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Numerical Analysis

On some matrix extrapolation methods

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Abstract

In the present Note we introduce new matrix extrapolation methods as a generalization of well known vector extrapolation methods. We give expressions of the obtained approximation via the Schur complement. We apply these methods to linearly generated sequences and give some theoretical results. ***To cite this article: K. Jbilou et al., C. R. Acad. Sci. Paris, Ser. I 341 (2005).***

Résumé

Sur des nouvelles méthodes d'extrapolation matricielle. Dans cette Note, nous introduisons de nouvelles méthodes d'extrapolation matricielle comme généralisation de certaines méthodes d'extrapolation vectorielle. Les approximations obtenues sont données sous forme de complément de Schur. Ces méthodes seront ensuite appliquées à des suites matricielles générées linéairement et des résultas théoriques sont proposés. ***Pour citer cet article : K. Jbilou et al., C. R. Acad. Sci. Paris, Ser. I 341 (2005).***

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Les transformations de suites vectorielles les plus connues sont la méthode MPE (Minimal Polynomial Extrapolation) de Cabay et Jackson [7], la méthode RRE (Reduced Rank Extrapolation) de Eddy [8] et Mesina [11] et la méthode MMPE (Modified Minimal Polynomial Extrapolation) de Sidi, Ford et Smith [15], Brezinski [1] et Pugatchev [12]. L'analyse et les procedures d'implémentation de ces méthodes d'extrapolation vectorielles sont présentées dans [4,9,10,14,15]. Une deuxième classe de transformations de suites vectorielles contient l'ϵ-algorithme topologique (TEA : Topological ϵ-Algorithm) de Brezinski [4,1] et l'ϵ-algorithme vectoriel (VEA : Vectorial ϵ-Algorithm) de Wynn [16]. Des généralisations de ces méthodes ont été données dans [5,2,3].

En utilisant les formules des compléments de Schur nous développons des généralisations de ces méthodes pour des suites de matrices. L'utilisation du complément de Schur permet de présenter ces méthodes de manière simple et pourra aider au developpement de nouveaux algorithmes pour l'implémentation des méthods proposées. Nous

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introduisons les versions par blocs de ces méthodes d'extrapolation vectorielle et nous montrons comment les appliquer pour résoudre des systèmes linéaires à plusieurs seconds membres. Nous montrons aussi que ces méthodes, lorsqu'elles sont appliquées à des suites de matrices générées linéairement, sont des méthodes des sous-espaces de Krylov par blocs et qu'elles sont mathématiquement équivalentes à des méthodes connues [2,13]. Dans la Section 2, nous introduisons les méthodes d'extrapolation par blocs Bl-RRE, Bl-MPE et Bl-MMPE. Nous verrons aussi comment appliquer ces méthodes à des suites de matrices générées linéairement, et montrer, dans ce cas, que les approximations produites sont les mêmes que celles produites par des méthodes connues des sous-espaces de Krylov par blocs. Dans la Section 3, nous définissons l'ϵ-transformation topologique par blocs.

Comme toutes ces transformations peuvent être exprimées sous forme de compléments de Schur, nous allons d'abord rappeler la définition de ces derniers [6,17]. Si M est la matrice partitionnée comme suit : $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$, alors le complément de Schur de D dans M, où la matrice D est supposée une matrice carrée et inversible, est donné par $(M/D) = A - BD^{-1}C$.

1. Introduction

The well known vector sequence transformations methods are the minimal polynomial extrapolation (MPE) method of Cabay and Jackson [7], the reduced rank extrapolation (RRE) method of Eddy [8] and Mesina [11] and the modified minimal polynomial extrapolation (MMPE) method of Sidi, Ford and Smith [15], Brezinski [1] and Pugatchev [12]. Analysis and computational procedures of these vector extrapolation methods could be found in [4,9,10,14,15]. A second class of vector sequence transformations contains the topological ϵ-algorithm (TEA) of Brezinski [4,1] and the vector ϵ-algorithms (VEA) of Wynn [16]. Block generalizations of these methods are given in [5,2,3].

Using the Schur complement formulae, we develop the generalizations of these methods for matrix sequences. The use of the Schur complement simplifies of the presentation of the proposed methods and could be used to develop algorithms for their implementation. We introduce block versions of these vector extrapolation methods and show how to apply them for solving linear systems of equations with multiple right-hand sides. We also show that when applied to linearly generated matrix sequences, these block extrapolation methods are block Krylov subspace methods and are mathematically equivalent to some known block Krylov subspace methods [2,13].

This Note is organized as follows. In Section 2, we introduce the polynomial block extrapolation methods Bl-RRE, Bl-MPE and Bl-MMPE. We will also see how these methods could be applied for linearly generated matrix sequences and show in this case that the approximations produced by these block extrapolation methods are the same as those produced by well known block Krylov subspace methods. In Section 3 we define the block topological ϵ-transformation. As all of these transformations could be expressed as a Schur complement, we will recall the definition of the Schur complement [6,17]. If M is the matrix partitioned as $M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$, then the Schur complement of D in M, where D is square and nonsingular, is given by $(M/D) = A - BD^{-1}C$.

2. The block extrapolation methods

2.1. The polynomial block extrapolation methods

Let (S_n) be a sequence of matrices of $\mathbb{R}^{N \times s}$ and consider the transformation T_k from $\mathbb{R}^{N \times s}$ to $\mathbb{R}^{N \times s}$ defined by

$$T_k : S_n \to T_k^{(n)} = S_n + \sum_{i=1}^{k} G_i(n) A_i^{(n)}, \quad n \geqslant 0 \tag{1}$$

where the auxiliary $N \times s$ matrix sequences $(G_i(n))_n$; $i = 1, \ldots, k$ are given and the $s \times s$ coefficients $A_i^{(n)}$ will be determined. Let $\widetilde{T}_k$ denotes the new transformation obtained from T_k as follows

$$\widetilde{T}_k^{(n)} = S_{n+1} + \sum_{i=1}^{k} G_i(n+1) A_i^{(n)}, \quad n \geqslant 0. \tag{2}$$

We define the generalized residual of $T_k^{(n)}$ by $\widetilde{R}(T_k^{(n)}) = \widetilde{T}_k^{(n)} - T_k^{(n)}$ also given by

$$\widetilde{R}\big(T_k^{(n)}\big) = \Delta S_n + \sum_{i=1}^{k} \Delta G_i(n) A_i^{(n)}.$$

The forward difference operator Δ acts on the index n, i.e., $\Delta G_i(n) = G_i(n+1) - G_i(n)$, $i = 1, \ldots, k$. We will see later that when solving linear systems of equations, the sequence $(S_n)_n$ is generated by a linear process and then the generalized residual coincides with the classical residual. The matrix coefficients $A_i^{(n)}$ are obtained from the orthogonality relation

$$\widetilde{R}\big(T_k^{(n)}\big) \in \operatorname{span}\big\{Y_1^{(n)}, \ldots, Y_k^{(n)}\big\}^{\perp} \tag{3}$$

where $Y_1^{(n)}, \ldots, Y_k^{(n)}$ are given $N \times s$ matrices. If $\widetilde{\mathcal{W}}_{k,n}$ and $\tilde{\mathcal{L}}_{k,n}$ denote the block subspaces $\widetilde{\mathcal{W}}_{k,n} = \operatorname{span}\{\Delta G_1(n), \ldots, \Delta G_k(n)\}$ (the subspace generated by the columns of $\Delta G_1(n), \ldots, \Delta G_k(n)$) and $\tilde{\mathcal{L}}_{k,n} = \operatorname{span}\{Y_1^{(n)}, \ldots, Y_k^{(n)}\}$ (generated by the columns of $Y_1^{(n)}, \ldots, Y_k^{(n)}$), then from (2) and (3), the generalized residual satisfy the following relations

$$\widetilde{R}\big(T_k^{(n)}\big) - \Delta S_n \in \widetilde{\mathcal{W}}_{k,n} \tag{4}$$

and

$$\widetilde{R}\big(T_k^{(n)}\big) \in \tilde{\mathcal{L}}_{k,n}^{\perp}. \tag{5}$$

The relations (4) and (5) show that the generalized residual $\widetilde{R}(T_k^{(n)})$ is obtained by projecting, orthogonally to $\tilde{\mathcal{L}}_{k,n}$, the columns of the matrix ΔS_n onto the block subspace $\widetilde{\mathcal{W}}_{k,n}$. In a matrix form, $\widetilde{R}(T_k^{(n)})$ can be written as $\widetilde{R}(T_k^{(n)}) = \Delta S_n - \Delta\mathcal{G}_{k,n}(L_{k,n}^{\mathrm{T}} \Delta\mathcal{G}_{k,n})^{-1} L_{k,n}^{\mathrm{T}} \Delta S_n$, where $\Delta\mathcal{G}_{k,n}$ and $L_{k,n}$ are the $N \times ks$ matrices generated by the columns of the matrices $\Delta G_1(n), \ldots, \Delta G_k(n)$ and $Y_1^{(n)}, \ldots, Y_k^{(n)}$ respectively. The approximation $T_k^{(n)}$ is given by

$$T_k^{(n)} = S_n - \mathcal{G}_{k,n}\big(L_{k,n}^{\mathrm{T}} \Delta\mathcal{G}_{k,n}\big)^{-1} L_{k,n}^{\mathrm{T}} \Delta S_n, \tag{6}$$

where $\mathcal{G}_{k,n}$ is the $N \times ks$ block matrix $\mathcal{G}_{k,n} = [G_1(n), \ldots, G_k(n)]$. Note that $T_k^{(n)}$ is well defined if and only if the $ks \times ks$ matrix $L_{k,n}^{\mathrm{T}} \Delta\mathcal{G}_{k,n}$ is nonsingular. Let $\mathcal{T}_{k,n}$ be the matrix given by

$$\mathcal{T}_{k,n} = \begin{pmatrix} S_n & \mathcal{G}_{k,n} \\ L_{k,n}^{\mathrm{T}} \Delta S_n & L_{k,n}^{\mathrm{T}} \Delta\mathcal{G}_{k,n} \end{pmatrix}. \tag{7}$$

The approximation $T_k^{(n)}$ is then expressed as a Shcur complement

$$T_k^{(n)} = \big(\mathcal{T}_{k,n} / L_{k,n}^{\mathrm{T}} \Delta\mathcal{G}_{k,n}\big). \tag{8}$$

If we set $G_i(n) = \Delta S_{n+i-1}$; $i = 1, \ldots, k$ and $Y_i(n) = \Delta G_i(n)$; $i = 1, \ldots, k$ we obtain the block Reduced Rank Extrapolation (Bl-RRE) method. In this case, the approximation $T_k^{(n)}$ is given by

$$T_{k,\text{Bl-RRE}}^{(n)} = \big(\mathcal{T}_{k,n} / \Delta\mathcal{G}_{k,n}^{\mathrm{T}} \Delta\mathcal{G}_{k,n}\big).$$

If $G_i(n) = \Delta S_{n+i-1}$; $i = 1, \ldots, k$ and $Y_i(n) = G_i(n)$; $i = 1, \ldots, k$ we get the block Minimal Polynomial Extrapolation (Bl-MPE) method.

Finally if $G_i(n) = \Delta S_{n+i-1}$; $i = 1, \ldots, k$ and $Y_i(n) = Y_i$; $i = 1, \ldots, k$ (arbitrary $N \times s$ matrices) we obtain the block Modified Minimal Polynomial Extrapolation (Bl-MMPE) method.

Note that if the $N \times ks$ matrix $\Delta\mathcal{G}_{k,n}$ is of full rank the approximations produced by the Bl-RRE method are well defined while those generated by the Bl-MPE and Bl-MMPE methods may not exist. As Bl-RRE is an orthogonal projection method, the corresponding generalized residual satisfies the following minimization property $\|\widetilde{R}(T_{k,\text{Bl-RRE}}^{(n)})\|_F = \min_{Z \in \tilde{W}_{k,n}} \|\Delta S_n - Z\|_F$; where $\|X\|$ denotes the Frobenius norm of X.

2.2. *The block topological ϵ-transformation*

In [1], Brezinski proposed a generalization of the scalar ϵ-algorithm [13] for vector sequences called the topological ϵ-algorithm (TEA). In this section we introduce the block topological ϵ-transformation (Bl-TET).
We consider approximations $E_k(s_n) = T_k^{(n)}$ of the limit or the anti-limit of the sequence (S_n) such that

$$T_k^{(n)} = S_n + \sum_{i=1}^{k} \Delta S_{n+i-1} A_i^{(n)}, \quad n \geqslant 0. \tag{9}$$

We introduce the new transformation $\widetilde{T}_{k,j}$, $j = 1, \ldots, k$ defined by

$$\widetilde{T}_{k,j}^{(n)} = S_{n+j} + \sum_{i=1}^{k} \Delta S_{n+i+j-1} A_i^{(n)}, \quad j = 1, \ldots, k. \tag{10}$$

We set $\widetilde{T}_{k,0}^{(n)} = T_k^{(n)}$ and define the j-th generalized residual as follows

$$\widetilde{R}_j\big(T_k^{(n)}\big) = \widetilde{T}_{k,j}^{(n)} - \widetilde{T}_{k,j-1}^{(n)}.$$

Therefore the coefficients involved in the expression (10) of $T_k^{(n)}$ are computed such that each j-th generalized residual is orthogonal to some chosen $N \times s$ matrix Y, that is

$$Y^{\mathrm{T}} \widetilde{R}_j\big(T_k^{(n)}\big) = 0; \quad j = 1, \ldots, k. \tag{11}$$

Let $\mathcal{D}_{k,n}$ denotes the following matrix

$$\mathcal{D}_{k,n} = \begin{bmatrix} Y^{\mathrm{T}}\Delta^2 S_n & Y^{\mathrm{T}}\Delta^2 S_{n+1} & \cdots & Y^{\mathrm{T}}\Delta^2 S_{n+k-1} \\ Y^{\mathrm{T}}\Delta^2 S_{n+1} & Y^{\mathrm{T}}\Delta^2 S_{n+2} & \ddots & Y^{\mathrm{T}}\Delta^2 S_{n+k} \\ \vdots & \vdots & \ddots & \vdots \\ Y^{\mathrm{T}}\Delta^2 S_{n+k-1} & Y^{\mathrm{T}}\Delta^2 S_{n+k} & \cdots & Y^{\mathrm{T}}\Delta^2 S_{n+2k-2} \end{bmatrix} \tag{12}$$

we also define the matrices $A_n = [(A_1^{(n)})^{\mathrm{T}}, \ldots, (A_k^{(n)})^{\mathrm{T}}]^{\mathrm{T}}$ and $Z_n = [(Y^{\mathrm{T}}\Delta S_n)^{\mathrm{T}}, \ldots, (Y^{\mathrm{T}}\Delta S_{n+k-1})^{\mathrm{T}}]^{\mathrm{T}}$. Then the relation (11) can be written as follows

$$\mathcal{D}_{k,n} A_n = -Z_n.$$

If the block matrix $\mathcal{D}_{n,k}$ is nonsingular then $A_n = -\mathcal{D}_{k,n}^{-1} Z_n$ and hence the matrix coefficients $A_1^{(n)}, \ldots, A_k^{(n)}$ are uniquely defined. In this case, the approximation $T_k^{(n)}$ exists, is unique and can be expressed by

$$T_k^{(n)} = S_n - \Delta\mathcal{S}_{k,n} \mathcal{D}_{k,n}^{-1} Z_n \tag{13}$$

where $\Delta\mathcal{S}_{k,n} = [\Delta S_n, \ldots, \Delta S_{n+k-1}]$. We can also express $T_k^{(n)}$ as the following Schur complement

$$T_k^{(n)} = (\mathcal{M}_{k,n}/\mathcal{D}_{k,n}) \quad \text{where } \mathcal{M}_{k,n} = \begin{bmatrix} S_n & \Delta\mathcal{S}_{k,n} \\ Z_n & \mathcal{D}_{k,n} \end{bmatrix}.$$

An interesting point will be to develop recursive algorithms for the block extrapolation methods defined in this note. This work is under investigation.

3. Application to linear systems with multiple right hand sides

Consider the multiple linear system of equations

$$AX = B \tag{14}$$

where A is a real $N \times N$ nonsingular matrix, B is a matrix of $\mathbb{R}^{N\times s}$ and X^* denotes the unique solution of (14). Starting from an initial guess S_0, we construct the sequence $(S_n)_n$ by

$$S_{n+1} = CS_n + B; \quad n = 0, 1, \ldots \tag{15}$$

with $C = I - A$. Note that if the sequence (S_n) is convergent, it's limit $S = X^*$ is the solution of the multiple linear system (14). From (15) we have $\Delta S_n = B - A\,S_n = R(S_n)$ the residual of the vector S_n. Therefore using (3) and (15), it follows that the generalized residual of the approximation $T_k^{(n)}$ becomes the true residual $\widetilde{R}(T_k^{(n)}) = R(T_k^{(n)})$. Note also that since $\Delta^2 S_n = -A\,\Delta S_n$ we have $\Delta\mathcal{G}_{k,n} = -A\,\mathcal{G}_{k,n}$. For simplicity and until specified, we shall set $n = 0$, denote $T_k^{(0)} = X_k$ and drop the index n in all our notations. When applied to the sequence generated by (15), the block extrapolation methods above produce approximations X_k such that the corresponding residuals $R_k = B - A\,X_k$ satisfy the relations

$$X_k^i - X_0^i \in \widetilde{\mathcal{W}}_k = A\widetilde{\mathcal{V}}_k \quad \text{and} \quad R_k^i \perp \tilde{\mathcal{L}}_k; \quad i = 1, \ldots, s$$

where R_k^i is the i-th column of R_k. Remark that $\widetilde{\mathcal{V}}_k = \mathcal{K}_k(A, R_0)$, ($\mathcal{K}_k(A, R_0)$ is the block Krylov subspace generated by the columns of the matrices $R_0, AR_0, \ldots, A^{k-1}R_0$) and $\widetilde{\mathcal{W}}_k = \mathcal{K}_k(A, AR_0)$. Then we have $\tilde{\mathcal{L}}_k \equiv \widetilde{\mathcal{W}}_k$ for Bl-RRE, $\tilde{\mathcal{L}}_k \equiv \widetilde{\mathcal{V}}_k$ for Bl-MPE and $\tilde{\mathcal{L}}_k \equiv \widetilde{Y}_k = \text{span}\{Y_1, \ldots, Y_k\}$ for Bl-MMPE where $Y_1, \ldots, Y_k$ are chosen $N \times s$ matrices.

Theorem 3.1. *When applied to linearly matrix sequences, the Bl-RRE, the Bl-MPE are block Krylov subspace methods and are mathematically equivalent to the block GMRES and the block FOM methods respectively.*

The acute angle $\theta_{k,i}$; $i = 1, \ldots, s$ between R_0^i and the block Krylov subspace $\widetilde{\mathcal{W}}_k$ is defined by

$$\cos\theta_{k,i} = \max_{z \in \widetilde{\mathcal{W}}_k - \{0\}} \left(\frac{|(R_0^i, z)|}{\|R_0^i\|_2 \|z\|_2} \right).$$

In the following theorem, we give some relations satisfied by the residual norms.

Theorem 3.2. *Let $\theta_{k,i}$ be the acute angle between R_0^i and $\widetilde{\mathcal{W}}_k$; $i = 1, \ldots, s$ and let $\phi_{k,i}$ denote the acute angle between R_0^i and $\mathcal{Q}_k\,R_0^i$; $i = 1, \ldots, s$ where $\mathcal{Q}_k$ is the oblique projector onto $\mathcal{K}_k(A, AR_0)$ and orthogonally to $\mathcal{K}_k(A, R_0)$. Then we have the following relations*

(1) $\|R_k^{\text{Bl-RRE}}\|_F^2 = \sum_{i=1}^s (1 - \cos^2\theta_{k,i})\|R_0^i\|_2^2$.
(2) $\|R_k^{\text{Bl-MPE}}\|_F^2 = \sum_{i=1}^s \tan^2\phi_{k,i}\|R_0^i\|_2^2$.
(3) $\|R_k^{\text{Bl-RRE}}\|_F^2 \leqslant (1 - \cos^2\theta_k)\|R_0\|_F^2$ *and* $\|R_k^{\text{Bl-MPE}}\|_F^2 \leqslant \tan^2\phi_k\|R_0\|_F^2$

where $\theta_k = \max_{1 \leqslant i \leqslant s}\theta_{k,i}$ *and* $\phi_k = \max_{1 \leqslant i \leqslant s}\phi_{k,i}$.

Let us apply now the block ϵ-transformation to the sequence (S_n) generated by the linear process (15). Using the fact that $\Delta^2 S_{n+i} = (I - A)\Delta^2 S_{n+i-1}$ and $\Delta^2 S_{n+i} = -A\Delta S_{n+i-1}$; $i = 1, \ldots, k$, the matrix $\mathcal{D}_{k,n}$ defined by (12) has now the following expression

$$\mathcal{D}_{k,n} = -\mathcal{L}_k^{\mathrm{T}} A \Delta\mathcal{S}_{k,n} \tag{16}$$

where $\mathcal{L}_k$ is the $N \times ks$ matrix whose block columns are $Y, C^{\mathrm{T}}Y, \ldots, C^{\mathrm{T}^{k-1}}Y$ with $C = I - A$. As n will be a fixed integer, we set $n = 0$ for simplicity and denote $\mathcal{D}_{k,0}$ by $\mathcal{D}_k$ and $\Delta\mathcal{S}_{k,0}$ by $\Delta\mathcal{S}_k$. On the other hand, it is not difficult to see that

$$Z_0 = \mathcal{L}_k^{\mathrm{T}} \Delta S_0. \tag{17}$$

Setting $X_0 = S_0$ and using the relations (13), (16) and (17), the approximation $X_k^{\text{Bl-TET}} = T_k^{(0)}$ is given by

$$X_k^{\text{Bl-TET}} = X_0 + \Delta\mathcal{S}_k \big(\mathcal{L}_k^{\mathrm{T}} A \Delta\mathcal{S}_k\big)^{-1} \mathcal{L}_k^{\mathrm{T}} R_0$$

where $R_0 = B - AX_0 = \Delta S_0$ and $\Delta\mathcal{S}_k = -[AR_0, A^2R_0, \ldots, A^{k-1}R_0]$. The k-th residual produced by Bl-TET is given as

$$R_k^{(\mathcal{L}_k^{\mathrm{T}} A \Delta\mathcal{S}_k)} = R_0 - A\,\Delta\mathcal{S}_k \left(\mathcal{L}_k^{\mathrm{T}} A \Delta\mathcal{S}_k\right)^{-1} \mathcal{L}_k^{\mathrm{T}} R_0.$$

Note that the k-th approximation defined by Bl-TET is uniquely defined iff the $ks \times ks$ matrix $\mathcal{L}_k^{\mathrm{T}} A \Delta\mathcal{S}_k$ is nonsingular.

Theorem 3.3. *When applied to linearly generated sequences, Bl-TET is a block Krylov subspace method and is mathematically equivalent to the block Lanczos method.*

The following result gives an expression of the residual norm in the case where $Y = R_0$.

Theorem 3.4. *Let $\varphi_{k,i}$ be the acute angle between R_0^i and $\mathcal{F}_k R_0^i$; $i = 1, \ldots, s$ where $\mathcal{F}_k$ denotes the oblique projector onto $\mathcal{K}_k(A, AR_0)$ and orthogonally to $\mathcal{K}_k(A^{\mathrm{T}}, Y)$. If $Y = R_0$, then we have*

$$\|R_k^{\text{Bl-TET}}\|_F^2 = \sum_{i=1}^{s}\left(\tan^2 \varphi_{k,i}\right)\|R_0^i\|_2^2.$$

Note that in practice, extrapolation methods as compared to Krylov subspace methods are quit difficult to implement for large linear systems.

4. Conclusion

We have presented in this Note new block extrapolations methods. We applied these block methods to matrix sequences generated by a linear process and show that, in this case, these methods are theoretically equivalent to some well known Krylov subspace methods. However, in practice the above extrapolation methods could not be applied for large linear systems and new algorithms for their computation are needed. This work is under investigation.

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