Vector Padé approximants and the Lanczos method for solving a system of linear equations

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Abstract
In the present paper we solve a system of linear equations by using the vectorPadé approximants of a matrix series. The connection with the Lanczos methodand the oblique projections on Krylov subspaces is made.
Key words : Lanczos method, vector orthogonal polynomials, vector Padé approximants, minimal polynomial, biorthogonality.

Introduction
The vector Padé approximants considered in this paper are those defined by Van Iseghem in [14]. Their definition and properties will be summarized in the section 1. Let us consider the function $F(z) = \sum_{n \geq 0} z^n A^n X_0$ from C to C^d where A is a square $d \times d$ matrix and $X_0 \in C^d$. For z small enoughwe have $F(z) = (I - zA)^{-1} X_0$. This function is rational and thus, some of the vector Padé approximants of the series will be identical to the series itself [9].On the other hand, the vector $(I - zA)^{-1} X_0$ is the solution of the linear system $X = zAX + X_0$. The vector Padé approximants of the series can be computed recursively, that gives a way to obtain the solution of the previous system. This method is related to a generalization to the vector case of the Shanks transform [13].Recently, Brezinski [4] generalized the method of moments of Vorobyev [15] and gave some generalizations of the Lanczos method for solving system of linear equations. The aim of this paper is to show the connection between the vector Padé approximants and the projections on Krylov subspaces. The vector orthogonal polynomials associated to the function $z \mapsto (I - zA)^{-1} X_0$ can be seen as the minimal polynomials of nonderogatory linear mappings into Krylov subspaces.This paper is organized as follows. In section 1 we deal with the linear system $X = AX + X_0$. We show how to solve it by using vector Padé approximants of the resolvent of A applied to the vector X_0. In section 2 we prove that a Lanczos type method is obtained by using vector orthogonal polynomials. Finally, the section 3 contains remarks about the different assumptions made before. Particularly, we make clearly the link between the Lanczos type method and the oblique projections on Krylov subspaces.

1 Vector Padé approximants of $z \mapsto (I - zA)^{-1}\ X_0$.

The notations are as follows.If p *and* q are two integers, $[p:q]$ is the integer part of $[\frac{p}{q}]$.$[p,q] = \frac{P}{Q}$ is the vector Padé approximant of degree (p,q) of the power series F, with coefficients in C^d, i.e we have

$$P = (P_1, \dots, P_d),$$

$$all\ P_i\ are\ polynomials\ of\ degree\ p,$$

$$Q\ is\ a\ polynomial\ of\ degree\ q,\ and$$

$$F(z) - [p,q]_F(z) = O(z^{p\ +\ [q\ :\ d]\ +\ 1}). \tag{1}$$

The polynomial $\widetilde{P}_r^s$ (i.e $\widetilde{P}_r^s = x^r P_r^s(\frac{1}{x})$ is the denominator of the vector Padé approximant $[r+s-1/r]$ (we assume of course, that the generalized Hankel's determinant [12] doesn't vanish).Let us now consider a linear operator A of C^d. If necessary, we will identify A to its matrix, still denoted by A, in the canonical basis of C^d.

1.1

Let F be the function $z \mapsto (I - zA)^{-1}\ X_0$. We assume that

$$the\ Krylov\ subspace\ span\left(X_0, AX_0, \dots, A^{d\ -\ 1}X_0\right)\ is\ equal\ to\ C^d.$$

It was proved in [9] that P_d^0 exists and is unique, and

$$P_d^0 = \Pi_A = P_A = \Pi_{A,X_0}$$

where Π_A is the minimal polynomial of A, P_A is the characteristic polynomial of A, Π_{A,X_0} is the minimal polynomial of A for the vector X_0, and P_d^0 is the vector orthogonal polynomial associated with the vector Padé approximant $[d-1/d]_F$. Moreover, since $s = 0$, we have even if A is singular

$$(I - zA)^{-1}X_0 = [d-1/d]_F(z). \tag{2}$$

Indeed we have

$$[d-1/d]_F(z) = \frac{\sum_{j=1}^d \alpha_j z^{d-j} \sum_{k=0}^{j-1} \Gamma_k z^k}{\alpha_0 z^d + \cdots + \alpha_d} \tag{3}$$

$(\Gamma_k = A^k X_0\ and\ the\ \alpha_i's\ are\ the\ coefficients\ of\ P_d^0)$.
But

$$\begin{aligned}
\sum_{j=1}^{d} \alpha_j z^{d-j} (\sum_{k \geq j} \Gamma_k z^k) &= \sum_{j=1}^{d} \alpha_j z^{d-j} (\sum_{k \geq 0} \Gamma_{k+j} z^{k+j}) &(4)\\
&= z^d (\sum_{j=1}^{d} \alpha_j A^j)(\sum_{k \geq 0} \Gamma_k z^k) &(5)\\
&= z^d(-\alpha_0)(I - zA)^{-1} X_0 &(6)
\end{aligned}$$

and thus

$$(I - zA)^{-1}X_0 = \frac{\sum_{j=0}^{d} \alpha_j z^{d-j}(\sum_{k\geq 0} \Gamma_k z^k)}{\sum_{j=0}^{d} \alpha_j z^{d-j}} \quad (7)$$

$$= \frac{\sum_{j=1} \alpha_j z^{d-j}(\sum_{k\geq 0} \Gamma_k z^k) \; - \; \alpha_0 z^d (I - zA)^{-1}X_0}{\sum_{j=0}^{d} \alpha_j z^{d-j}} \quad (8)$$

$$= \frac{\sum_{j=1}^{d} \alpha_j z^{d-j}(\sum_{k=0}^{j-1} \Gamma_k z^k)}{\sum_{j=0}^{d} \alpha_j z^{d-j}} \quad (9)$$

$$= [d - 1/d]_F(z). \quad (10)$$

Remark 1.1 *If I-A is nonsingular, we get*

$$(I - A)^{-1}X_0 = [d - 1/d]_F(1) = Q_{d-1}(A)X_0 \quad (11)$$

where Q_{d-1} is the polynomial of degree $d - 1$ defined by

$$1 - \frac{P_d^0(t)}{P_d^0(1)} = (1 - t)Q_{d-1}(t)$$

(clearly $\sum_{j=1}^{d} \alpha_j(\sum_{k=0}^{j-1} A^k) = \sum_{j=0}^{d-1}(\sum_{k=j+1}^{d} \alpha_j)A^j$ and$Q_{d-1}(t) = \frac{\sum_{j=1}^{d-1}(\sum_{k=j+1}^{d} \alpha_k t^j}{\alpha_0+\alpha_1+\cdots+\alpha_d}$).

1.2

More generally, let r be an integer smaller or equal to d, the dimensionof the space. Let us assume that

$$span(X_0, AX_0, \ldots, A^{r-1}X_0) = span(e_1, \ldots, e_r) = E_r, \; (e_i)_{i=1}^{d} \; being \; the \; canonical \; basis \; of C^d.$$

According to [9], the vector Padé approximant $[r - 1/r]_F(z)$ of $F(z) = (I - zA)^{-1}X_0$ exists and is unique. Its generating polynomial, i.e P_r^0, is the characteristic polynomial of the operator $A_r = \delta_r A$ restricted to the subspace E_r (δ_r denotes the orthogonal projection operator on E_r). The operator A_r is the operator which appears in the moments method (see [15]). Moreover, we have

$$[r - 1/r]_F(z) = (I_r - zA_r)^{-1}X_0 \quad (12)$$

(I_r is the identity operator of E_r). Indeed, after noticing that

$$A_r^k = A^k for \; k = 0, \ldots, r - 1,$$

we work on E_r and apply the result of the section 1.1 which is true for every finite space, and for every nonderogatory operator.
If $I - A$ is nonsingular, when we are allowed to choose z=1 and the remark 1.1 is still valid with, of course, r replacing d.

Remark 1.2 *If, for example, we assume that*

$$span(X_0, AX_0, \ldots, A^{r-1}X_0) = \ span(e_1, \ldots, e_r) \ for \ all \ r, r = 1 \ to \ d,$$

the canonical basis should mean the Gram-Schmidt basis.

We have now to see for which condition $P_r^0(1)$ doesn't vanish. Let us give the following condition

Lemma 1.1 *Let B be an operator of C^d and $X_0 \in C^d$.*
Let us assume that

$$span(X_0, BX_0, \ldots, B^{r-1}X_0) = E_r.$$

Then the operator B_r, i.e $\delta_r B$ restricted to E_r, is nonsingular if and only if

$$\begin{vmatrix} (X_0, BX_0) & \ldots & (X_0, B^r X_0) \\ \vdots & & \vdots \\ (B^{r-1}X_0, BX_0) & \ldots & (B^{r-1}X_0, B^r X_0) \end{vmatrix} \neq 0 \tag{13}$$

Proof
Let $X = \sum_{i=0}^{r-1} x_i B^i X_0 \in E^r$, then we have $BX = \sum_{i=0}^{r-1} x_i B^{i+1} X_0$.
Thus $\delta_r(BX) = 0$ if and only if

$$for \ k = 0, \ldots, r-1 \ \ (B^k X_0, BX) = 0,$$

i.e

$$\forall k \in \{0, \ldots, r-1\} \ \ \sum_{i=0}^{r-1} x_i (B^k X_0, B^{i+1} X_0) = 0.$$

B_r, operator de E_r, is then nonsingular if and only if the linear system

$$\sum_{i=0}^{r-1} x_i (B^k, B^{i+1}), \ k = 0, \ldots, r-1$$

is a nonsingular system and so we have the condition of the lemma. We need also

Lemma 1.2 *Let B be an operator of C^d and $X_0 \in C^d$.*
Let us assume that the vectors $X_0, BX_0, \ldots, B^{r-1}X_0$ are linearly independent. Then

$$span(X_0, BX_0, \ldots, BX^{r-1}X_0) = span(X_0, (I-B)X_0, \ldots, (I-B)^{r-1}X_0).$$

Proof
The proof is quite trivial by virtue of the binomial formula.Let us denote by A_r the operator $\delta_r A$ restricted to E_r. By using the lemma 1.1 and the lemma 1.2, we obtain finally the

Theorem 1.1 *Let A be an operator of C^d and $X_0 \in C^d$. Let us asumme that*

$$span(X_0, AX_0, \ldots, A^{r-1}X_0) = E_r.$$

The generating polynomial P_r^0 of $[r-1/r]_F$ is also the characteristic polynomial of A_r.If

$$\begin{vmatrix} (X_0,(I-A)X_0 & \dots & (X_0,(I-A)^r X_0) \\ \vdots & & \vdots \\ ((I-A)^{r-1}X_0,(I-A)X_0) & \dots & ((I-A)^{r-1}X_0,(I-A)^r X_0) \end{vmatrix} \neq 0 \tag{14}$$

then $P_r^0(1) \neq 0$ (i.e $I_r - A_r$ is nonsingular) and if Q_{r-1} denotes the polynomial defined by

$$1 - \frac{P_r^0(t)}{P_r^0(1)} = (1-t)Q_{r-1}(t),$$

then

$$\begin{aligned} (I_r - A_r)^{-1}X_0 &= [r-1/r]_F(1) && (15) \\ &= Q_{r-1}(A_r)X_0 && (16) \\ &= Q_{r-1}(A)X_0. && (17) \end{aligned}$$

1.3

Let us give the following example

$$A = \begin{pmatrix} 1 & 3 & 1 \\ 1 & 2 & 4 \\ 0 & 1 & 1 \end{pmatrix},\ X_0 = (1,0,0)^T.$$

We have

$$(I-A)^{-1}X_0 = (4,0,-1)^T,\ AX_0 = (1,1,0)^T, A^2X_0 = (4,3,1)^T,$$
$$A^3X_0 = (14,14,4)^T,\ A^4X_0 = (80,58,18)^T.$$

It is easy to see that the assumptions of the theorem 1.1 are satisfied. By using directly the determinantal expressions of the vector Padé approximants (see [14]), we obtain

$$[0/0](t) = (1,0,0)^T \tag{18}$$

$$[1/0](t) = (1+t,t,0)^T \tag{19}$$

$$[1/1](t) = \left(\frac{3t-1}{4t-1}, \frac{-t}{4t-1}, 0\right)^T \tag{20}$$

$$[1/2](t) = \left(\frac{-2t+1}{-t^2-3t+1}, \frac{t}{-t^2-3t+1}, 0\right)^T \tag{21}$$

$$[2/1](t) = \left(\frac{-t^2+5t-2}{7t-2}, \frac{t^2-2t}{7t-2}, \frac{-2t^2}{7t-2}\right)^T \tag{22}$$

$$[2/2](t) = \left(\frac{10t^2+5t-2}{14t^2-1}, \frac{-3t^2-t}{14t^2-1}, \frac{-t^2}{14t^2-1}\right)^T \tag{23}$$

$$[3/2](t) = \left(\frac{-20t3-12t^2-19t+14}{-14t^2-26t+14}, \frac{6t^3-5t^2+14t}{-14t^2-26t+14}, \frac{2t^3+14t^2}{-14t^2-26t+14}\right)^T \tag{24}$$

$$[2/3](t) = \left(\frac{2t^2+3t-1}{-4t^3+2t^2+4t-1}, \frac{t^2-t}{-4t^3+2t^2+4t-1}, \frac{-t^2}{-4t^3+2t^2+4t-1}\right)^T \tag{25}$$

and

$$[2/3](1) = (4, 0, -1)^T.$$

Remark 1.3 *The vector Padé approximants can be also computed by using the generalizedcross rule (see [11]). Numerical examples using this rule can be found in [13].*
In the generalized cross rule, determinants of dimension d occur. Thus, it will be difficult to compute them when d increases. Other algorithms can be used to compute the vector Padé approximants (see [5]). Let us mention for example, the recursive projection algorithm (R.P.A). The same problem of implementation occurs in the initialization of the vector Q.D algorithm ([12]) (in [9], an initialization using the R.P.A is given).

2 The Lanczos method.

2.1

Let us now consider the linear system $AX = X_0$ (A is nonsingular). It can be written as $(I - B)X = X_0$ with $B = I - A$.
First of all, let us give the following result

Lemma 2.1 *Let Π_A be the minimal polynomial of A and Π_B be the minimal polynomial of B.*

$$If\ \ B = I - A,\ \ then\ \Pi_B(x) = \Pi_A(1 - x). \tag{26}$$

This result remains true if we consider the characteritic polynomials or the minimal polynomials for a vector.

Proof
This result comes from the Jordan decomposition of the matrix A and from the notion of elementary polynomials, after having noticed that the spectrum of B is the set $\{1 - \lambda / \lambda\ eigenvalue\ of\ A\}$ (see [7]).We have now the

Theorem 2.1 *Let A be a linear operator of C^d and $X_0 \in C^d$. Let us denote by A_r the operator $\delta_r A$ restricted to $E_r = span(e_1, \ldots, e_r)$.*
Let us assume that

$$span(X_0, AX_0, \ldots, A^{r-1}X_0) = E_r$$

and

$$\begin{vmatrix} (X_0, AX_0) & \ldots & (X_0, A^r X_0) \\ \vdots & & \vdots \\ (A^{r-1}X_0, AX_0) & \ldots & (A^{r-1}X_0, A^r X_0) \end{vmatrix} \neq 0.$$

Then A_r is nonsingular and the solution of the system $\delta_r AX = X_0,\ X \in E_r$ is

$$X = V_{r-1}(A)X_0, \tag{27}$$

where V_{r-1} is the polynomial defined by the relation

$$1 - \frac{P_r^x}{P_r^0} = xV_{r-1}(x) \tag{28}$$

with P_r^0 *the generating polynomial of the vector Padé approximant* $[r-1/r]$ *of the function* $z \mapsto (I - zA)^{-1}X_0$*.*

Proof
The nonvanishing condition of the previous determinant implies that A_r is nonsingular.Moreover, we have

$$span(X_0, AX_0, \ldots, A^{r-1}X_0) = span(X_0, BX_0, \ldots, B^{r-1}X_0) = E_r$$

and

$$B_r = I_r - A_r.$$

Let us denote by P_r^0 the generating polynomial of $[r-1/r]_F$ where $F(z) = (I - zA)^{-1}X_0$ and by P the generating polynomial of $[r-1/r]_G$ where $G(z) = (I - zB)^{-1}X_0$. Applying the theorem 1.1 to B, we obtain $(I_r - B_r)^{-1}X_0 = Q(B)X_0$ where Q is the polynomial defined by $1 - \frac{P(x)}{P(1)} = (1-x)Q(x)$.
Since P is the characteristic polynomial (and also the minimal polynomial) of B_r, then it follows from lemma 2.1 that $P(x) = P_r^0(1-x)$.
We deduce that

$$1 - \frac{P_r^0(1-x)}{P_r^0(0)} = (1-x)Q(x),$$

and thus

$$1 - \frac{P_r^0(x)}{P_r^0(0)} = xQ(1-x) = xV_{r-1}(x).$$

In conclusion, the following result is obtained

$$A_r^{-1}X_0 = (I_r - B_r)^{-1}X_0 = V_{r-1}(I - B)X_0 \tag{29}$$

that is

$$A_r^{-1}X_0 = V_{r-1}(A)X_0 \tag{30}$$

2.2

Let us now study the connection between the vector orthogonal polynomials and the Lanczos method.We consider in C^d the linear system

$$(\star)\ Ax = b\ (A\ \textit{is nonsingular}).$$

Let $x_0 \in C^d$, we set $r_0 = b - Ax_0$. Throughout this section we are assuming that

$$\textit{for } k = 1, \ldots, m,\ span(r_0, Ar_0, \ldots, A^{k-1}r_0) = E_k = span(e_1, \ldots, e_k)$$

(m being the degree of the minimal polynomial of A for the vector r_0).

Remark 2.1 *This assumption seems very strong. In the section 3 some remark about this assumption will be made. Besides, an important example of such a matrix is an Hessenberg's matrix.*

Putting $x = x_0 + z$, the system $(\star)$ becomes $Az = r_0$. Then we solve the linear system $\delta_k Az = r_0$ in E_k. To do this, let us apply the theorem 2.1.
The condition

$$\begin{vmatrix} (r_0, Ar_0) & \dots & (r_0, A^k r_0) \\ \vdots & & \vdots \\ (A^{k-1}r_0, Ar_0) & \dots & (A^{k-1}r_0, A^k r_0) \end{vmatrix} \neq 0 \tag{31}$$

must be satisfied. Thus the solution of the system $(\star)$ is

$$z_k = V_{k-1}(A) r_0 \tag{32}$$

where V_{k-1} is the polynomial defined by

$$1 - \frac{P_k^0(x)}{P_k^0(0)} = x V_{k-1}(x), \tag{33}$$

P_k^0 being the generating polynomial of the vector Padé $[k-1/k]$ of the function $z \mapsto (I - zA)^{-1} r_0$.
Then we set

$$\begin{cases} x_k &= x_0 + z_k \\ r_k &= b - Ax_k \end{cases} \tag{34}$$

So it follows

$$\begin{aligned} r_k &= b - Ax_k & (35)\\ &= b - A(x_0 + V_{k-1}(A) r_0) & (36)\\ &= r_0 - AV_{k-1}(A) r_0 & (37)\\ &= \frac{P_k^0(A)}{P_k^0(0)} r_0 & (38) \end{aligned}$$

According to the definition of the vector orthogonal polynomials, we get see that $P_k^0(A) r_0$ is orthogonal to E_k,i.e

$$r_k \textit{ is orthogonal to } E_k.$$

Moreover, since $r_m = 0$, we obtain

$$Ax_m = b. \tag{39}$$

Remark 2.2 *The computation of the P_k^0 can be made, for example, by using the recurrence relations proved by Van Iseghem in [12]. But these polynomials don't allow an implementation as easy as in the standard Lanczos method (see [10]). Thus, the connection with the Lanczos method as described above, is the theoritical aspect of the method of for solving a system of linear equations, of the section 1.*

Let us now make some remarks about the different assumptions made before.

3 Biorthogonal polynomials. Oblique projection.

3.1 Biorthogonal polynomials.

Let us consider the most general biorthogonal polynomials, $(P_k)_{k\geq 0}$, with the respect to the independent linear functionals $(L_i)_{i\geq 0}$ on $C[X]$. They satisfy

$$L_i(P_k) = 0 \ for \ i = 0,\dots,k-1. \tag{40}$$

The vector orthogonal polynomials of dimension n are a special case, when the funtionals $(L_i)_{i\geq 0}$ satisfy

$$L_i(x^{j+1}) = L_{i+n}(x^j). \tag{41}$$

In the sections 1 and 2, we considered the vector polynomials of dimension $n = d$ where d is the dimension of the space on which we work. We only considered the polynomials $(P_k)_{k\leq d}$. Thus we did not make use of the relation (41).
Further generalizations of the Lanczos method using biorthogonal polynomials are given in [4].

3.2 The assumption $span(X_0, AX_0, \dots, A^{k-1}X_0) = span(e_1,\dots,e_k)$.

We still denote by $(e_i)_{i=1}^d$ the canonical basis of C^d. The orthogonal polynomials P_k^0 are defined by

$$(e_i, P_k^0(A)X_0) = 0 \ for \ i = 1,\dots,k.$$

Let us try to express these relations as projection on the subspace $span(X_0, AX_0, \dots, A^{k-1}X_0)$. If we assume that

$$span(X_0, AX_0, \dots, A^{k-1}X_0) = span(e_1,\dots,e_k),$$

this projection is the orthogonal projection on $span(X_0, AX_0, \dots, A^{k-1}X_0)$. Moreover we immediatly have the matrix of the linear transformation A_k in the basis $(e_i)_{i=1}^k$. This is the matrix formed by the first k rows and columns of the matrix A.Let us now assume that $span(X_0, AX_0, \dots, A^{k-1}X_0) = E_k$ with $dim E_k = k$ (E_k is not necessary equal to $span(e_1,\dots,e_k)$).
Can we write

$$C^d = E_k \oplus (span(e_1,\dots,e_k))^{\perp} \ ?$$

It is necessary and sufficient that

$$E_k \bigcap (span(e_1,\dots,e_k))^{\perp} = \{0\},$$

which is equivalent to

$$\begin{vmatrix} (e_1, X_0) & \dots & (e_1, A^{k-1}X_0) \\ \vdots & & \vdots \\ (e_k, X_0) & \dots & (e_k, A^{k-1}X_0) \end{vmatrix} \neq 0. \tag{42}$$

We recover the condition of existence and uniqueness of the polynomial P_k^0.
On the other hand, since the vectors $X_0, AX_0, \dots, A^{k-1}X_0$ are linearly independent, this condition implies that the functionals $e_i, i = 1,\dots,k$, considered as linear functionals on E_k are

independent (see [6]). Thus, we can take the oblique projection on E_k along $(span(e_1, \ldots, e_k))^\perp$. We obtain a nonderogatory operator A_k of E_k whose characteristic polynomial is P_k^0.**Conclusion** There is a strong connection between the Lanczos method for solving a system of linear equations and the the vector Padé approximants. Particularly, the Lanczos and the vector Padé approximants give the same iterates when the matrix A is Hessenberg.**References**

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