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# Chebyshev acceleration techniques for large complex non Hermitian eigenvalue problems

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We propose an extension of the Arnoldi-Chebyshev algorithm to the large complex non Hermitian case. We demonstrate the algorithm on two applied problems.

# Техника ускорения по Чебышеву для больших задач нахождения собственных значений не-эрмитовых комплексных матриц

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Предлагается обобщение алгоритма Арнольди-Чебышева для случая больших комплексных не-эрмитовых матриц. Работа алгоритма продемонстрирована на примере двух прикладных задач.

## 1. Introduction

The computation of a few eigenvalues and the corresponding eigenvectors of large complex non hermitian matrices arises in many applications in science and engineering such as magnetohydrodynamic or electromagnetism [6], where the eigenvalues of interest often belong to some region of the complex plane.

If the size of the matrices is relatively small, then the problem can be solved by the standard and robust QZ algorithm [9]. The QZ algorithm computes all the eigenvalues while only a few eigenvalues may be of interest, requires a high computational cost and does not exploit the sparsity of the matrices and is therefore only suitable for small matrices.

When the size of the matrices becomes large, then Krylov subspace methods are a good alternative since these methods take into account the structure of the matrix and approximate only a small part of the spectrum. Among these methods, Arnoldi's algorithm appears to be the most suitable. Arnoldi's method builds an orthogonal basis in which the matrix is represented in a Hessenberg form whose spectrum, or at least a part of it, approximates the sought eigenvalues. Saad [11] has proved that this method gives a good approximation to the outermost part of the spectrum. However, convergence can be very slow especially when the distribution of the spectrum is unfavorable. On the other hand, to ensure convergence, the dimension of the Krylov subspace must be large, which increases the cost and the storage. To overcome these difficulties, one solution is to use the method iteratively, that is, the process must be restarted periodically with the best estimated eigenvectors associated with the required eigenvalues. These eigenvectors can also be improved by choosing a polynomial that amplifies

the components of the required eigendirections while damping those in the unwanted ones. This amounts to finding, at each restart, a polynomial $p^*$ that solves the minimax problem

$$\min_{p \in \mathcal{P}} \max_{z \in D} |p(z)| \tag{1}$$

where $\mathcal{P}$ is some set of polynomials and $D$ is a domain that contains the unwanted eigenvalues. These techniques have already been used for linear systems [7, 8] and for eigenvalue problems [1, 5, 11–13]. The domain $D$ is often delimited by an ellipse and the polynomial $p^*$ is a Chebyshev polynomial. However, the acceleration schemes described in these works deal with real matrices and take into great account the symmetry with respect to the real axis of the spectrum of these matrices. This property does not hold for complex matrices and therefore the construction of the domain $D$ and the polynomial $p^*$ is more difficult.

In this paper, we consider a new acceleration scheme for the complex non hermitian eigenvalue problem. We will restrict ourselves to the case where the rightmost eigenvalues are needed. Section 2 provides background and notations for the Chebyshev-Arnoldi method. Section 3 exhibits a new polynomial acceleration scheme for complex non hermitian matrices. Section 4 is devoted to numerical tests taken from practical problems.

# 2. The Arnoldi-Chebyshev method

Let $A$ be a large sparse complex non Hermitian diagonalizable $n \times n$ matrix whose eigenvalues $\lambda_1, \ldots, \lambda_n$ are labeled in decreasing order of their real parts: $\Re e\lambda_1 \geq \cdots \geq \Re e\lambda_n$ and $u_1, \ldots, u_n$ their corresponding eigenvectors. We suppose that we are interested in computing $(\lambda_i, u_i)$ $i = 1, \ldots, r$ $(r \ll n)$. These eigenpairs may be approximated in the following way: From $V_1 \in C^{n \times r}$, let $\mathcal{V}_m = [V_1, \ldots, V_m] \in C^{n \times mr} (r < m \ll n)$ be the block Arnoldi[1] basis of the Krylov subspace $\mathcal{K}_m = \text{span}\{V_1, AV_1, \ldots, A^{m-1}V_1\}$ satisfying:

$$A\mathcal{V}_m = \mathcal{V}_m H_m + [0, \ldots, 0, V_{m+1}H_{m+1,m}] \tag{2}$$

where $H_m = \mathcal{V}_m^H A \mathcal{V}_m$ is a block Hessenberg matrix and $H_{m+1,m} = V_{m+1}^H A V_m$. Let $H_m Y = Y\Theta$ with $\Theta = \text{diag}(\theta_1, \ldots, \theta_r)$, $Y = [y_1, \ldots, y_r]$ corresponding to the $r$ rightmost eigenpairs of $H_m$ and $X = \mathcal{V}_m Y$ the matrix whose columns approximate the sought eigenvectors of $A$. Then (2) reduces to

$$\|AX - X\Theta\|_2 = \|H_{m+1,m}\tilde{Y}\|_2 \tag{3}$$

where $\tilde{Y}$ is the last $r \times r$ block of $Y$. In order to improve the approximate eigenpair $(\Theta, X)$ of $A$, we look for a polynomial $p^*$ such that the columns of $p^*(A)X$ will be a better approximation of $u_1, \ldots, u_r$ than $X$. This may be done in the following way:

**Algorithm 1: Arnoldi-Chebyschev**

1. **Start:**
   Choose an initial block $V_1 \in C^{n \times r}$ and the size $m$ of the Krylov subspace.
2. **Block-Arnoldi:**
   Orthonormalize the columns of $V_1$ and generate an orthogonal basis $\mathcal{V}_m$ of the Krylov subspace $\mathcal{K}_m(A, V_1) = \text{span}\{V_1, AV_1, \ldots, A^{m-1}V_1\}$.

[1]The block version may, in certain cases, be more efficient than the standard one [12].

Compute the rightmost eigenpairs $(\tilde{\lambda}_i, \tilde{y}_i)_{1\leq i\leq r}$ of $H_m \equiv \mathcal{V}_m^H A \mathcal{V}_m$.

**3. Restart:**

Compute the corresponding approximate eigenvectors $\tilde{u}_i = \mathcal{V}_m \tilde{y}_i$ $i = 1, \ldots, r$.
If convergence stop. Else compute polynomial $p^*$ that solves approximately (1) and set $V_1 = [p^*(A)\tilde{u}_1, \ldots, p^*(A)\tilde{u}_r]$. Go to 2.

The aim of the polynomial acceleration is to enhance the columns of the restarting block $V_1$ in the needed eigendirections $\{u_i\}_{1\leq i\leq r}$. We see that each $p(A)u_j$ $j = 1, \ldots, r$ can be expanded in the basis $u_1, \ldots, u_n$ as follows:

$$p(A)u_j = \alpha_j p(\lambda_j)u_j + \sum_{k\neq j} \alpha_k p(\lambda_k)u_k, \quad j = 1, \ldots, r. \tag{4}$$

Obviously we are thus seeking a polynomial $p^*$ which achieves the minimum

$$\min_{\substack{p\in\Pi_k \\ p(\lambda_r)=1}} \max_{\lambda\in\mathcal{E}} |p(\lambda)| \tag{5}$$

where $\mathcal{E}$ is a domain containing the unwanted eigenvalues $\lambda_i$ for $i \in [r+1, n]$, and $\Pi_k$ denotes the space of all polynomials of degree not exceeding $k$. The condition $p(\lambda_r) = 1$ is only used for normalization purpose.

Let $\mathcal{E} = \mathcal{E}(c, e, a)$ be an ellipse containing the set $\{\lambda_{r+1}, \ldots, \lambda_n\}$ and having center $c$, focis $c+e$, $c-e$ and major semi-axis $a$. An asymptotically best min-max polynomial for (5) is the polynomial [3]

$$p^*(z) = \frac{T_k\left(\dfrac{z-c}{e}\right)}{T_k\left(\dfrac{\lambda_r - c}{e}\right)} \tag{6}$$

where $T_k$ is the Chebyshev polynomial of degree $k$ of the first kind.

In the next section we discuss the strategy that we have adopted for constructing the ellipse $\mathcal{E}$.

# 3. Computation of the ellipse $\mathcal{E}$

In practice we replace the set $\{\lambda_{r+1}, \ldots, \lambda_n\}$ by $\tilde{\mathcal{R}}_u = \{\tilde{\lambda}_{r+1}, \ldots, \tilde{\lambda}_{mr}\}$ which corresponds to the rest of the spectrum of $H_m$. An infinity of ellipses may enclose the unwanted eigenvalues in $\tilde{\mathcal{R}}_u$ and exclude the wanted ones $\tilde{\mathcal{R}}_w = \{\tilde{\lambda}_1, \ldots, \tilde{\lambda}_r\}$. Hence we will add two more conditions that ensure the uniqueness of the desired ellipse.

Considering $\tilde{\lambda}_l \in \tilde{\mathcal{R}}_u$ the nearest approximate unwanted eigenvalue to the wanted ones with respect to the Euclidean norm, then we want the following conditions to be fulfilled:

- $\tilde{\lambda}_l$ belongs to the ellipse and is a minimal point of $|p^*(z)|$ on the ellipse.
- The desired ellipse has the minimal surface.

The motivation of the first condition is to discriminate as much as possible between the wanted and the unwanted eigenvalues which are close to each other. Indeed it is well known that

Arnoldi's method may have very slow convergence on clustered eigenvalues. Moreover, the approximate wanted eigenvalues may, at least at the beginning of the process, be far from the exact ones and therefore there is no guarantee that $\tilde{\mathcal{R}}_u$ and the wanted eigenvalues will not intersect.

The motivation of the second condition is to minimize the risk mentioned in the first situation. Notice that even in the real case, there is no way to fully circumvent this difficulty.

Considering the above conditions, the computation the ellipse $\mathcal{E}(c,e,a)$ occurs in two steps: (1) Choice of the center $c$ and (2) Computation of the main axis direction, $|a|$ and $|e|$. These two points are discussed in more details in [4]. We only mention them briefly here:

- **Choice of the center:** The choice of the center of the ellipse is difficult considering the fact that it greatly depends on the location of the wanted and unwanted eigenvalues. Moreover, an inappropriate choice may imply that any ellipse enclosing the unwanted eigenvalues, contains also the wanted ones.

  To avoid such situations we have considered a set of centers $\{c_i\}_{i=1,\ldots,n_c}$ defined by the heuristic scheme

$$c_i = \frac{\sum_{k=r+1}^{m} w_k^{(i)} \tilde{\lambda}_k}{\sum_{k=r+1}^{m} w_k^{(i)}}, \quad i = 1, \ldots, n_c \tag{7}$$

  which ensures that the centers are in the convex hull of the unwanted eigenvalues $\tilde{\mathcal{R}}_u$. The choice of the weights $\{w_k^{(i)}\}$ is discussed in [4].

- **Computation of the main axis direction:** Considering the Joukowski mapping we can show that the Chebyshev polynomial of degree $k$, $T_k(\frac{z-c}{e})$ maps the ellipse $\mathcal{E}(c,e,a)$ onto the ellipse $\mathcal{E}(0,1,a')$ with $a' > 1$ [4, 10]. Moreover, one rotation on the initial ellipse $\mathcal{E}(c,e,a)$ is mapped on $k$ rotations onto the target ellipse $\mathcal{E}(0,1,a')$. Consequently, for $z \in \mathcal{E}(c,e,a)$, $|p^*(z)|$ as defined in (6) has $2k$ minimums. We impose $\tilde{\lambda}_l$ defined above to correspond to one of these minimums. Scanning for all possible constructions such that the searched ellipse contains $\tilde{\mathcal{R}}_u$ and excludes $\tilde{\mathcal{R}}_w$ we then choose the ellipse of minimal surface.

These two steps involve only scalar operations and therefore the computation of the ellipse is cheap.

# 4. Numerical experiments

The numerical experiments described in this section have been performed on an IBM/RISC 6000–590 computer using double precision. The stopping criterion is such that the relative residual corresponding to the computed pair $(\lambda, x)$ must satisfy $\frac{\|Ax-\lambda x\|_2}{\|x\|_2} \leq \varepsilon \|A\|_2$ with $\varepsilon = 10^{-6}$. If the spectral norm $\|A\|_2$ is not known we use the Frobenius norm $\|A\|_F$. Before considering our test examples, it is worth mentioning that the code we have implemented uses a block version of Arnoldi with a deflation technique that eliminates all the converged eigenpairs in previous steps. Let us illustrate the behavior of the algorithm on two representative test problems.

- **The Orr-Sommerfeld operator [6]:** Consider the operator defined by $\frac{1}{\alpha R}L^2y - i(ULy - U''y) - \lambda Ly = 0$, where $\alpha$ and $R$ are positive parameters, $\lambda$ is a spectral parameter number, $U = 1 - x^2$, $y$ is a function defined on $[-1, +1]$ with $y(\pm 1) = y'(\pm 1) = 0$, $L = \frac{d^2}{dx^2} - \alpha^2$. Discretizing this operator using the following approximation $x_j = -1 + jh$, $h = \frac{2}{n+1}$, $L_h = \frac{1}{h^2}\text{Tridiag}(1, -2 - \alpha^2h^2, 1)$, $U_h = \text{diag}(1 - x_1^2, \ldots, 1 - x_n^2)$ gives rise to the eigenvalue problem $\mathcal{A}u = \lambda u$ with $\mathcal{A} = \frac{1}{\alpha R}L_h - iL_h^{-1}(U_hL_h + 2I_n)$. Taking $\alpha = 1$, $R = 5000$, $n = 2000$ yields a complex non Hermitian matrix $\mathcal{A}$ (order = 2000, number of nonzero elements $= 4 \cdot 10^6$, $||\mathcal{A}||_F = 21929$), whose spectrum is plotted in Figure 1. We computed the five rightmost eigenpairs of $\mathcal{A}$. The results are shown in Figure 1 and Table 1.

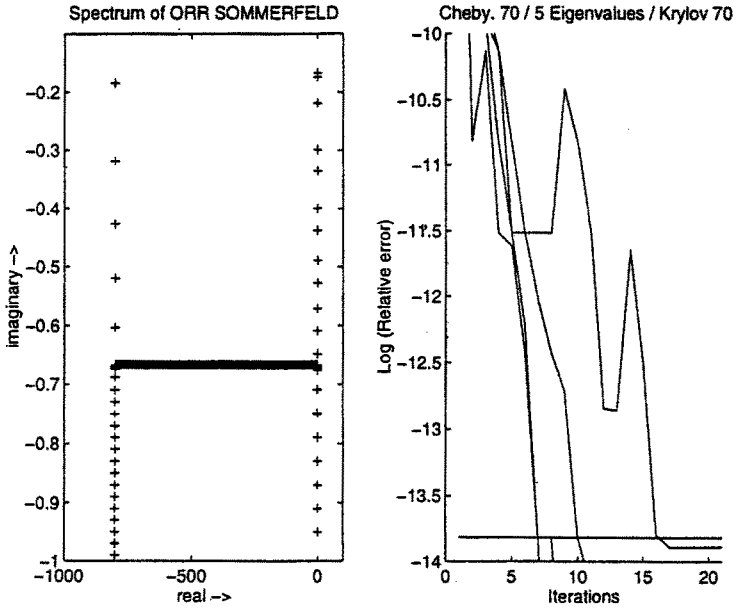


Figure 1. Spectrum (left) and the residual norm versus the number of iterations (right) for Orr-Sommerfeld

| Method for Orr-Sommerfeld $\alpha = 1$, $R = 5000$, $n = 2000$ | | | 5 eigenvalues | |
|---|---|---|---|---|
| Krylov Basis | Deflation | Cheby. Degree | nmult | Iterations |
| 40 | No | No | $\infty$ | $\infty$ |
| 40 | Yes | No | $\infty$ | $\infty$ |
| 40 | Yes | 40 | 67840 | 189 |
| 40 | Yes | 70 | 48530 | 81 |
| 70 | No | No | $\infty$ | $\infty$ |
| 70 | Yes | No | 103000 | 1482 |
| 70 | Yes | 40 | 38940 | 101 |
| 70 | Yes | 70 | 9620 | 21 |

Table 1. nmult: Number of matrix vector multiplications

- **The matrix Young1c:** This matrix comes from the Harwell-Boeing [2] set of test matrices. It arises when modeling the acoustic scattering phenomenon. It is complex with order 841 and contains 4089 nonzero elements. $||A||_F = 6484$. The spectrum is plotted in Figure 2. The results obtained with a basis $m = 40$ are given in Figure 2 and Table 2.

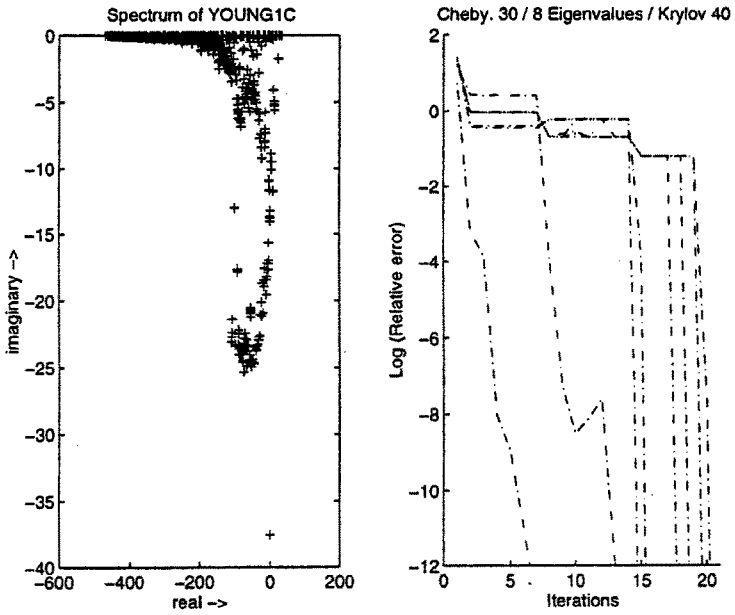


Figure 2. Spectrum (left) and the residual norm versus the number of iterations (right) for Young1c

| Method | 6 eigenvalues | | 8 eigenvalues | |
|---|---|---|---|---|
| | nmult | Iterations | nmult | Iterations |
| Block Arnoldi | 36000 | 1000 | $\infty$ | $\infty$ |
| + Deflation | 1908 | 53 | 14160 | 354 |
| + Chebyshev $T_{30}$ | 1182 | 7 | 4723 | 21 |

Table 2. nmult: Number of matrix vector multiplications

# 5. Conclusion

We have shown how to apply Chebyshev eigenvalue acceleration in the complex case. Numerical results indicate that the algorithm performs well and that the acceleration is useful and may be necessary in some practical problems.

# References

[1] Chatelin, F., Ho, D., and Bennani, M. *Arnoldi-Tchebychev procedure for large scale nonsymmetric matrices.* Mathematical Modelling and Numerical Analysis **1** (1990), pp. 53–65.

[2] Duff, I. S., Grimes, R. G., and Lewis, J. G. *Sparse matrix test problems.* ACM Trans. Math. Softw. **15** (1989), pp. 1–14.

[3] Fischer, B. and Freund, R. *Chebyshev polynomials are not always optimal.* J. Approximation Theory **65** (1991), pp. 261–273.

[4] Heuveline, V. *Polynomial acceleration in the complex plane.* Technical report, Irisa/Inria, 1995.

[5] Ho, D. *Tchebychev acceleration technique for large scale nonsymmetric matrices.* Numer. Math. **56** (1990), pp. 721–734.

[6] Kerner, W. *Large-scale complex eigenvalue problems.* J. Comp. Phys. **85** (1989), pp. 1–85.

[7] Manteuffel, T. A. *The Tchebychev iteration for nonsymmetric linear system.* Numer. Math. **28** (1977), pp. 307–327.

[8] Manteuffel, T. A. *Adaptive procedure for estimating parameters for the nonsymmetric Tchebychev iteration.* Numer. Math. **31** (1978), pp. 183–208.

[9] Moler, C. B. and Stewart, G. W. *An algorithm for generalized matrix eigenvalue problems.* SIAM J. Num. Anal. **10** (1973), pp. 241–256.

[10] Rivlin, T. J. *The Chebyshev polynomials: from approximation theory to algebra and number theory.* J. Wiley and Sons Inc., New-York, 1990.

[11] Saad, Y. *Numerical methods for large eigenvalue problems. Algorithms and architectures for advanced scientific computing.* Manchester University Press, Manchester, 1992.

[12] Sadkane, M. *A block Arnoldi-Chebyshev method for computing the leading eigenpairs of large sparse unsymmetric matrices.* Numer. Math. **64** (1993), pp. 181–193.

[13] Yamamoto, Y. and Ohtsubo, H. *Subspace iteration accelerated by using Chebyshev polynomials for eigenvalue problems with symmetric matrices.* Int. J. Numer. Methods Eng. **10** (1976), pp. 935–944.

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