Theory and software for Krylov methods for the computation of the frequency response of large acoustic finite element models.

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ABSTRACT.
The frequency analysis of acoustic cavities and structures often requires the solution of a large number of linear systems with the frequency as a parameter. The aim of this talk is to review theory and software for Krylov methods for solving this problem efficiently, and pose remaining open questions. We also introduce a memory efficient Arnoldi algorithm and present numerical examples from applications that show the behaviour of the various techniques. We show the connection with the vector-Padé method.

1 Introduction

The goal is to solve the sequence of linear systems

$$(K + \omega C + \omega^2 M)x(\omega) = f_0 + \omega f_1 \tag{1}$$

where ω is a parameter. In the frequency analysis of acoustics and structures, the engineer is interested in $x(\omega)$ for ω in the frequency range $\Omega = [\omega_{\min}, \omega_{\max}]$. The matrices K, $-iC$, and $-M$ are the stiffness, damping, and mass matrices respectively. They are large $n \times n$ matrices and usually sparse. In practical computations, the interval Ω is discretized into the set $\{\omega_1, \ldots, \omega_k\}$, where k typically ranges from 10 to 1000. Usually, the solution of (1) is obtained by a direct method, so that k sparse matrix factorizations and k backtransformations are required. Simoncini et al. [14, 15] and Meerbergen [10] suggest the use of Krylov subspaces to speed-up the computation, which is strongly related to the Ritz vector technique [16] [7] [3]. In other situations, the Padé via Lanczos method is used [4] [2] [9]. The properties of Krylov methods cannot be fully exploited because of the quadratic term in ω. Instead, (1) is 'linearized' into a problem of the form

$$(A - \omega B)y(\omega) = g \tag{2}$$

of double dimension to which a Krylov method is applied [14, 15]. The fact that the Krylov vectors have length $2n$ instead of n may limit their practical use, especially when the Arnoldi method is used for which a large number of vectors need to be stored [1, 8] : m iterations of the Arnoldi method require the storage of the order of $(2m + 3)n$ floating point numbers (real or complex). In this paper, we introduce an adapted Arnoldi scheme, that uses the structure of the linearized problem (2) to reduce the memory requirements to $(m + 2)n$ floating point numbers.

The paper is organized as follows. In §2, we review the Arnoldi method for (2): we introduce a linearization for (1) and present a modification of Arnoldi's method that saves memory. We call this the Q-Arnoldi method, where Q stands for 'quadratic'. In §5 we show a numerical example arising from acoustics.

2 The Arnoldi method

Assume that we want to compute the solution of (2) for ω near zero. The first step consists of preconditioning (2) into

$$A^{-1}(A - \omega B)y(\omega) = A^{-1}g \tag{3}$$

with N-by-N matrices A and B and where it is important to note that g does not depend on ω. We refer to the books on iterative linear system solvers by Greenbaum [6] and Saad [13] for convergence properties. If $\omega \approx 0$ then $A^{-1}(A - \omega B) \approx I$ so it is clear that A^{-1} is a suitable preconditioner.

The Arnoldi method applied to $S = A^{-1}B$ and $b = A^{-1}g$ produces the Krylov subspace

$$\mathcal{K}_m(S, b) = \text{span}\{b, Sb, S^2b, \ldots, S^{m-1}b\} .$$

It computes the $N \times m$ matrix $\mathbf{V}_m = [\mathbf{v}_1, \ldots, \mathbf{v}_m]$ of iteration vectors, the upper Hessenberg matrix H_m and the residual term $\mathbf{v}_{m+1}\beta_m$ so that

$$A^{-1}B\mathbf{V}_m - \mathbf{V}_m H_m \quad = \quad \mathbf{v}_{m+1}\beta_m e_m^T \tag{4}$$

where $\mathbf{V}_{m+1}^* \mathbf{V}_{m+1} = I$. Equation (4) is called the Arnoldi recurrence relation. An algorithm for computing $\mathbf{V}_m$ and H_m is now given.

Algorithm 2.1 (Arnoldi method)
1. Set the initial vector $\mathbf{v}_1 = b/\|b\|_2$.
2. For $j = 1, \ldots, m$ *do*
2.1. Compute $\hat{\mathbf{v}}_j = A^{-1}B\mathbf{v}_j$
2.2. Compute the Arnoldi coefficients $h_j = \mathbf{V}_j^* \hat{\mathbf{v}}_j$.
2.3. Update $\tilde{\mathbf{v}}_j = \hat{\mathbf{v}}_j - \mathbf{V}_j h_j$.
2.4. Get the scalar $\beta_j = \|\tilde{\mathbf{v}}_j\|_2$ *and compute* $\mathbf{v}_{j+1} = \tilde{\mathbf{v}}_j/\beta_j$.
End do

Steps 2.2–2.4 orthogonalize $A^{-1}B\mathbf{v}_j$ against $\mathbf{v}_1, \ldots, \mathbf{v}_j$ into $\mathbf{v}_{j+1}$. The coefficients h_j form the jth column of H_m and β_j is the $j+1, j$ element of H_m.

An approximate solution to (3) is computed in Arnoldi's method [12] as $\tilde{y}(\omega) = \mathbf{V}_m z(\omega)$ where

$$z(\omega) \quad = \quad \|A^{-1}g\|(I - \omega H_m)^{-1} e_1 .$$

Let us now return to the solution of (1). We consider the case for which $f_1 = 0$. The case $f_1 \neq 0$ is discussed by Meerbergen and Robbé [11]. We need to find a pair of matrices A and B so that the solution of (1) can be easily extracted from (2). A straightforward choice is

$$A = \begin{bmatrix} K & \\ & D \end{bmatrix}, \quad B = \begin{bmatrix} -C & -M \\ D & \end{bmatrix}, \quad g = \begin{pmatrix} f_0 \\ 0 \end{pmatrix}, \quad y = \begin{pmatrix} x \\ \omega x \end{pmatrix} \tag{5}$$

where D can be any nonsingular matrix. It is easy to see that

$$A^{-1}B = \begin{bmatrix} -K^{-1}C & -K^{-1}M \\ I & \end{bmatrix} \tag{6}$$

from which D disappears. Usually, we shift K, C into

$$\begin{aligned} K &:= K + \sigma C + \sigma^2 M \\ C &:= C + 2\sigma M , \end{aligned}$$

where σ is chosen near the ω's of interest. This improves the speed of convergence.

The storage of the Arnoldi vectors in Algorithm 2.1 requires $2n(m+1)$ floating point numbers. We decompose the jth Arnoldi vector into $\mathbf{v}_j = \begin{pmatrix} v_j \\ w_j \end{pmatrix}$ with $v_j, w_j \in \mathbf{C}^n$. From (4), it can be demonstrated that

$$v_j = W_j H_j + w_{j+1}\beta_j e_j^* . \tag{7}$$

The Q-Arnoldi algorithm [11] does not store v_j but applies (7) when needed. This implies that m Arnoldi iterations require only the storage of the vectors W_m, v_{m+1} and w_{m+1} to evaluate the recurrence relation, i.e. $(2+m)n$ floating point numbers.

Algorithm 2.2 (Q-Arnoldi)
1. Let $v_1 = K^{-1}f_0/\|K^{-1}f_0\|_2$ and $w_1 = 0$.
2. For $j = 1, \ldots, m$ do
   2.1. Compute $\hat{v}_j = K^{-1}(-Cv_j - Mw_j)$ and $\hat{w}_j = v_j$.
   2.2. Compute the Arnoldi coefficients

$$h_j = \begin{bmatrix} \underline{H}_{j-1}^*(W_j^*\hat{v}_j) + W_{j-1}^*\hat{w}_j \\ v_j^*\hat{v}_j + w_j^*\hat{w}_j \end{bmatrix} .$$

   2.3. Update

$$\begin{aligned} \tilde{v}_j &= \hat{v}_j - [W_j \;\; v_j]\left(\begin{bmatrix} \underline{H}_{j-1} & 0 \\ 0 & 1 \end{bmatrix} h_j\right) \\ \tilde{w}_j &= \hat{w}_j - W_j h_j \; . \end{aligned}$$

   2.4. Normalize $v_{j+1} = \tilde{v}_j/\beta_j$ and $w_{j+1} = \tilde{w}_j/\beta_j$ with $\beta_j = (\|\tilde{v}_j\|^2 + \|\tilde{w}_j\|^2)^{1/2}$.
   2.5. Set the jth column of $\underline{H}_j$ as $[h_j; \beta_j]$.
   End for

From the finite precision arithmetic analysis in [11], it appears that the Q-Arnoldi algorithm is as numerically stable as the Arnoldi algorithm, if $\kappa(H_m)$ is of the order of 1.

3 Vector-Padé connection

The Arnoldi solution is computed as $x(\omega) = V_k z(\omega)$ and it can be shown that it can be written in the form

$$x(\omega) = \sum_{j=1}^{m} \frac{x_j}{1 + \omega\theta_j}$$

where θ_j is an eigenvalue of H_m. This is a partial fraction form and is called a vector-Padé approximation. For the Padé connection, see [4, 10]. The poles are the Ritz values, which are good approximations to the frequencies for which peaks are produced (eigenfrequencies). This shows that if the spectral density of the underlying physical problem is high, a large m is required to accurately approximate $x(\omega)$.

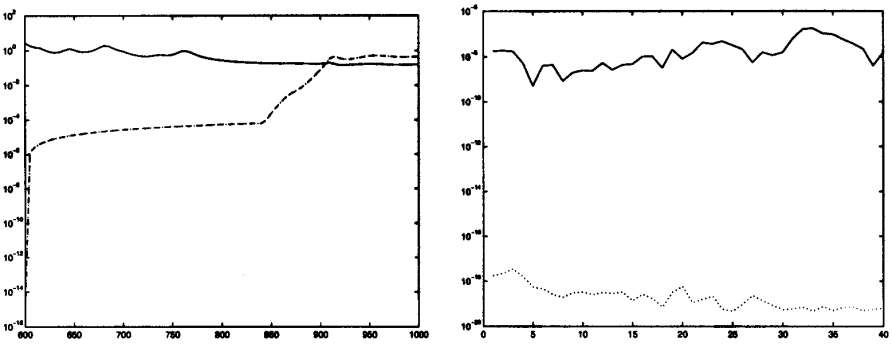
4 Software

Free Field Technologies has developed a Fortran subroutine that solves (1). The major features are the following:

- a reverse communication interface for the operations with the matrices K, C and M and returning the solution $x(\omega)$ to the user ;
- Availability of both Arnoldi's method and Lanczos' method ;
- Out-of-core storage of Krylov vectors ;
- Error estimation ;
- Automatic selection of shifts σ to make the solution more efficient.

5 Numerical example

In this section we study the problem of an acoustic box with walls covered with carpet with dimensions 0.54m × 0.54m × 0.55m. The material has a complex speed of sound $340 + i3.4$ and the density is 1.225kg/m^3. The box is discretized with 64710 hexahedral elements. The excitation consists of an acceleration in a disk on a corner of one face of the box. It consists of a constant (unit) contribution 1



a. solid: $\|x(\omega)\|$
dashed: $\rho(\omega)$ for Arnoldi
dotted: $\rho(\omega)$ for Q-Arnoldi

b. solid: (9) for Arnoldi
dashed: (9) for Q-Arnoldi
dotted: (10) for Q-Arnoldi

Figure 1: Comparison of Arnoldi and Q-Arnoldi for the numerical example. Figure a shows the residual norms (8), Figure b shows the error on (4) and (10).

Table 1: Timings in seconds for the box problem. Comparison between the Arnoldi, Lanczos and direct methods.

	Arnoldi	Lanczos	direct
factorizations	5	7	181
time	522	601	7501

and a frequency dependent component 0.001ω on a few nodes of the disk ; therefore, the excitation has the form $f_0 + \omega f_1$.

The matrices and right-hand side are produced by ACTRAN [5]. The problem to be solved has the form (1) and $n = 13,623$. The frequencies of interest are $\omega = 600, \ldots, 1000$. The problem is shifted with a shift $\sigma = 600$. We solved this problem by running 40 iterations of the Algorithms 2.1 and 2.2. The computations were carried out in ACTRAN on an IBM RS/6000. In this section we compare the quality of the results. Figure 1.a shows the residual norms

$$\rho(\omega) := \|(K + \sigma C + \sigma^2 M)^{-1}((K + \omega C + \omega^2 M)\tilde{x}(\omega) - f_0 - \omega f_1)\| \tag{8}$$

for both methods in function of ω. We notice no visual difference between the residual norm curves for both algorithms. Figure 1.b shows the error on the recurrence relation (4)

$$\left\| S \begin{pmatrix} v_j \\ w_j \end{pmatrix} - \begin{pmatrix} V_{j+1} \\ W_{j+1} \end{pmatrix} \underline{H}_j e_j \right\| \tag{9}$$

for both methods and

$$\|v_j - W_{j+1}\underline{H}_j e_j\| \tag{10}$$

for Q-Arnoldi for $j = 1, \ldots, m$. We notice that the recurrence error norm curves for both algorithms show no visual difference. Also note that (10) is significantly smaller than (9). Note that $\kappa(\underline{H}_m) \approx 967.5$, which indicates that we expect the Q-Arnoldi algorithm to be as accurate as the Arnoldi algorithm.

In Table 1, we compare timings using the direct method and the Arnoldi and Lanczos method for the frequencies $\omega = 600, 605, 610, \ldots, 1500$. The Arnoldi and Lanczos method use a subspace of dimension 40. The Lanczos method requires two more factorizations, i.e. new shifts σ because of loss of orthogonality [10].

References

[1] W. ARNOLDI, *The principle of minimized iterations in the solution of the matrix eigenvalue problem*, Quart. Appl. Math., 9 (1951), pp. 17–29.

[2] Z. BAI AND Q. YE, *Error estimation of the Padé approximation of transfer functions via the Lanczos process*, ETNA, 7 (1998), pp. 1–17.

[3] J.-P. COYETTE, *Evaluation of different computational strategies for acoustic finite element modelling*, in Proceedings of the Institute of Acoustics, vol. 12, 1990, pp. 851–864.

[4] P. FELDMAN AND R. W. FREUND, *Efficient linear circuit analysis by Padé approximation via the Lanczos process*, IEEE Trans. Computer-Aided Design, CAD-14 (1995), pp. 639–649.

[5] FREE FIELD TECHNOLOGIES, *ACTRAN Rev.2.0, User's Manual*, 2002.

[6] A. GREENBAUM, *Iterative methods for solving linear systems*, SIAM, Philadelphia, PA, USA, 1997.

[7] H. C. IBRAHIMBEGOVIC, E. L. CHEN, E. L. WILSON, AND R. L. TAYLOR, *Ritz method for dynamic analysis of large discrete linear systems with non-proportional damping*, Earthquake Engineering and Structural Dynamics, 19 (1990), pp. 877–889.

[8] R. B. LEHOUCQ, D. C. SORENSEN, AND C. YANG, *ARPACK USERS GUIDE: Solution of Large Scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods*, SIAM, Philadelphia, PA, USA, 1998.

[9] M. MALHOTRA AND P. M. PINSKY, *Efficient computation of multi-frequency far-field solutions of the Helmholtz equation using Padé approximation*, J. Comput. Acoustics, 8 (2000), pp. 223–240.

[10] K. MEERBERGEN, *The solution of parametrized symmetric linear systems*, SIAM J. Matrix Anal. Appl., (2002). To appear.

[11] K. MEERBERGEN AND M. ROBBÉ, *The Arnoldi method for the solution of the quadratic eigenvalue problem and parametrized equations*, Technical Report KM-2002-2, Free Field Technologies, 16 place de l'Université, 1348 Louvain-la-Neuve, Belgium, 2002.

[12] Y. SAAD, *Krylov subspace methods for solving unsymmetric linear systems*, Math. Comp., 37 (1981), pp. 105–126.

[13] ——, *Iterative Methods for Linear Systems*, PWS Publishing, Boston, 1996.

[14] V. SIMONCINI, *Linear systems with a quadratic parameter and application to structural dynamics*, in Iterative Methods in Scientific Computation II, D. R. Kincaid and A. Elster, ed., vol. 5 of IMACS Series in Computational and Applied Mathematics, 1999, pp. 451–461.

[15] V. SIMONCINI AND F. PEROTTI, *On the numerical solution of* $(\lambda^2 A + \lambda B + C)x = b$ *and application to structural dynamics*, SIAM J. Sci. Comput., 23 (2002), pp. 1876–1898.

[16] E. L. WILSON, M.-W. YUAN, AND J. M. DICKENS, *Dynamic analysis by direct superposition of Ritz vectors*, Earthquake Engineering and Structural Dynamics, 10 (1982), pp. 813–821.