The Padé-Rayleigh-Ritz Method for Solving Large Symmetric Eigenproblem

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Abstract

We make use of the Padé approximants and Krylov's sequence $x, Ax, , \ldots, A^{m-1}x$ in the projection methods to compute a few Ritz values of a hermitian matrix A of order n. This process consists of approaching the poles of $\mathcal{R}_x(\lambda) = ((I-\lambda A)^{-1}x, x)$, the mean value of the resolvant of A, by those of $[m-1/m]_{\mathcal{R}_x}(\lambda)$, where $[m-1/m]_{\mathcal{R}_x}(\lambda)$ is the Padé approximant of order m of the function $\mathcal{R}_x(\lambda)$. This is equivalent to approach some eigenvalues of A by the roots of the polynomial of degree m of the denominator of $[m-1/m]_{\mathcal{R}_x}(\lambda)$. This projection method, called the Padé-Rayleigh-Ritz (PRR) method, provides a simple way to determine the minimum polynomial of x in the Krylov's method for the symmetrical case. The numerical stability of the PRR method can be ensured if there is not "considerable" variation in the matrix elements of A and if the projection subspace m is "sufficiently" small. The mainly expensive portion of this method is its projection phase, which is composed of the matrix-vector multiplications and, consequently, is well suited for parallel computing. This is also true when the matrices are sparse, as recently demonstrated, especially on massively parallel machines. This paper points out a relationship between the PRR and Lanczos methods and presents a comparison between them with regard to stability and parallelism. We then try to justify the use of this method under some assumptions.

Keywords : *projection method, large symmetrical eigenproblem, Padé approximant, Krylov's vectors, numerical stability, parallelism.*

1 Introduction Given a complex matrix A of dimension $n \times n$, and two subspaces $\mathcal{K}_m$ and $\mathcal{L}_m$ of $\mathcal{C}^n$. The projection method on the subspace $\mathcal{K}_m$ along subspace $\mathcal{L}_m$ aims to approximate an eigenpair (λ_i, u_i) of A by a pair $\lambda_i^{(m)}$, $u_i^{(m)}$ satisfying:

$$\begin{cases} \lambda_i^{(m)} \in \mathcal{C}, u_i^{(m)} \in \mathcal{K}_m \\ (A - \lambda_i^{(m)} I) u_i^{(m)} - \mathcal{L}_m \end{cases} \tag{1}$$

Let $V_m = [v_1, v_2, \cdots, v_m]$ and $W_m = [w_1, w_2, \cdots, w_m]$ be two bases of the subspaces $\mathcal{K}_m$ and $\mathcal{L}_m$. Writing $u_i^{(m)} = V_m y_i^{(m)}$, then $\lambda_i^{(m)}$ and $y_i^{(m)} \in \mathcal{C}^m$ are eigenelements of the generalized eigenvalues problem:

$$(\hat{C}_m - \lambda_i^{(m)} \hat{B}_m) y_i^{(m)} = 0 \tag{2}$$

where the $m \times m$ matrices C_m and B_m are defined by $C_m = W_m^H A V_m$, $B_m = W_m^H V_m$ (with W_m^H transpose conjugate of W_m). It is clear that, $\lambda_i^{(m)}$ and $u_i^{(m)}$ can be defined as the solution of the classical eigenvalue problem:

$$(\hat{B}_m^{-1}\hat{C}_m - \lambda_i^{(m)} I) y_i^{(m)} = 0 \tag{3}$$

All the solution $\lambda_i^{(m)}$ of the problem (1) are usually called Ritz values on the subspace $\mathcal{K}_m$. To each Ritz value $\lambda_i^{(m)}$is associated a Ritz vector $u_i^{(m)}$.

The above process is the principle of the oblique projection method. The most applications of the projection method involve an biorthogonal system $W_m^H V_m$, so that $\hat{B}_m$ in (2) and (3) reduce to the identity matrix. The problem (3) will reduced then to the following:

$$(\hat{C}_m - \lambda_i^{(m)} I) y_i^{(m)} = 0 \tag{4}$$

In the particular case of the orthogonal projection method $\mathcal{L}_m = \mathcal{K}_m$. The $V_m = W_m$ can be an orthonormal basis of the subspace $\mathcal{K}_m$. An orthogonal projection method is also called the Rayleigh-Ritz approximation method when A is a hermitian matrix. This method allows one to compute, for every couple (λ_i, u_i) of matrix A, a sequence of approximated eigenelements $(\lambda_i^{(m)}, u_i^{(m)})_m$. One can show[**?**] that $(\lambda_i^{(m)})_m$ is a monotonic sequence (with $\lambda_i^{(n)} = \lambda_i$). The drawback of a possible lack of strict monotonicity of the $(\lambda_i^{(m)})_m$ sequence is that one can choose the m parameter larger and larger ($m < n$) without significantly approaching the exact solution.

The Padé-Raleigh-Ritz (PRR) method, developed by D. Bessis and M. Villani [**?**] is a version of the Rayleigh-Ritz method and is used in quantum mechanics and physics. The PRR method uses the Padé approximants and the Krylov's subspace for solving the spectral problem of the Hamiltonian operator H, which has an important role in quantum mechanics. The authors carried out calculations for a `semi-bounded self-adjoint` operator H having the `discrete` (resp. `continuous`) part of the spectrum `positive` (resp. `non-positive`).

This paper presents an adaption of the PRR method to the case of large matrices in the scope of numerical analysis ($n < \infty$), generalizing it to the case of hermitian matrices (`definite positive or not`). Also, a new projection method for solving a hermitian eigenproblem is formulated and studied. Furthermore, we propose to use this method iteratively; that is, restarting a PRR step on a new Krylov's subspace with the same dimension until achieving satisfactory accuracy for the approximated eigenpairs.

In PRR method the subspace $\mathcal{K}_m$ is spanned by the Krylov's vectors $x, Ax, \ldots, A^{m-1}x$ where x is any non zero vector in $\mathcal{C}^n$. Then if V_m is the matrix of this Krylov's vectors sequence, the matrices $\hat{B}_m$ and $\hat{C}_m$ are the Hankel matrices of order m:

$$\hat{B}_m = \begin{pmatrix} C_{00} & C_{10} & \cdots & C_{(m-1)0} \\ C_{01} & C_{11} & \cdots & C_{(m-1)1} \\ \vdots & \vdots & \ddots & \vdots \\ C_{0(m-1)} & C_{1(m-1)} & \cdots & C_{(m-1)(m-1)} \end{pmatrix}$$

and

$$\hat{C}_m = \begin{pmatrix} C_{10} & C_{20} & \cdots & C_{m0} \\ C_{11} & C_{21} & \cdots & C_{m1} \\ \vdots & \vdots & \ddots & \vdots \\ C_{1(m-1)} & C_{2(m-1)} & \cdots & C_{m(m-1)} \end{pmatrix}$$

with $C_{ij} = (A^i x, A^j x)$ where (a, b) denote the Euclidean inner product between a and b vectors and $i, j \in \{0, 1, \cdots, m-1\}$. Nevertheless, to compute the Ritz values with PRR method the system (3) will not be used. Indeed, this system can be used in order to compute the corresponding Ritz vectors. In this method we make use of the Padé approximant and Krylov sequence to compute the Ritz values: Let $\mathcal{P}_m$ be the projector from $\mathcal{C}^n$ to $\mathcal{K}_m$. By using the same notation for linear operator A and its matrix representation, it can be shown that the problem (1) can also represented by:

$$\begin{cases} \lambda_i^{(m)} \in \mathcal{C}, u_i^{(m)} \in \mathcal{C}^n \\ \mathcal{P}_m A \mathcal{P}_m u_i^{(m)} = \lambda_i^{(m)} u_i^{(m)} \end{cases} \tag{5}$$

The PRR method consists of approximating the poles of $\mathcal{R}_x(\beta) = ((I-\beta A)^{-1}x, x)$, the mean value of the resolvant of A[1], by those of $\mathcal{R}_x^m(\beta) = ((I - \beta A_m)^{-1}x, x)$, the mean value of the resolvant of $A_m = \mathcal{P}_m A \mathcal{P}_m$[2]. We will show that this is equivalent to approximating some eigenvalues of the matrix A by the roots of the polynomial of degree m of the denominator of $[m-1/m]_{\mathcal{R}_x}(\beta)$ where $[m-1/m]_{\mathcal{R}_x}(\beta)$ is the Padé approximant of order m of the function $\mathcal{R}_x(\beta)$.

Let $(\lambda_i^{(m)})_m$ be a Ritz values sequence obtained by this method. We state that it is a `strictly monotonic` sequence for $m \leq s$ where s is the number of poles of the mean value of the resolvant of A. Consequently, two different choices, m_1 and m_2, of the parameter m allow us to have two different approximated eigenvalues, $\lambda_i^{(m_1)}$ and $\lambda_i^{(m_2)}$, for the exact eigenvalue λ_i of A with :

$$|\lambda_i^{(m_2)} - \lambda_i| < |\lambda_i^{(m_1)} - \lambda_i| \tag{6}$$

for $m_2 > m_1$. We give also a `necessary and sufficient condition` for the linear dependence of a Krylov's vectors sequence. This allows us to suggest possible choices for the initial vector x and the projection subspace size m. We use this condition in the study of the PRR method, in which an assumption of linear dependence or independence takes place at every step.

The connection of the Padé approximants with the theory of orthogonal polynomials allows to establish a relationship between the Padé approximants and Lanczos method [**?**, **?**, **?**]. We point out then a relationship between the PRR and Lanczos methods and observe that by using the Lanczos method we reproduce the results of PRR. As a consequence the Ritz values sequence obtained by the Lanczos method is a strictly monotonic sequence.

[1] We posed $\beta = \lambda^{-1}$ in the original form of the mean value of the resolvant of A: $((\lambda I - A)^{-1}x, x)$ where x is any non null vector in $\mathcal{C}^n$.

[2] We use also the same notation for the projector $\mathcal{P}_m$ and its matrix representation (consequently, we do it for A_m too).

In Sec.2 we recall some properties of the mean value of the resolvant of A and define a regular function from the resolvant. This function will be used in the section 4 to show the strict monotonicity of the Ritz values computed by the PRR method. In Sec.3 we show the essence of PRR method which is the equality between $\mathcal{R}_x^m(\beta)$ and the Padé approximant of order m of $\mathcal{R}_x(\beta)$. The strict monotonicity of the Ritz values sequence $(\lambda_i^{(m)})_m$ will be pointed out in Sec.4. In Sec.5 we give a necessary and sufficient condition for linear dependence of $x, \cdots, A^{m-1}x$ in function of x and m. Sec.6 is devoted to a global description of the PRR method. In Sec.7 we point out the connection between the PRR and the well-known Lanczos method. An important question is then whether PRR is a numerically stable method with respect to Lanczos. We try to answer to this question and give a comparison of these methods in viewpoint of computation cost in this section. Finally we present a conclusion in the last section.

2 Background and some definitions

Some properties of the mean value of the resolvant of A.

Let x be any non zero vector in $\mathcal{C}^n$. The mean value of the resolvant of A is defined by $((\lambda I - A)^{-1}x, x)$. By posing $\beta = \lambda^{-1}$ it can also be expressed by $\beta((I - \beta A)^{-1}x, x)$. The spectral decomposition of the resolvant of A allows us to redefine the mean value of the resolvant of A by:

$$\beta((I - \beta A)^{-1}x, x) = \sum_{i=1}^{p} \frac{a_i \beta \beta_i}{(\beta_i - \beta)} \tag{7}$$

where $a_i = (q_i x, x) \geq 0$, with q_i the eigenprojection corresponding to the eigenvalue $\lambda_i = (\beta_i)^{-1}$ and p the number of the `distinct` eigenvalues of A.

• The function $\beta \mapsto \beta\mathcal{R}_x(\beta) = \beta((I - \beta A)^{-1}x, x)$ is well defined for all $\beta \in \mathcal{C}$, except for some poles. These poles $\beta_1, \cdots, \beta_s$ are given by the inverse of the eigenvalues for which x is not orthogonal to the corresponding eigenspace M_i:

$$x \neq M_i \quad \text{for i=1,..,s} \tag{8}$$

with $s \leq p$. Thus, (7) can be write:

$$\beta\mathcal{R}_x(\beta) = \sum_{i=1}^{s} \frac{a_i \beta \beta_i}{(\beta_i - \beta)} \tag{9}$$

• Since for all $\beta \in \mathcal{R}$ $(\beta \neq \beta_i)$:

$$\frac{d}{d\beta}(\beta\mathcal{R}_x(\beta)) = \sum_{i=1}^{s} \frac{a_i \beta_i^2}{(\beta - \beta_i)^2} > 0 \tag{10}$$

the function $\beta \mapsto \beta\mathcal{R}_x(\beta)$ is `strictly increasing` in β.

• We note by $\overline{\beta}_i$ (resp. $\tilde{\beta}_i$) the positive (resp. negative) poles of $\beta\mathcal{R}_x(\beta)$. Suppose that they are ordered following the scheme:

$$\overline{\beta}_{s^-} < \cdots < \overline{\beta}_1 < 0 < \tilde{\beta}_1 < \cdots < \tilde{\beta}_{s^+} \tag{11}$$

where $s^+ + s^- = s$. The function $\beta \mapsto \beta\mathcal{R}_x(\beta)$ is positive for $0 < \beta < \tilde{\beta}_1$, null in $\beta = 0$ and negative for $\overline{\beta}_1 < \beta < 0$. Therefore, it has `exactly` one zero between each two successive poles.

The definition of a regular function from the mean value of the resolvant.

We want to show [?] that the sequence of Ritz values $(\lambda_i^{(m)})_m$, obtained by the PRR method, is strictly monotonic. In other words, $(\lambda_i^{(m)})_m$ (for $m < n$) is a strictly monotonic sequence of bounds for the exact eigenvalue λ_i of A. For this, the function $\beta \mapsto \beta\mathcal{R}_x(\beta)$ not being determinate in the position of the poles, one defines the auxiliary function $f(\beta) = arctg(\beta\mathcal{R}_x(\beta))$. This function has the remarkable properties that it is holomorphic and monotonic on the real axis. Consequently, the poles have been changed into points of holomorphy of $f(\beta)$. It is now possible to obtain bounds for $f(\beta)$. This enables us to build up a strictly monotonic sequence of bounds for the poles $\lambda_1, \cdots, \lambda_s$ of $\beta\mathcal{R}_x(\beta)$, and consequently for some of the eigenvalues of A [?].

• We define the function $f(\beta)$, for $\beta \in \mathcal{R}$ by:

$$f(\beta) = \arctan(\beta\mathcal{R}_x(\beta)) \tag{12}$$

by normalizing it at $\beta = -\infty$ and prolonging it by continuity:

$$f(-\infty) = \arctan(\lim_{\beta \to -\infty} \beta R_x(\beta)) \tag{13}$$

with

$$-(2s^- + 1)\frac{\pi}{2} < f(-\infty) < -(2s^- - 1)\frac{\pi}{2} \tag{14}$$

We have:

$$\frac{d}{d\beta} f(\beta) = \frac{\frac{d}{d\beta}(\beta R_x(\beta))}{1 + \beta^2 \mathcal{R}_x^2(\beta)} \tag{15}$$

The function $\beta \mapsto \beta\mathcal{R}_x(\beta)$ being meromorphic in $\mathcal{C}$, equation (15) shows that $\frac{d}{d\beta} f(\beta)$ is holomorphic for $\beta \in \mathcal{R}$. Therefore, f is also holomorphic in a vicinity of $\mathcal{R}$. On the other hand, equation (15) shows that we have always $\frac{d}{d\beta} f(\beta) > 0$, then, f is a strictly increasing function of β. Consequently, this function passes through the values $-(2k-1)\frac{\pi}{2}$ (resp. $+(2k-1)\frac{\pi}{2}$) for $\beta = \overline{\beta}_k$ (resp. $\beta = \tilde{\beta}_k$) and tends to a finite limit $f(+\infty)$ when $\beta \to +\infty$ with:

$$(2s^+ - 1)\frac{\pi}{2} < f(+\infty) < (2s^+ + 1)\frac{\pi}{2} \tag{16}$$

• We define, in the same way as f, the function f_m by:

$$f_m(\beta) = \arctan(\beta\mathcal{R}_x^m(\beta)) \tag{17}$$

This function has the same properties as f.

3 Padé-Rayleigh-Ritz = (Rayleigh-Ritz) + Krylov + Padé

By expanding the functions $\mathcal{R}_x(\beta)$ and $\mathcal{R}_x^m(\beta)$, in power of β, we have formally:

$$\mathcal{R}_x(\beta) = ((I - \beta A)^{-1}x, x) = \sum_{k=0}^{\infty} C_k \beta^k \tag{18}$$

$$\mathcal{R}_x^m(\beta) = ((I - \beta A_m)^{-1}x, x) = \sum_{k=0}^{\infty} C_k^m \beta^k \tag{19}$$

with $C_k = (A^k x, x)$ and $C_k^m = (A_m^k x, x)$. Let us note by S_x^m the Krylov's vectors sequence $x, Ax, \cdots, A^{m-1}x$. We have the following fundamental result [**?**, **?**] :

Theorem 1 *Suppose S_x^m is a linearly independent Krylov's vectors sequence. Then, the Padé approximation $[m-1/m]\mathcal{R}_x(\beta)$ constructed out of the first $2m$ moments $C_k = (A^k x, x)$, $k = 0, 1, \cdots, 2m-1$, fulfills $[m-1/m]_{\mathcal{R}_x}(\beta) = \mathcal{R}_x^m(\beta)$. If the sequence S_x^m is linearly dependent, then $[j-1/j]_{\mathcal{R}_x}(\beta) = \mathcal{R}_x(\beta)$ for all $j \in \{m, \cdots, n\}$.*

Demonstration 1 *The hypothesis of linear independence of the vectors $x, Ax, \cdots, A^{m-1}x$ spanning the subspace $\mathcal{K}_m$ implies:*

$$A_m^\ell x = (\mathcal{P}_m A \mathcal{P}_m)^\ell x = A^\ell x \qquad for \quad 0 \le \ell \le m-1 \tag{20}$$

and

$$A_m^{\ell'+1} x = (\mathcal{P}_m A \mathcal{P}_m) A^{\ell'} x = \mathcal{P}_m A^{\ell'+1} x \qquad for \quad 0 \le \ell' \le m-1 \tag{21}$$

The matrices A and $\mathcal{P}_m$ are hermitian. By using the inner product of (20) and (21), for $1 \le \ell + \ell' + 1 \le 2m-1$, we have then:

$$(A_m^{\ell'+\ell+1} x, x) = (\mathcal{P}_m A^{\ell'+1} x, A^\ell x) = (A^{\ell'+1} x, \mathcal{P}_m A^\ell x) = (A^{\ell'+\ell+1} x, x) \tag{22}$$

or

$$C_k^m = (A_m^k x, x) = (A^k x, x) = C_k \qquad for \quad 0 \le k \le 2m-1 \tag{23}$$

Then, by using the equations (18,19) and the equalities (23), we have:

$$\mathcal{R}_x(\beta) - \mathcal{R}_x^m(\beta) = \sum_{k=0}^{\infty} (C_k - C_k^m)\beta^k = O(\beta^{2m}) \tag{24}$$

Consider the spectral decomposition of the matrix A_m (which is of rank m):

$$A_m = \sum_{j=1}^{m} \lambda_j^{(m)} h_j^m \tag{25}$$

where h_j^m is the eigenprojection corresponding to the eigenvalue $\lambda_j^{(m)}$ of A_m. Since:

$$\mathcal{R}_x^m(\beta) = ((I - \beta A_m)^{-1}x, x) = \left(\frac{I}{I - \beta \sum_{j=1}^m \lambda_j^{(m)} h_j^m} x, x\right) = \sum_{j=1}^{m} \left(\frac{(h_j^m)^2}{h_j^m (1 - \beta \lambda_j^{(m)})} x, x\right) \tag{26}$$

and $(h_j^m)^2 = h_j^m$. *We have, then:*

$$\mathcal{R}_x^m(\beta) = \sum_{j=1}^{m} \frac{(h_j^m x, x)}{(1 - \beta\lambda_j^m)} \tag{27}$$

This equation shows that $\mathcal{R}_x^m(\beta)$ *is a rational fraction with a denominator of degree* m *and a numerator of degree* $m-1$ *in* β. *On the other hand, equation (24) shows that it differs from* $\mathcal{R}_x(\beta)$ *by a factor of order* β^{2m}. *Consequently, according to the definition of the Padé approximations[?], we have:*

$$[m - 1/m]_{\mathcal{R}_x}(\beta) = \mathcal{R}_x^m(\beta) \tag{28}$$

If the vectors $x, Ax, ..., A^{m-1}x$ *are linearly dependent, we have:*

$$A_m^\ell x = (\mathcal{P}_m A \mathcal{P}_m)^\ell x = A^\ell x \qquad \textit{for all} \quad \ell \geq 0 \tag{29}$$

Hence:

$$[m - 1/m]_{\mathcal{R}_x}(\beta) = \mathcal{R}_x^m(\beta) = \mathcal{R}_x(\beta) \tag{30}$$

□

The Padé approximant of order m of $\mathcal{R}_x(\beta)$ is defined by[?] (with $C_{-i} = 0$):

$$[m - 1/m]_{\mathcal{R}_x}(\beta) = \frac{det \begin{pmatrix} \sum_{i=0}^{-1} C_i \beta^{m+i} & \sum_{i=0}^{0} C_i \beta^{m+i-1} & \cdots & \sum_{i=0}^{m-1} C_i \beta^i \\ C_0 & C_1 & \cdots & C_m \\ \vdots & \vdots & \ddots & \vdots \\ C_{m-1} & C_m & \cdots & C_{2m-1} \end{pmatrix}}{det \begin{pmatrix} \beta^m & \beta^{m-1} & \cdots & 1 \\ C_0 & C_1 & \cdots & C_m \\ \vdots & \vdots & \ddots & \vdots \\ C_{m-1} & C_m & \cdots & C_{2m-1} \end{pmatrix}} \tag{31}$$

The above theorem show that approaching the poles of $\mathcal{R}_x(\beta)$ by the ones of $\mathcal{R}_x^m(\beta)$ is equivalent to approach them by the poles of $[m-1/m]_{\mathcal{R}_x}(\beta)$. As we see from (31), the poles of $[m-1/m]_{\mathcal{R}_x}(\beta)$ are the roots of the polynomial of degree m:

$$\tilde{Q}_m(\beta) = det \begin{pmatrix} C_0 & C_1 & \cdots & C_m \\ \vdots & \vdots & \ddots & \vdots \\ C_{m-1} & C_m & \cdots & C_{2m-1} \\ \beta^m & \beta^{m-1} & \cdots & 1 \end{pmatrix} \tag{32}$$

The PRR method consists in approaching some eigenvalues of A by the inverse of the roots of this polynomial.

4 Strict Monotonicity of the Ritz Values. According to the theorem 1 of the last section and some properties of the Padé approximants [**?**, **?**, **?**], the function $f_m(\beta)$ can also be define by:

$$f_m(\beta) = \arctan \beta [m-1/m]_{\mathcal{R}_x}(\beta) = \arctan [m/m]_{\beta \mathcal{R}_x}(\beta) \tag{33}$$

The definition of f_m and some properties [**?**, **?**, **?**] of Padé approximations allow us to show[**?**]:

Theorem 2 *For $\beta > 0$, we have always $f_{m+1}(\beta) > f_m(\beta)$. If at one point $\beta^* \neq 0$, we have $f_{m+1}(\beta^*) = f_m(\beta^*)$, then, for all k $(0 \leq k \leq n-m)$, we have $f_{m+k}(\beta) = f_m(\beta) = f(\beta)$, and for $\beta < 0$ we always have $f_{m+1}(\beta) < f_m(\beta)$.*

Demonstration 2 *Suppose:*

$$[m-1/m]_{R_x}(\beta) = \frac{P_{m-1}(\beta)}{Q_m(\beta)} \tag{34}$$

where $P_{m-1}(\beta)$ and $Q_m(\beta)$ are polynomials in β of degree $m-1$ and m respectively, and $Q_m(0) = 1$. Let $D(0,j) = det(\Delta(0,j))$ where

$$\Delta(i,j) = \begin{pmatrix} C_i & C_{i+1} & \cdots & C_{i+j} \\ C_{i+1} & C_{i+2} & \cdots & C_{i+j+1} \\ \vdots & \vdots & \ddots & \vdots \\ C_{i+j} & C_{i+j+1} & \cdots & C_{i+2j} \end{pmatrix} \tag{35}$$

*From now, we note $D(0,j)$ and $\Delta(0,j)$ by D_j and Δ_j respectively. We recall the following identity [**?**]:*

$$[m/m+1]_{R_x}(\beta) - [m-1/m]_{R_x}(\beta) = \frac{\beta^{2m} D_m^2}{Q_m(\beta) Q_{m+1}(\beta)} \tag{36}$$

For a hermitian matrix, we can show that D_m is always positive. In fact, we have the following relationship:

$$D_m = \gamma_m D_{m-1} \tag{37}$$

where $(\gamma_m)_m$ is some sequence of the real positive values and $D_{-1} = 1$. The above equality shows that if for some m_0, $D_{m_0} = 0$, we have then:

$$D_{m_0+k} = 0 \qquad \text{for all } k \text{ such that} \quad 0 \leq k \leq (n-1) - m_0 \tag{38}$$

and the mean value of the resolvant of A will be reduced to its Padé approximant of order m:

$$R_x(\beta) = [n-1/n]_{R_x}(\beta) = \cdots = [m_0 - 1/m_0]_{R_x}(\beta)$$

On the other hand, by using equation (36) we see that if a point $\beta^* \neq 0$ exists such that $f_{m+1}(\beta^*) = f_m(\beta^*)$, then $D_m = 0$ and therefore:

$$f_{m+k}(\beta) = f_m(\beta) = f(\beta) \qquad \text{for all } k \text{ such that} \quad 0 \leq k \leq (n-1) - m \tag{39}$$

Apart from this particular case, we see that for $\beta > 0$ the $f_{m+1}(\beta)$ and $f_m(\beta)$ functions have no point of intersection. Consequently, in order to fix their relative position, we consider their relative values in the vicinity of zero. In fact, we deduce from (36) that:

$$f_{m+1}(\beta) - f_m(\beta) = (D_m)^2 \beta^{2m+1} + O(\beta^{2m+2}) \tag{40}$$

Because the Taylor's development, in the vicinity of zero of the function $f_m(\beta) = \arctan(z_m)$ (with $z_m = \beta[m-1/m]_{R_x}(\beta)$) provides:

$$f_m(\beta) = \arctan(z_m) = z_m + O(\beta^{2m+1}) = [m/m]_{\beta R_x}(\beta) + O(\beta^{2m+1}) \tag{41}$$

we have:

$$\begin{cases} f_{m+1}(\beta) > f_m(\beta) & \text{for } \beta > 0 \\ f_{m+1}(\beta) < f_m(\beta) & \text{for } \beta < 0 \end{cases}$$

□

As long as the Krylov's vectors $x, Ax, ..., A^{m-1}x$ are linearly independent, the poles of $[m-1/m]_{R_x}(\beta)$ are all `real` and `distinct`. Suppose they are ordered in the following scheme:

$$\overline{\beta}_{m^-}^{(m)} < \cdots < \overline{\beta}_1^{(m)} < 0 < \tilde{\beta}_1^{(m)} < \cdots < \tilde{\beta}_{m^+}^{(m)} \tag{42}$$

where $m^+ + m^- = m$. According to the definition of f_m (for $k = 1, \cdots, m^-$ and $j = 1, \cdots, m^+$) we have:

$$f_m(\overline{\beta}_k^{(m)}) = -(2k-1)\frac{\pi}{2} \quad \text{and} \quad f_m(\tilde{\beta}_j^{(m)}) = (2j-1)\frac{\pi}{2} \tag{43}$$

On the other hand, the orthogonality properties of the denominators of the Padé approximations $[m/m]_{\beta R_x}(\beta)$ imply that between two successive poles of $[m/m]_{\beta R_x}(\beta)$, we have `exactly` one pole of $[m+1/m+1]_{\beta R_x}(\beta)$, except between the two poles nearest to the origin of the $[m/m]_{\beta R_x}(\beta)$. In fact, between those two poles (i.e.: $\tilde{\beta}_1^{(m)}$ and $\overline{\beta}_1^{(m)}$), there are two poles of $[m+1/m+1]_{\beta R_x}(\beta)$, one positive and one negative. In other words:

$$\overline{\beta}_1^{(m)} < \overline{\beta}_1^{(m+1)} < 0 < \tilde{\beta}_1^{(m+1)} < \tilde{\beta}_1^{(m)} \tag{44}$$

Because in the contrary case, we have:

$$\overline{\beta}_1^{(m+1)} < \overline{\beta}_1^{(m)} < 0 \quad \text{or} \quad 0 < \tilde{\beta}_1^{(m)} < \tilde{\beta}_1^{(m+1)} \tag{45}$$

Then, the function $\beta \mapsto f_m(\beta)$ is strictly increasing and the sequence $(f_m(\beta))_m$ is strictly monotonic. Combining theses two properties of f_m with equation (45), we have:

$$-\frac{\pi}{2} = f_{m+1}(\overline{\beta}_1^{(m+1)}) < f_m(\overline{\beta}_1^{(m)}) = -\frac{\pi}{2} \tag{46}$$

$$\frac{\pi}{2} = f_m(\tilde{\beta}_1^{(m)}) < f_{m+1}(\tilde{\beta}_1^{(m+1)}) = \frac{\pi}{2} \tag{47}$$

which are not true. Consequently, the sequence of the poles $(\tilde{\beta}_k^{(m)})_m$ (resp. $(\overline{\beta}_k^{(m)})_m$) is strictly decreasing (resp. strictly increasing)

Hence, if the eigenvalues $\tilde{\lambda}_i = (\tilde{\beta}_i)^{-1}$ and $\overline{\lambda}_i = (\overline{\beta}_i)^{-1}$ of the matrix A and ones $\tilde{\lambda}_i^{(m)} = (\tilde{\beta}_i^{(m)})^{-1}$ and $\overline{\lambda}_i^{(m)} = (\overline{\beta}_i^{(m)})^{-1}$ of the matrix A_m are ordered as follows:

$$\overline{\lambda}_1 < \cdots < \overline{\lambda}_{s^-} < 0 < \tilde{\lambda}_{s^+} < \cdots < \tilde{\lambda}_1 \tag{48}$$

$$\overline{\lambda}_1^{(m)} < \cdots < \overline{\lambda}_{m^-}^{(m)} < 0 < \tilde{\lambda}_{m^+}^{(m)} < \cdots < \tilde{\lambda}_1^{(m)} \tag{49}$$

they fulfill:

$$\overline{\lambda}_k^{(m_{end})} < \cdots < \overline{\lambda}_k^{(m+1)} < \overline{\lambda}_k^{(m)} < 0 \tag{50}$$

$$0 < \tilde{\lambda}_k^{(m)} < \tilde{\lambda}_k^{(m+1)} < \cdots < \tilde{\lambda}_k^{(m_{end})} \tag{51}$$

In other words, for $m = 1, \cdots, m_{end}$, the sequence of `positive` Ritz values $(\tilde{\lambda}_k^{(m)})_m$ is `strictly increasing` and the sequence of `negatives` Ritz values $(\overline{\lambda}_k^{(m)})_m$ is `strictly decreasing`.

But, what is the m_{end}? It is clear that the `strict monotonicity` of the Ritz values sequence is true as long as the poles of $[m-1/m]_{\mathcal{R}_x}(\beta)$ are all real and distinct. We have seen before that this is true as long as the sequence of the Krylov's vectors S_x^m is `linearly independent`. Therefore, m_{end} is the value of the parameter m beyond which we have linear dependence of S_x^m. Consequently, we are interested in locating the moment from where the Krylov's vectors sequence S_x^m is no longer linearly independent. We will address this question in the next section.

5 A Necessary and Sufficient Condition for the Linear Dependence of a Krylov's Vectors Sequence. Let $M_1, \cdots, M_p$ be the eigenspaces corresponding to p distinct eigenvalues of A. We denote the orthogonality of the vector x with the subspace M_i by $x - M_i$. We can show the following result:

Theorem 3 *Let A be a normal (in particular hermitian) matrix of order n and let x be any non null vector of $\mathcal{C}^n$. Suppose $x \neq M_i$ for $i = 1, \cdots, t$ and $x - M_i$ for $i = t+1, \cdots, p$ (`hypothese H`), then S_x^t is linearly independent and S_x^m is linearly dependent for all $m > t$.*

Demonstration 3 *Since A is a `normal` matrix, there is an orthogonal basis $u_1, \cdots, u_n$ of its eigenvectors. Let $u_{i_1}, \cdots, u_{i_d}$ be the eigenvectors associated to the eigenvalue λ_i, and let $M_i = span\{u_{i_1}, \cdots, u_{i_d}\}$ be the eigenspace corresponding to λ_i. Then $n = \sum_{i=1}^p i_d$, $\mathcal{C}^n = \oplus_{i=1}^p M_i$ and $x = \sum_{i=1}^p x_i$ with $x_i \in M_i$. Our hypothesis for x implies $x_i \neq 0$ for $i = 1, \cdots, t$ and $x_i = 0$ for $i = t+1, \cdots, p$. Hence:*

$$x = \sum_{i=1}^{t} x_i \tag{52}$$

Consider now $\sum_{j=0}^{m-1} \alpha_j A^j x$ for nonzero vector $y = (\alpha_0, \cdots, \alpha_{m-1})^t \in \mathcal{C}^m$. Equation (52) implies $A^j x = \sum_{i=1}^t A^j x_i$ for all $j \geq 0$. On the other hand, for all $i \in \{1, \cdots, t\}$, there exists a nonzero

vector $(\beta_{i_1}, \cdots, \beta_{i_d})^t \in \mathcal{C}^t$ *such that* $x_i = \sum_{k=1}^{d} \beta_{i_k} u_{i_k}$. *Hence, for all* $j \geq 0$ *and* $i \in \{1, \cdots, t\}$, *we have* $A^j x_i = A^j \sum_{k=1}^{d} \beta_{i_k} u_{i_k} = \lambda_i^j x_i$. *We can write then:*

$$\sum_{j=0}^{m-1} \alpha_j A^j x = \sum_{i=1}^{t} (\sum_{j=0}^{m-1} \alpha_j \lambda_i^j) x_i \tag{53}$$

Linear independence of the vectors $x_1, \cdots, x_t$ *implies:*

$$\sum_{j=0}^{m-1} \alpha_j A^j x = 0 \Leftrightarrow \sum_{j=0}^{m-1} \alpha_j \lambda_i^j = 0 \quad \forall i \in \{1, \cdots, t\} \tag{54}$$

This is equivalent to the following system:

$$\begin{pmatrix} 1 & \lambda_1 & \cdots & \lambda_1^{m-1} \\ 1 & \lambda_2 & \cdots & \lambda_2^{m-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_t & \cdots & \lambda_t^{m-1} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{m-1} \end{pmatrix} = V_m y = 0 \tag{55}$$

As the eigenvalues $\lambda_1, \cdots, \lambda_t$ *are distinct, the Vander Monde matrix* V_m *is invertible for* $m = t$. *Hence* $V_t y = 0 \Leftrightarrow y = 0$. *Consequently, the sequence* S_x^t *is linearly independent. For* $m = t + 1$ *the above system of equations has at least one (nonzero) solution. This is equivalent to the linear dependence of* S_x^m *for* $m > t$. *These results allow us to say:*

$$S_x^m \textit{ is linearly dependent} \Leftrightarrow m > t \tag{56}$$

□

An immediate consequence of this theorem is that, if x fulfills the `H` hypothese, for $m \geq t$ the projection subspace $\mathcal{K}_m$ is an invariant subspace for the `normal` matrix A. The restriction of A_m to $\mathcal{K}_m$ is no longer a projection of A onto $\mathcal{K}_m$ but the restriction of A to $\mathcal{K}_m$. Consequently, the eigenvalues of the restriction of A_m to $\mathcal{K}_m$ are the `exact` eigenvalues of A. We propose then, a suggestion for possible choices of the initial vector x and the parameter m: the number t is unknown in practice, but for any x and large n, it is, in general, large. This means that if we choose m `large`, we can hope to have $m \geq t$. But this choice is in disagreement with the general principle of projection methods for computing a few eigenvalues of a very large matrix (i.e.: $m \ll n$). Now, with m small, according to the above result, we must choose an initial vector x in such a way that it belongs to an invariant subspace $M^t = M_1 \oplus \cdots \oplus M_t$ and does not belong to any other invariant subspace (i.e. $x \notin M^{p-t} = M_{t+1} \oplus ... \oplus M_p$).

Suppose now we want to compute r Ritz values of matrix A ($r \leq m \ll n$). As a consequence of the above theorem, we must attempt to find an initial vector x whose components are `nonzero` (resp. `zero`) in the r eigenspaces corresponding to the `wanted` (resp. `unwanted`) eigenvalues. The research of such initial vectors has been the aim of much investigation, particularly in [**?**, **?**, **?**, **?**].

Application to PRR Method

In the specific case of the PRR method, we can consider that the vector x defined in this method

fulfills the condition of the above theorem for $t = s$, the poles number of $R_x(\beta)$. In other words, the vector x belongs to the invariant subspace $M^s = M_1 \oplus ... \oplus M_s$ and does not belong to the rest of invariant subspaces: $M^{p-s} = M_{s+1} \oplus ... \oplus M_p$. Consequently, for $m \geq s$ the Ritz values obtained by PRR are the `exact` eigenvalues of A and the m_{end} parameter, defined in the last section, is equal to s. In other words, $Q_s(A)x$ is the minimal polynomial of x. The inequalities (50, 51) can now be rewritten:

$$\overline{\lambda}_k = \overline{\lambda}_k^{(s)} = \overline{\lambda}_k^{(m_{end})} < \cdots < \overline{\lambda}_k^{(m+1)} < \overline{\lambda}_k^{(m)} < 0 \tag{57}$$

$$\tilde{\lambda}_k = \tilde{\lambda}_k^{(s)} = \tilde{\lambda}_k^{(m_{end})} > \cdots > \tilde{\lambda}_k^{(m+1)} > \tilde{\lambda}_k^{(m)} > 0 \tag{58}$$

This shows that the ideal choice of parameter m is $m = s = m_{end}$. As we have just seen, this is accomplished by a "good" choice of the initial vector x.

Combining the strict monotonicity of the Ritz values sequence $(\lambda_k^{(m)})_m$ obtained by the PRR method and the above theorem, it is easy to show that if x is not orthogonal to any of the eigenspaces, the Ritz values in the extremity of the spectrum converge to the corresponding exact eigenvalues. Furthermore, the error bounds given by [**?**] show that these approximations are more and more precise as they go up to the extremity of the spectrum of A.

6 The PRR Method Suppose the Krylov's vectors sequence S_x^m is linearly independent. Consider an even number of moments $C_0, C_1, ..., C_{2m-1}$. We consider the polynomial (32) of the denominator of the Padé approximation $[m/m]_{\beta R_x}(\beta)$ built up on the mean value of the resolvant of A. Computing the roots of this polynomial can be done by finding the inverse of the ones of the following[3]:

$$Q_m(\lambda) \quad = det \begin{pmatrix} C_0 & C_1 & \cdots & C_m \\ \vdots & \vdots & \ddots & \vdots \\ C_{m-1} & C_m & \cdots & C_{2m-1} \\ 1 & \lambda & \cdots & \lambda^m \end{pmatrix} \tag{59}$$

The PRR method consists of approximating the poles of $\mathcal{R}_x(\beta)$, the mean value of the resolvant of A, by those of $\mathcal{R}_x^m(\beta)$, the mean value of the resolvant of $A_m = \mathcal{P}_m A \mathcal{P}_m$. We have shown that this is equivalent to approaching some eigenvalues of the matrix A by the inverse of the poles of $[m/m]_{\beta \mathcal{R}_x}(\beta)$. In other words, the PRR method permits to approach m distinct eigenvalues of A by the m real and distinct roots $\lambda_i^{(m)}$, $i \in \{1, \cdots, m\}$, of the polynomial $Q_m(\lambda)$. The $\lambda_i^{(m)}$ are the eigenvalues of the projection of A onto $\mathcal{K}_m = span(x, Ax, \cdots, A^{m-1}x)$ which is the restriction of A_m to $\mathcal{K}_m$. Let $\theta_j = det(\Theta_j)$ with

$$\Theta_j = \begin{pmatrix} C_0 & \cdots & C_{j-1} & C_{j+1} & \cdots & C_m \\ C_1 & \cdots & C_j & C_{j+2} & \cdots & C_{m+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ C_{m-1} & \cdots & C_{j+m-2} & C_{j+m} & \cdots & C_{2m-1} \end{pmatrix} \tag{60}$$

[3] We posed $\lambda = \beta^{-1}$ in (32). Hence, the roots λ_i^m of $Q_m(\lambda)$ are the inverse of the roots of polynomial (32).

Notice that $\Theta_m = \Delta_{m-1}$, hence $\theta_m = D_{m-1}$. The polynomial $Q_m(\lambda)$ can be rewritten by:

$$Q_m(\lambda) = D_{m-1}(\lambda^m + b_{m-1}\lambda^{m-1} + \cdots + b_0) \tag{61}$$

where

$$b_j = \frac{\theta_j}{(-1)^{m-j} D_{m-1}} \tag{62}$$

Computing roots of $Q_m(\lambda)$ requires first computation of the polynomial coefficients b_j. This can be done using the above relation. Another way to determine these coefficients is solving the following Yule Walker system:

$$\begin{pmatrix} C_0 & C_1 & \cdots & C_{m-1} \\ C_1 & C_2 & \cdots & C_m \\ \vdots & \vdots & \ddots & \vdots \\ C_{m-1} & C_m & \cdots & C_{2m-2} \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_{m-1} \end{pmatrix} = - \begin{pmatrix} C_m \\ C_{m+1} \\ \vdots \\ C_{2m-1} \end{pmatrix} \tag{63}$$

This linear system can be obtain easily from the definition of the Padé approximants[**?**]. As soon as the vector $b = (b_0, \cdots, b_{m-1})^t$ is known, to compute the Ritz values $\lambda_i^{(m)}$, we can use either:

1. a method to compute the roots of an explicit polynomial (for example: Bairstow).
2. a method to compute the eigenvalues of a non-symmetric and sparse matrix (for example: QR):

$$H_m = \begin{pmatrix} -b_{m-1} & -b_{m-2} & \cdots & -b_1 & -b_0 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \ddots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix} \tag{64}$$

   Since H_m is the companion matrix of $D_{m-1}^{-1} Q_m(\lambda)$.

Ritz Vector Computation

Once the Ritz value $\lambda_i^{(m)}$ is computed, in order to compute the associated Ritz vector $u_i^{(m)}$ we consider the matrix $\hat{B}_m^{-1}\hat{C}_m$ defined in (3):

$$\hat{B}_m^{-1}\hat{C}_m = \Delta^{-1}(0, m-1)\Delta(1, m-1) = (V_m^H V_m)^{-1}(V_m^H A V_m) \tag{65}$$

where V_m represents the matrix of $x, Ax, \cdots, A^{m-1}x$ vectors. The system (3) can then be rewritten by the following relation:

$$(\Delta^{-1}(0, m-1)\Delta(1, m-1) - \lambda_i^{(m)} I) y_i^{(m)} = 0 \tag{66}$$

To compute $u_i^{(m)}$ we just need to obtain the eigenvector $y_i^{(m)}$ from (66) and then to calculate the following matrix vector product:

$$u_i^{(m)} = V_m y_i^{(m)} \tag{67}$$

Iterative PRR Method

Suppose, we want to compute some number r of the eigenelements of a matrix A of order n ($r \leq m \ll n$). By using the PRR method, the realized accuracy of approximated eigenvalues can be unsatisfactory. We propose to use this method iteratively. That is, to restart a PRR step with a new initial vector, until obtaining the desired accuracy. Concerning the choice of an initial vector, according to the results of the previous section, we need to find a vector with `nonzero` (resp. `zero`) components in the eigenspaces corresponding to the `wanted` (resp. `unwanted`) eigenvalues.

6.1 Iterative PRR Algorithm

1. Choice of m.
2. Choice of initial vector x.
3. Normalization of x: $y_0 = x / \parallel x \parallel$, $C_0 = \parallel y_0 \parallel^2 = 1$
4. Computation of $C_1, , \cdots, C_{2m-1}$.
   - $y_1 = Ay_0$
   - For $k = 1, m-1$, do
     $$C_{2k-1} = (y_k, y_{k-1})$$
     $$C_{2k} = (y_k, y_k)$$
     $$y_{k+1} = Ay_k$$
   - End for k
   - $C_{2m-1} = (y_m, y_{m-1})$
5. Linear system solving (63).
6. Computation of the roots of $Q_m(\lambda)$ polynomial.
7. Computation of the Ritz vectors $u_i^{(m)}$ by (66) and (67).
8. If ($\min_{1 \leq i \leq r} \parallel (A - \lambda_i^{(m)} I) u_i^{(m)} \parallel > p$: *requested precision*) then
   with a new initial vector go to 3.

7 Connection with the Lanczos method. Suppose $x, Ax, \cdots, A^{m-1}x$ are linearly independent. If we orthogonalize this sequence by Gramm Schimdt process, we obtain a vectors sequence:

$$\begin{cases} y_0 = \overline{Q}_0(A)x \\ y_1 = \overline{Q}_1(A)x \\ \qquad\qquad \vdots \\ y_{m-1} = \overline{Q}_{m-1}(A)x \end{cases} \tag{68}$$

where $\overline{Q}_j(\lambda)$ is related to the polynomial $\tilde{Q}_j(\beta)$ of the denominator of the Padé Approximation $[m-1/m]$ of $\mathcal{R}_x(\beta)$ by:

$$\overline{Q}_j(t) = \delta(j) t^j \tilde{Q}_j(t^{-1}) \tag{69}$$

the constant $\delta(j)$ being adjusted in such a way that the polynomial $\overline{Q}_j(t)$ form an orthogonalized set. Now, it can be shown that for a hermitian matrix A the $y_0, \cdots, y_{m-1}$ vectors fulfill the

following recursive relation:

$$\beta_j y_{j+1} = Ay_j - \alpha_j y_j - \beta_{j-1} y_{j-1} \tag{70}$$

This means that in the basis (68), the matrix A is represented by a tridiagonal and symmetrical matrix. In fact, if Y represents the matrix of $y_0, \cdots, y_{m-1}$ vectors, we have:

$$T_m = Y^H A Y \tag{71}$$

with $(T_m)_{i,j} = (Ay_i, y_j)$. The orthogonality properties of the basis (68) imply:

$$(T_m)_{i,i} = \alpha_i, \quad (T_m)_{i,i+1} = \beta_{i+1}, \quad (T_m)_{i,j} = 0 \quad \text{pour } j \geq i+2 \tag{72}$$

This process of tridiagonalization of a matrix by orthogonalization of the corresponding Krylov's sequence is the Lanczos method. Note that it can be shown [**?**] that the restriction of A_m to the projection subspace $\mathcal{K}_m$ is represented by the matrix T_m with respect to the basis Y. Consequently the eigenvalues of T_m are also eigenvalues of A_m.

If $w_i^{(m)}$ is the eigenvector of T_m corresponding to the eigenvalue $\lambda_i^{(m)}$, then the Ritz vector $v_i^{(m)}$ of A corresponding to $\lambda_i^{(m)}$ can be obtained by:

$$v_i^{(m)} = Y w_i^{(m)} \tag{73}$$

Because the PRR and Lanczos methods produce the same mathematical results it is natural to compare them. Recall an iterative Lanczos algorithm:

7.1 Iterative Lanczos Algorithm

1. Choice of m.
2. Choice of initial vector x.
3. Normalization of x : $y_0 = x / \parallel x \parallel$ and $\beta_{-1} = 0$
4. Computation of T_m matrix elements.
   - For $j = 0, m-2$, do
     $\alpha_j = (Ay_j, y_j)$
     $y'_{j+1} = Ay_j - \alpha_j y_j - \beta_{j-1} y_{j-1}$
     $\beta_j = \parallel y'_{j+1} \parallel$
     $y_{j+1} = y'_{j+1} / \beta_j$
   - End for j
   - $\alpha_{m-1} = (Ay_{m-1}, y_{m-1})$
5. Computation of the eigenvalues of T_m matrix.
6. Computation of the eigenvectors $w_i^{(m)}$ of T_m matrix.
7. Computation of the Ritz vectors $v_i^{(m)}$ by (73).
8. If $(\min_{1 \leq i \leq r} \parallel (A - \lambda_i^{(m)} I) v_i^{(m)} \parallel > p$: *requested precision*) Then
   with a new initial vector go to 3.

PRR Vs Lanczos

A drawback of the Lanczos method, calling into question its stability, is that the vectors obtained by the algorithm loose their orthogonality very rapidly. Several strategies of re-orthogonalization[**?**, **?**, **?**] can be used, but this can become very expensive.

The PRR method does not have this problem. Instead, the matrix in the projection subspace whose eigenvalues approximate those of A is a non-symmetric and sparse upper Hessenberg matrix: our symmetric eigenproblem is reduced to a non-symmetric eigenproblem! In order to circumvent this difficulty, an alternative seems to compute the roots of the characteristic polynomial $Q_m(\lambda)$ of this matrix.

In the PRR method, we must solve a symmetric linear system (i.e.: 63) which is well conditioned if there is not "considerable" variation in the size of matrix elements of A and if the system size is "sufficiently" small. This because the moments C_k $(0 \leq k \leq 2(m-1))$ increase very rapidly and for fixed x, the increasing rate of C_k is a function of the variation in the matrix elements of A. Furthermore, the special form of this system permits to solve it by the use of the Bordering method [**?**] or the triangular decomposition method proposed by Phillips [**?**], which are particularly well suited to these kind of systems. Consider now the following real and symmetrical matrix:

$$A = \begin{pmatrix} 9 & 1 & -2 & 1 \\ 1 & 8 & -3 & -2 \\ -2 & -3 & 7 & -1 \\ 1 & -2 & -1 & 6 \end{pmatrix} \tag{74}$$

which the exact eigenvalues are 3, 6, 9 and 12. If $m = 2$ with the initial vector $x = (1,0,0,0)^t$, the PRR method allow us to solve the linear system:

$$\begin{pmatrix} 1 & 9 \\ 9 & 87 \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = - \begin{pmatrix} 87 \\ 891 \end{pmatrix} \tag{75}$$

Thus the roots $\lambda_1^{(2)} = 11.44949$ and $\lambda_2^{(2)} = 6.5505103$ of $Q_2(\lambda) = \lambda^2 - 18\lambda + 75$ are the Ritz values obtained by PRR. By application of Lanczos to the matrix A with the same initial vector we obtain:

$$T_2 = \begin{pmatrix} 9 & \sqrt{6} \\ \sqrt{6} & 9 \end{pmatrix} \tag{76}$$

The eigenvalues of T_2 are exactly the roots of $Q_2(\lambda)$. Another initial vector: $x = (0,0,1,0)^t$ allows again to the exactly the same Ritz values $\lambda_1^{(2)} = 11.523512$, $\lambda_2^{(2)} = 3.9050595$ with the PRR and Lanczos methods. Nevertheless, with the initial vector $x = \frac{1}{2}(1,1,1,1)^t$ we obtain $\lambda_1^{(2)} = 10.732745$, $\lambda_2^{(2)} = 3.1763457$ with PRR and $\lambda_1^{(2)} = 13.239141$, $\lambda_2^{(2)} = 1.2154043$ with Lanczos[4]. We see that approximately the same results are obtained by both of these methods. Nevertheless, these examples are not very significant because n is too small.

Computing Ritz vectors $u_i^{(m)}$ requires the evaluation of the matrix $\Delta^{-1}(0, m-1)\Delta(1, m-1)$. The special form of these matrices implies that we can obtain the inverse matrix $\Delta^{-1}(0, m-1)$

[4] All these Ritz values are obtained by only one iteration of the PRR and Lanczos methods.

by the recursive Trench's algorithm [?] and there will not be "big" variation in the size of the matrix elements of $\Delta^{-1}(0, m-1)\Delta(1, m-1)$.

Computing Cost

The essential expensive part of the Lanczos and PRR algorithms is the projection phase. The complexity of which is $m(\alpha + 2\beta + 5\gamma) - (\beta + 7\gamma)$ for Lanczos and $m(\alpha + 2\beta) - \beta$ for PRR, where α, β and γ are respectively the complexity of a matrix-vector multiplication, an inner product of two vectors and an elementary operations between a scalar and a vector of order n.

Suppose that, we have $O(n^2)$ processors. Then, if we don't consider the communications time and the mapping problems, we have $\alpha = \beta$ and $\gamma \approx 1$. Nevertheless, we must recall that this is target machine dependent. Consequently, with $O(n^2)$ processors, the complexity of the projection phase of PRR and Lanczos are respectively $\alpha(3m-1)$ and $\alpha(3m-1) + 5m - 7$ ps with $\alpha = 1 + \log_2 n$ for the case of dense matrices and $\alpha = 1 + \log_2 c$ for the case of sparse matrices. where c is the maximum number of the non zero elements in a column of A.

Consequently, for this portion of algorithm, PRR can be more interesting than the Lanczos method. Furthermore, the inclusion of reorthogonalization makes the projection phase of Lanczos method almost `twice` as expensive. Now for the Arnoldi projective method it has been observed on the massively parallel architecture of the Connection Machine 2 [?] that with $O(n^2)$ processors in the general case and with $O(nc)$ processors in the sparse case, for $\frac{n}{m}$ large, we have:

$$d(\text{projection method}) \rightarrow d(\text{projection phase})$$

where $d(x)$ is the throughput of x. Then we can conclude that for $\frac{n}{m}$ large, the PRR method can be less expensive by a factor of two than Lanczos (with reorthogonalization) on such architectures.

8 Conclusion The method developed in this paper compute some Ritz elements of a `very large` hermitian matrix. The problems to be solved in the subspace are well conditioned when the projection subspace size, m, is very small.

We have seen that PRR and the well known Lanczos method produce mathematically the same results. The examples presented in the last section show that the Ritz values obtained by PRR have a "good" precision with respect of those obtained by Lanczos. But, this is not significant because of very small size of A. A reliable assessment of the PRR method requires using it for realistic n and m parameters and verifying numerical results. Now, for n very large, the use of the powerful machines and consequently the parallel architectures is necessary. We have seen that in this viewpoint, theoretically, PRR can be more efficient than Lanczos algorithm. In other hand, a study on the data parallelism behavior of the projection phase of these two methods [?] show that the memory requirements of Lanczos is larger than those of PRR. The experiments done on a CM5 for this study have shown that for n in some interval, Lanczos can not be executed but PRR can. In other words, for some large value of n, PRR can be used and Lanczos can not.

Now, it is well known that the Lanczos method is a numerically stable method. The stability

of PRR can be ensured for `very small` m and in some cases the use of Lanczos is impossible. Consequently, under some assumptions, PRR can be an efficient method to compute the Ritz values and vectors of a large hermitian matrix. To give a reliable assessment of PRR we have to implement it and to compare numerical results with those of Lanczos.

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