonormal basis of $\mathcal{K}_k(\tilde{A}, f)$ where $\tilde{A} = A + \Delta + O(\|\Delta\|^2)$ ($\|\Delta\| \ll 1$) and $\tilde{f}_1 = f_1 = (1, 0, \ldots, 0)^T$. Then,

$$F = \begin{pmatrix} I_k \\ 0 \end{pmatrix} \qquad \tilde{F} = \left(\begin{array}{c|c} 1 & \\ 0 & \\ \vdots & \tilde{f}_2, \ldots, \tilde{f}_k \\ 0 & \end{array}\right)$$

If we find a matrix $X \in \mathbb{R}^{n \times n}$ ($\|X\| \ll 1$) such that $\tilde{F} = (I + X + O(\|\Delta\|^2))F$ with $X^* = -X$, then, thanks to Lemma 1, we will be able to estimate $d(F, \tilde{F})$, and then, the condition number of the Krylov subspace and basis (see Definition 3).

3.1 Structure of the matrix X

Definition 4 *(Definition of the operator $\mathcal{L}_k$)*
Let $M \in \mathbb{R}^{n \times n}$ then $\mathcal{L}_k\{M\}$ designs the first $k-1$ columns below the subdiagonal of M, i.e. $\mathcal{L}_k\{M\} = \begin{pmatrix} 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & & & & & \\ m_{3,1} & \ddots & & \mathbf{0} & & \\ \vdots & \ddots & \ddots & & & \\ \vdots & & m_{k+1,k-1} & 0 & \ldots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ m_{n,1} & \ldots & m_{n,k-1} & 0 & \ldots & 0 \end{pmatrix}$

Remark *$\mathcal{L}_k$ is linear and its kernel is the subspace of Hessenberg matrices for the first $k-1$ columns.*

We have to find X such that $X^* = -X, \quad \tilde{f}_1 = f_1, \quad$. Therefore X has the following structure :

$$X = \begin{pmatrix} 0 & 0 & \ldots\ldots\ldots\ldots & & 0 \\ 0 & 0 & -x_{3,2} & \ldots\ldots & -x_{n,2} \\ \vdots & x_{3,2} & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & -x_{n,n-1} \\ 0 & x_{n,2} & \ldots\ldots & x_{n,n-1} & 0 \end{pmatrix}$$

Moreover, X has to be such that $\tilde{F} = (I + X + O(\|\Delta\|^2))F$ is an orthonormal basis of $\mathcal{K}_k(\tilde{A}, f)$, i.e.

$$\left(I - X + O(\|\Delta\|^2)\right)\left(A + \Delta + O(\|\Delta\|^2)\right)\left(I + X + O(\|\Delta\|^2)\right) = \hat{A} + O(\|\Delta\|^2)$$

where $\hat{A}$ is an Hessenberg matrix for the first $k-1$ columns. This previous equation is equivalent to :

$$\begin{aligned} &\mathcal{L}_k\left\{\left(I - X + O(\|\Delta\|^2)\right)\left(A + \Delta + O(\|\Delta\|^2)\right)\left(I + X + O(\|\Delta\|^2)\right)\right\} = O(\|\Delta\|^2) \\ &\iff \quad \mathcal{L}_k\left\{A + \Delta + AX - XA + O(\|\Delta\|^2)\right\} = O(\|\Delta\|^2) \end{aligned}$$

$$\boxed{\iff \quad \mathcal{L}_k\{XA - AX\} = \mathcal{L}_k\{\Delta\} + O(\|\Delta\|^2) \qquad (1)}$$

Therefore the part under the diagonal of the $n-k$ last columns of X can be arbitrarily chosen (for $j > k$ and $i > k, x_{i,j} = 0$) :

$$\boxed{X = \begin{pmatrix} 0 & 0 & \ldots\ldots\ldots\ldots\ldots\ldots & & & & 0 \\ 0 & 0 & -x_{3,2} & \ldots\ldots\ldots\ldots & & & -x_{n,2} \\ \vdots & x_{3,2} & \ddots & \ddots & & & \vdots \\ \vdots & \vdots & \ddots & 0 & -x_{k+1,k} & \ldots & -x_{n,k} \\ \vdots & \vdots & & x_{k+1,k} & & & \\ \vdots & \vdots & & \vdots & & \mathbf{0} & \\ 0 & x_{n,2} & \ldots\ldots & x_{n,k} & & & \end{pmatrix} \qquad (ST_X)}$$

3.2 Computation of X

We are searching X with the structure (ST_X) and solution of (1). Therefore, at the first order in $\|\Delta\|$, we are searching X solution of :

$$\boxed{\left\{\begin{array}{l} X \text{ has the structure } (ST_X) \text{ defined in subsection 3.1} \\ \mathcal{L}_k\,\{XA - AX\} = \mathcal{L}_k\{\Delta\} \end{array}\right. \qquad (2)}$$

Let m be the number of unknown components of X,

$$m = (k-1)n + 1 - k(k+1)/2,$$

$$x^{(k)} = (x_{3,2}, \ldots, x_{n,2} \,|\, x_{4,3}, \ldots \,|\, \ldots \,|\, x_{k+1,k}, \ldots, x_{n,k})^T \in \mathbb{R}^m$$

$$\text{and} \quad \delta^{(k)} = (\delta_{3,1}, \ldots, \delta_{n,1} \,|\, \ldots \,|\, \delta_{k+1,k-1}, \ldots, \delta_{n,k-1})^T \in \mathbb{R}^m$$

Then, we can prove (see section 4) that

$$\boxed{X \text{ solution of } (2) \iff x^{(k)} \text{ solution of } B^{(A,k)} x^{(k)} = \delta^{(k)}}$$

where $B^{(A,k)} \in \mathbb{R}^{m\times m}$ is a triangular matrix built with the elements of A.
$B^{(A,k)}$ is non singular because its diagonal elements ($a_{j+1,j}$, for $1 \leq j \leq k-1$) are non zero.

3.3 Condition number of Krylov subspace and basis

Let us write $X = X_k^{(1)} + X_k^{(2)} + X_k^{(3)}$ where

$$X_k^{(1)} = \left(\begin{array}{ccccc|c} 0 & 0 & \ldots\ldots\ldots\ldots & & 0 & \\ 0 & 0 & -x_{3,2} & \ldots\ldots & -x_{k,2} & \\ \vdots & x_{3,2} & 0 & \ddots & \vdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \ddots & -x_{k,k-1} & \\ 0 & x_{k,2} & \ldots\ldots & x_{k,k-1} & 0 & \\ \hline & & \mathbf{0} & & & \mathbf{0} \end{array}\right) \quad \begin{array}{c} \text{is such that } I + X_k^{(1)} \\ \text{is a rotation} \\ \text{in } \mathcal{K}_k(A,f) \end{array}$$

$$X_k^{(2)} = \left(\begin{array}{cccc|ccc} & & & & 0 & \dots & 0 \\ & & & & -x_{k+1,2} & \dots & -x_{n,2} \\ & & \mathbf{0} & & \vdots & & \vdots \\ & & & & -x_{k+1,k} & \dots & -x_{n,k} \\ \hline 0 & x_{k+1,2} & \dots & x_{k+1,k} & & & \\ \vdots & \vdots & & \vdots & & \mathbf{0} & \\ 0 & x_{n,2} & \dots & x_{n,k} & & & \end{array} \right) \text{ moves } \mathcal{K}_k(A,f)$$

$X_k^{(3)} = X - X_k^{(1)} - X_k^{(2)}$ is such that $I + X_k^{(3)}$ is a rotation in $\mathcal{K}_k^{\perp}(A,f)$

Remark *In subsection 3.1, we decided to take* $X_k^{(3)} = 0$*. Indeed,* $I + X_k^{(3)}$ *is a rotation in* $\mathcal{K}_k^{\perp}(A,f)$*, so it does not perturb the computation of* $\mathcal{K}_k(A,f)$ *and of its Krylov basis.*

We give here the condition numbers of the Krylov subspace and of its natural orthonormal basis defined in Definition 3.

Theorem 2 *Let* l *be the dimension of* $\mathcal{K}_n(A,f)$*, then for* $k \in [2, \min(l, n-1)]$*, the matrix* $C^{(A,k)} = \left(B^{(A,k)}\right)^{-1}$ *exists, and then :*

The condition number of the natural orthonormal basis of $\mathcal{K}_k(A,f)$ *is*

$$\mu_b\{\mathcal{K}_k(A,f)\} = \|C^{(A,k)}\|_2 \|A\|_F$$

The condition number of $\mathcal{K}_k(A,f)$ *is*

$$\mu\{\mathcal{K}_k(A,f)\} = \|\hat{C}^{(A,k)}\|_2 \|A\|_F$$

where $\hat{C}^{(A,k)}$ *is the matrix composed by a few rows of* $C^{(A,k)}$ *such that*

$$\hat{x}^{(k)} = (x_{k+1,2}, \dots, x_{n,2} \,|\, \dots \,|\, x_{k+1,k}, \dots, x_{n,k})^T = \hat{C}^{(A,k)} \delta^{(k)}.$$

Proof Definition 3 gives us :

$$\mu_b\{\mathcal{K}_k(A,f)\} = \inf_{\epsilon > 0} \left\{ \sup_{\|\Delta\|_F \le \epsilon} \left(\frac{d(F, \tilde{F})}{\|\Delta\|_F} \|A\|_F \right) \right\}$$

We have to remark that if Δ is an Hessenberg matrix for the $k-1$ first columns (i.e. $\mathcal{L}_k\{\Delta\}=0$) then $d(F,\tilde{F})=0$. Therefore

$$\mu_b\{\mathcal{K}_k(A,f)\} = \inf_{\epsilon>0}\left\{\sup_{\|\mathcal{L}_k\{\Delta\}\|_F\le\epsilon}\left(\frac{d(F,\tilde{F})}{\|\mathcal{L}_k\{\Delta\}\|_F}\|A\|_F\right)\right\}$$

Then, using Lemma 1 and the egality $\|\delta^{(k)}\|_2 = \|\mathcal{L}_k\{\Delta\}\|_F$, we find

$$\begin{aligned}\mu_b\{\mathcal{K}_k(A,f)\} &= \inf_{\epsilon>0}\left\{\sup_{\|\delta^{(k)}\|_2\le\epsilon}\left(\frac{\frac{1}{\sqrt{2}}\|X_k^{(1)}+X_k^{(2)}\|_F}{\|\delta^{(k)}\|_2}\|A\|_F\right)\right\}\\ &= \inf_{\epsilon>0}\left\{\sup_{\|\delta^{(k)}\|_2\le\epsilon}\frac{\|x^{(k)}\|_2}{\|\delta^{(k)}\|_2}\right\}\|A\|_F = \|C^{(A,k)}\|_2\|A\|_F\end{aligned}$$

Thus, we find $\mu\{\mathcal{K}_k(A,f)\} = \inf_{\epsilon>0}\left\{\sup_{\|\Delta\|_F\le\epsilon}\left(\frac{d(\mathcal{K},\tilde{\mathcal{K}})}{\|\Delta\|_F}\|A\|_F\right)\right\}$

$$= \inf_{\epsilon>0}\left\{\sup_{\|\mathcal{L}_k\{\Delta\}\|_F\le\epsilon}\left(\frac{d(\mathcal{K},\tilde{\mathcal{K}})}{\|\mathcal{L}_k\{\Delta\}\|_F}\|A\|_F\right)\right\}$$

But $d(\mathcal{K},\tilde{\mathcal{K}}) = \min_{F,\tilde{F}} d(F,\tilde{F}) = \min_X \frac{1}{\sqrt{2}}\|X_k^{(1)}+X_k^{(2)}\|_F$, then

$$\begin{aligned}\mu\{\mathcal{K}_k(A,f)\} &= \inf_{\epsilon>0}\left\{\sup_{\|\delta^{(k)}\|_2\le\epsilon}\left(\frac{\frac{1}{\sqrt{2}}\|X_k^{(2)}\|_F}{\|\delta^{(k)}\|_2}\|A\|_F\right)\right\}\\ &= \inf_{\epsilon>0}\left\{\sup_{\|\delta^{(k)}\|_2\le\epsilon}\frac{\|\hat{x}^{(k)}\|_2}{\|\delta^{(k)}\|_2}\right\}\|A\|_F = \|\hat{C}^{(A,k)}\|_2\|A\|_F\end{aligned}$$

where $\hat{x}^{(k)}$ and $\hat{C}^{(A,k)}$ are defined in the theorem. $\square$

4 The matrix $B^{(A,k)}$

Let $A,\Delta,\delta^{(k)}$ and the operator $\mathcal{L}_k$ be defined as in section 3. We are going to prove that X solution of (2) $\iff x^{(k)}$ solution of $B^{(A,k)}x^{(k)}=\delta^{(k)}$ where $B^{(A,k)}\in$

$\mathbb{R}^{m \times m}$ is a triangular matrix built with the elements of A.

X has the structure (ST_X) defined in subsection 3.1, therefore we can write $X = X_L + X_U$ where

$$X_L = \begin{pmatrix} 0 & & & & \\ 0 & 0 & & & \\ \vdots & x_{3,2} & 0 & \mathbf{0} & \\ \vdots & \vdots & \ddots & \ddots & \\ 0 & x_{n,2} & .. & x_{n,n-1} & 0 \end{pmatrix}, X_U = \begin{pmatrix} 0 & 0 & \dots\dots\dots & & 0 \\ & 0 & -x_{3,2} & .. & -x_{n,2} \\ & & 0 & \ddots & \vdots \\ & \mathbf{0} & & \ddots & -x_{n,n-1} \\ & & & & 0 \end{pmatrix}$$

As A is an Hessenberg matrix, we see that $X_U A - AX_U$ is an upper triangular matrix, then $\mathcal{L}_k\{X_U A - AX_U\} = 0$, and therefore

$$\boxed{\mathcal{L}_k\{XA - AX\} = \mathcal{L}_k\{\Delta\} \quad \Longleftrightarrow \quad \mathcal{L}_k\{X_L A - AX_L\} = \mathcal{L}_k\{\Delta\}}$$

$$\Longleftrightarrow \quad \sum_{l=1}^{j+1} x_{i,l} a_{l,j} - \sum_{l=i-1}^{n} a_{i,l} x_{l,j} = \delta_{i,j} \qquad \forall\, 1 \le j \le k-1 \text{ and } j+2 \le i \le n$$

But $\forall i,\ x_{i,1} = 0$, so $\quad \forall\, 1 \le j \le k-1$ and $j+2 \le i \le n,\quad$ we have :

$$\left(\sum_{l=2}^{j-1} a_{l,j} x_{i,l}\right) + \left(a_{j,j} x_{i,j} - \sum_{l=i-1}^{n} a_{i,l} x_{l,j}\right) + (a_{j+1,j} x_{i,j+1}) = \delta_{i,j}$$

$$\Longleftrightarrow \forall j \in [1, k-1], \qquad \sum_{l=2}^{j-1} a_{l,j} \left(\mathbf{0}_{j-l+1} \,\middle|\, \mathbf{I}_{n-j-1} \right) \begin{pmatrix} x_{l+1,l} \\ \vdots \\ x_{n,l} \end{pmatrix}$$

$$+ \left(a_{j,j} \left(\begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} \middle| \mathbf{I}_{n-j-1} \right) - \begin{pmatrix} a_{j+2,j+1} & \dots\dots\dots & a_{j+2,n} \\ & \ddots & \vdots \\ \mathbf{0} & a_{n,n-1} & a_{n,n} \end{pmatrix} \right) \begin{pmatrix} x_{j+1,j} \\ \vdots \\ x_{n,j} \end{pmatrix}$$

$$+ a_{j+1,j} \mathbf{I}_{n-j-1} \begin{pmatrix} x_{j+2,j+1} \\ \vdots \\ x_{n,j+1} \end{pmatrix} = \begin{pmatrix} \delta_{j+2,j} \\ \vdots \\ \delta_{n,j} \end{pmatrix}$$

$$\iff \sum_{l=2}^{j-1} a_{l,j} J_{n-j-1}^{n-l} \begin{pmatrix} x_{l+1,l} \\ \vdots \\ x_{n,l} \end{pmatrix} + \left(a_{j,j} J_{n-j-1}^{n-j} - A^{(j+2)}\right) \begin{pmatrix} x_{j+1,j} \\ \vdots \\ x_{n,j} \end{pmatrix}$$

$$+ a_{j+1,j} \mathbf{I}_{n-j-1} \begin{pmatrix} x_{j+2,j+1} \\ \vdots \\ x_{n,j+1} \end{pmatrix} = \begin{pmatrix} \delta_{j+2,j} \\ \vdots \\ \delta_{n,j} \end{pmatrix}, \qquad \forall j \in [1, k-1]$$

where $J_i^j = \left(\mathbf{0}_{j-i} \,\middle|\, \mathbf{I}_i \right) \in \mathbb{R}^{i \times j}$

$$\text{and } A^{(i)} = \begin{pmatrix} a_{i,i-1} & \cdots\cdots\cdots & a_{i,n} \\ & \ddots & \vdots \\ \mathbf{0} & a_{n,n-1} & a_{n,n} \end{pmatrix} \in \mathbb{R}^{(n-i+1)\times(n-i+2)}$$

This last system of equations is equivalent to $B^{(A,k)} x^{(k)} = \delta^{(k)}$ where $B^{(A,k)}$ is the following triangular matrix built with the elements of A :

$$\begin{pmatrix} a_{2,1} I_{\text{n-2}} & & & & \\ a_{2,2} J_{\text{n-3}}^{\text{n-2}} - A^{(4)} & a_{3,2} I_{\text{n-3}} & & & \\ a_{2,3} J_{\text{n-4}}^{\text{n-2}} & \ddots & \ddots & \mathbf{0} & \\ \vdots & \ddots & \ddots & \ddots & \\ a_{2,\text{k-1}} J_{\text{n-k}}^{\text{n-2}} & \cdots & a_{\text{k-2,k-1}} J_{\text{n-k}}^{\text{n-k+2}} & a_{\text{k-1,k-1}} J_{\text{n-k}}^{\text{n-k+1}} - A^{(\text{k+1})} & a_{\text{k,k-1}} I_{\text{n-k}} \end{pmatrix}$$

5 The algorithm

Let $A \in \mathbb{R}^{n \times n}$ and $f \in \mathbb{R}^n$. We propose here an algorithm to compute the condition numbers of the Krylov subspaces $\mathcal{K}_k(A, f)$ and of their natural orthonormal bases, for k from 2 to $n-1$.

This algorithm consists in the construction of a large triangular matrix $B^{(A,n-1)}$, for which we have to estimate the norm of its inverse. We need to have a good precision of the computations in order to ensure the results. To realize this, we compute the inverse by using a special technique for scalar products, in order to avoid in mosts cases underflow and overflow.

In the second part, we bound the computed condition numbers. These bounds will be improved [2] because the study of the algorithm stability is not enough sharp at this time. Indeed, we cannot ensure the exactness of the result for some examples.

5.1 Algorithms

We give first the algorithm of computation of the condition numbers (Algorithm 1) and then we give in detail the algorithm of computation of the inverse matrix (Algorithm 2).

5.1.1 Algorithm 1 : computation of the condition numbers

1. Compute the reflections of Householder $P_0, P_1, \ldots, P_{n-2}$ such that $P_0 f = (1, 0, \ldots, 0)^T$, and $P^T A P$ is an Hessenberg matrix, where $P = P_0 P_1 \ldots P_{n-2}$.

   Let now $A := P^T A P$ *and* $f := (1, 0, \ldots, 0)^T$

2. Compute the lower triangular matrix $B^{(A,n-1)}$ of section 4

3. Compute the lower triangular matrix $C^{(A,l)} = \left(B^{(A,l)}\right)^{-1}$ by Algorithm 2

4. For $k = 2 \ldots l$, give the condition numbers using subsection 3.3 :

   - For the basis : $\|C^{(A,k)}\|_2$,
   - For the subspace $\mathcal{K}_k(A, f)$: $\|\hat{C}^{(A,k)}\|_2$, where $\hat{C}^{(A,k)}$ is defined in subsection 3.3.

5.1.2 Computation of the inverse

Let $B = (b_{i,j})_{i,j=1}^m = B^{(A,n-1)}$, and $C = (c_{i,j})_{i,j=1}^m = C^{(A,n-1)}$. The classic algorithm of computation of the $c_{i,j}$ is the next :

for $\quad i = 1, m \quad$ **do** $\quad c_{i,i} = \dfrac{1}{b_{i,i}}$

  for $\quad j = 1, i-1 \quad$ **do** $\quad c_{i,j} = \dfrac{-1}{b_{i,i}} \left(\displaystyle\sum_{k=j}^{i-1} b_{i,k} c_{k,j} \right)$

We have to take into account that the diagonal of the matrix B may contain some elements which are very close from 0. Indeed, if it exists i_0 such that $b_{i_0,i_0} \approx 0$

then the computation of the $c_{i_0,j}$ can failed if $\sum_{k=j}^{i_0-1} b_{i_0,k}c_{k,j}$ is very small too : underflow. On the other hand, if $\sum_{k=j}^{i_0-1} b_{i_0,k}c_{k,j}$ is not small, then $c_{i_0,j}$ is very big ($b_{i_0,i_0} \approx 0$). Therefore, for $i_1 > i_0$, $\sum_{k=j}^{i_1-1} b_{i_1,k}c_{k,j}$ can be very big : overflow. By using the following method to compute the $c_{i,j}$, we can avoid such problems.

Algorithm 2

$$\textbf{for} \quad i = 1, m \quad \textbf{do} \quad c_{i,i} = 2^{-r}\frac{1}{\frac{b_{i,i}}{2^r}}$$

$$\textbf{for} \quad j = 1, i-1 \quad \textbf{do} \quad c_{i,j} = -2^{(p+q-r)}\frac{\sum_{k=j}^{i-1}\frac{b_{i,k}}{2^p}\frac{c_{k,j}}{2^q}}{\frac{b_{i,i}}{2^r}} \tag{3}$$

where $r = 1 + \lfloor \log_2 |b_{i,i}| \rfloor$, $p = 1 + \max_{j \leq k \leq i-1} \lfloor \log_2 |b_{i,k}| \rfloor$ and $q = 1 + \max_{j \leq k \leq i-1} \lfloor \log_2 |c_{k,j}| \rfloor$.

5.2 Validation of the result

Let $B = B^{(A,k)}$ and $C = C^{(A,k)}$, then we have to be sure that the computed matrix C_{mach} is not too far from B^{-1}. The study of the stability of this algorithm allows us to estimate a majorant M of $\|\Omega\|_F$ where $\Omega = BC_{mach} - I$. Then, we can bound the computed condition numbers :

$$\|C_{mach}\|_2 \frac{1-2M}{1-M}\|A\|_F \leq \mu_b\{\mathcal{K}_k(A,f)\} \leq \|C_{mach}\|_2 \frac{1}{1-M}\|A\|_F$$

$$\|\hat{C}_{mach}\|_2 \frac{1-2M}{1-M}\|A\|_F \leq \mu\{\mathcal{K}_k(A,f)\} \leq \|\hat{C}_{mach}\|_2 \frac{1}{1-M}\|A\|_F$$

6 Examples

We give now some examples of computation of the condition numbers of Krylov bases and subspaces.

For each example, we give a table in which we can see the lower and upper bounds of the condition numbers of the basis :

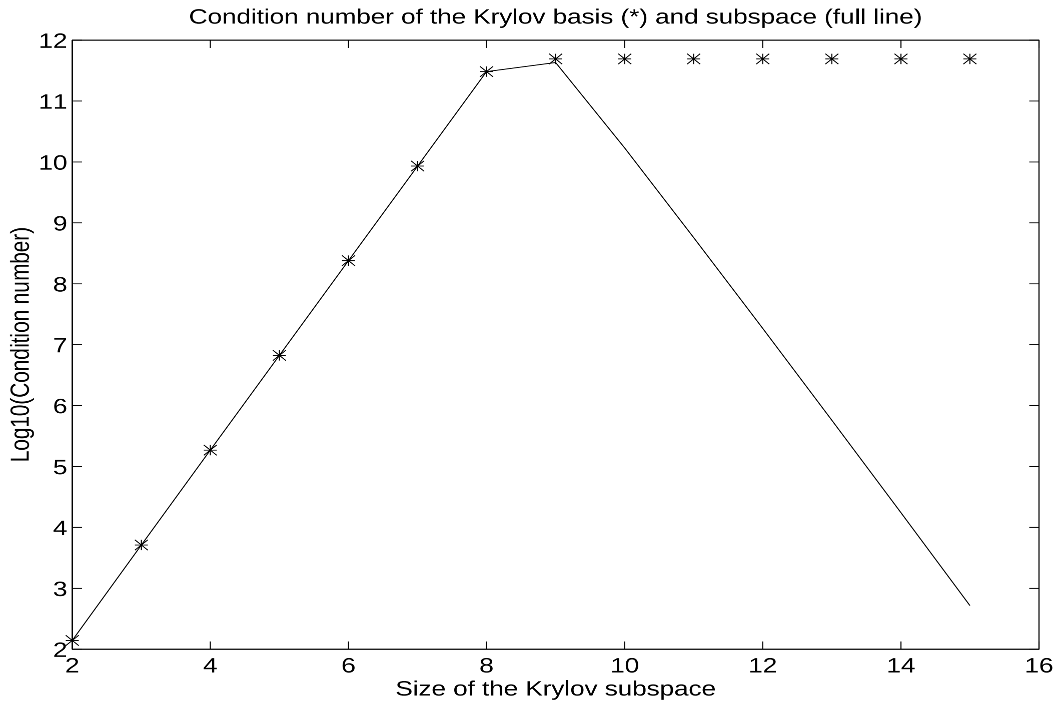
$$\text{Lower bound} = \|C_{mach}\|_2 \frac{1-2M}{1-M} \|A\|_F$$
$$\text{and Upper bound} = \|C_{mach}\|_2 \frac{1}{1-M} \|A\|_F$$

Indeed, these bounds, which can only be computed if $M < 1$, allow us to validate the result when they are close enough from each other. Moreover, we can validate the result, by computing the quantity $\|\Omega\|_2 = \|BC_{mach} - I\|_2$.

6.1 Example 1

Let us consider the following matrix $A \in \mathbb{R}^{16\times 16}$ and $f \in \mathbb{R}^{16}$:

$$A = \begin{pmatrix} -7 & 36 & & \\ -1 & 0 & \ddots & \mathbf{0} \\ & \ddots & \ddots & 36 \\ \mathbf{0} & & -1 & 0 \end{pmatrix} \qquad f = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$



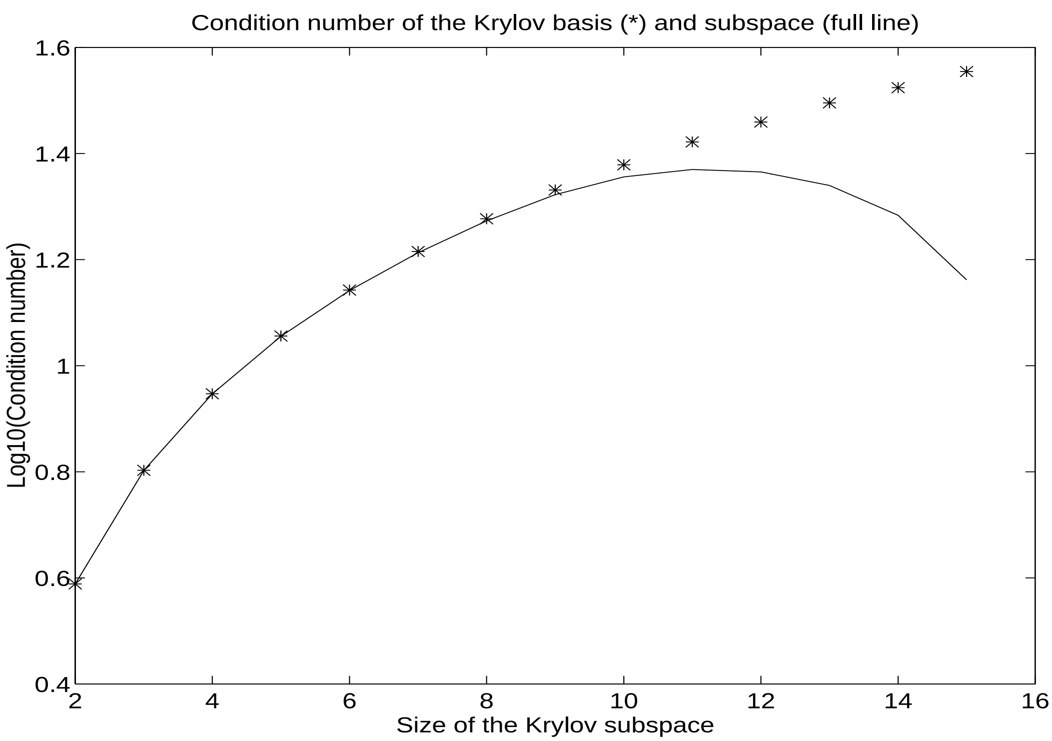
k	lower bound	$\mu_b\{\mathcal{K}_k(A,f)\}$	upper bound	$\mu\{\mathcal{K}_k(A,f)\}$	$(\|\Omega\|_2)_{mach}$
2	1.397e+02	1.397e+02	1.397e+02	1.397e+02	-0.0e+00
3	5.158e+03	5.158e+03	5.158e+03	5.158e+03	-0.0e+00
4	1.856e+05	1.856e+05	1.856e+05	1.856e+05	-0.0e+00
5	6.671e+06	6.671e+06	6.671e+06	6.671e+06	-0.0e+00
6	2.395e+08	2.395e+08	2.395e+08	2.395e+08	-0.0e+00
7	8.556e+09	8.573e+09	8.589e+09	8.573e+09	-0.0e+00
8	2.851e+11	3.045e+11	3.238e+11	3.045e+11	-0.0e+00
9	4.393e+11	4.924e+11	5.455e+11	4.304e+11	-0.0e+00
10	4.322e+11	4.924e+11	5.526e+11	1.691e+10	-0.0e+00
11	4.260e+11	4.924e+11	5.588e+11	5.755e+08	-0.0e+00
12	4.208e+11	4.924e+11	5.640e+11	1.847e+07	-0.0e+00
13	4.169e+11	4.924e+11	5.679e+11	5.737e+05	-0.0e+00
14	4.144e+11	4.924e+11	5.704e+11	1.746e+04	-0.0e+00
15	4.132e+11	4.924e+11	5.716e+11	5.225e+02	-0.0e+00

The condition number of the Krylov basis increases with its size, and becomes quickly bad. It is interesting to see that the condition number of the Krylov subspace increases first up to a large value then decreases.

6.2 Example 2

Let us now take the transposed of the previous matrix and the same vector :

$$A = \begin{pmatrix} -7 & -1 & & \\ 36 & 0 & \ddots & \text{\huge 0} \\ & \ddots & \ddots & -1 \\ \text{\huge 0} & & 36 & 0 \end{pmatrix} \in \mathbb{R}^{16\times 16} \quad \text{and} \quad f = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \in \mathbb{R}^{16}$$



size	lower bound	$\mu_b\{\mathcal{K}_k(A,f)\}$	upper bound	$\mu\{\mathcal{K}_k(A,f)\}$	$(\|\Omega\|_2)_{mach}$
2	3.879e+00	3.879e+00	3.879e+00	3.879e+00	-0.0e+00
3	6.349e+00	6.349e+00	6.349e+00	6.348e+00	-0.0e+00
4	8.856e+00	8.856e+00	8.856e+00	8.851e+00	-0.0e+00
5	1.138e+01	1.138e+01	1.138e+01	1.136e+01	3.4e-21
6	1.389e+01	1.389e+01	1.389e+01	1.386e+01	5.5e-21
7	1.641e+01	1.641e+01	1.641e+01	1.633e+01	7.7e-21
8	1.892e+01	1.892e+01	1.892e+01	1.875e+01	9.8e-21
9	2.144e+01	2.144e+01	2.144e+01	2.101e+01	1.1e-20
10	2.391e+01	2.391e+01	2.391e+01	2.269e+01	1.2e-20
11	2.642e+01	2.642e+01	2.642e+01	2.344e+01	1.2e-20
12	2.881e+01	2.881e+01	2.881e+01	2.319e+01	1.2e-20
13	3.130e+01	3.130e+01	3.130e+01	2.187e+01	1.2e-20
14	3.343e+01	3.343e+01	3.343e+01	1.922e+01	1.2e-20
15	3.586e+01	3.586e+01	3.586e+01	1.452e+01	1.2e-20

The only difference between this example and the previous is that we consider here the transposed matrix. But, as we can see in the tables the results are quite different. Here, the condition numbers of the Krylov basis and subspaces are always good.

7 Conclusion

We provide an algorithm to measure the sensitivity of the Krylov subspace and basis to a matrix perturbation. This tool will be very useful to understand unstabilities of a Krylov subspace or basis. We plan to use it on various examples and to analyze the results thoroughly. Another direction of study is to understand the links between the stability of the Krylov subspace and the convergence of iterative methods in linear algebra using these subspaces.

For example, this algorithm could be used in the future to validate the computation of an invariant subspace by the Arnoldi process.

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