Arnoldi methods for structure-preserving dimension reduction of second-order dynamical systems

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1 Introduction

Consider the multi-input multi-output (MIMO) time-invariant second-order problem

$$\Sigma_N : \begin{cases} M\ddot{q}(t) + D\dot{q}(t) + Kq(t) = F\,u(t) \\ y(t) = L^T q(t) \end{cases} \tag{1}$$

with initial conditions $q(0) = q_0$ and $\dot{q}(0) = \dot{q}_0$. Here t is the time variable. $q(t) \in \mathcal{R}^N$ is a vector of state variables. N is the state-space dimension. $u(t)$ and $y(t)$ are the input force and output measurement functions, respectively. M, D, $K \in \mathcal{R}^{N\times N}$ are system matrices, such as mass, damping and stiffness as known in structural dynamics, and acoustics. We have $F \in \mathcal{R}^{N\times p}$ and $L \in \mathcal{R}^{N\times m}$ are input distribution and output measurement matrices, respectively.

Second-order systems Σ_N of the form (1) arise in the study of many types of physical systems, with common examples being electrical, mechanical and structural systems, electromagnetics and microelectromechanical systems (MEMS) [Cra81, Bal82, CZB+00, BBC+00, RW00, Slo02, WMSW02].

We are concerned with the system Σ_N of very large state-space dimension N. The analysis and design of large models becomes unfeasible with reasonable computing resources and computation time. It is necessary to obtain a reduced-order model which retains important properties of the original system, and yet is efficient for practical use. A common approach for reduced-order modeling is to first rewrite Σ_N as a mathematically equivalent linear system and then apply linear system dimension reduction techniques, such as explicit and implicit moment-matching and balanced truncation. The reader can find surveys of these methods, for example, in [Fre00, ASG01, Bai02].

There are two major drawbacks with such a linearization approach: the corresponding linear system has a state space of double dimension which increases memory requirements, and the reduced system is typically linear and the second-order structure of the original system is not preserved.

The preservation of the second-order structure is important for physical interpretation of the reduced system in applications. In addition, respecting the second-order structure also leads more stable, accurate and efficient reduced systems. This book contains three chapters on second (or higher) order systems. Chapter **??** discusses Krylov-subspace based and SVD-based methods for second-order structure preserving model reduction. For the Krylov-subspace based techniques, conditions on the projectors that guarantee the reduced second-order system tangentially interpolates the original system at given frequencies are derived. For SVD-based techniques, a second-order balanced truncation method is derived from second order gramians. Chapter **??** presents Krylov methods based on projections onto a subspace which is spanned by a properly partitioned Krylov basis matrices obtained by applying standard Krylov-subspace techniques to an equivalent linearized system. In this chapter, we present modified Arnoldi methods which are specifically designed for the second-order system, without via linearization. We call them as second-order Krylov subspace techniques. In a unified style, we will review recently developed Arnoldi-like dimension reduction methods that preserve the second-order structure. We will focus on the presentation of essential ideas behind these methods, without going into details on elaborate issues on robustness and stability of implementations and others.

For simplicity, we only consider the single-input single output (SISO) system in this paper. Denote $F = f$ and $L = l$, where f and l are column vectors of dimension N. The extension to the MIMO case requires block Arnoldi-like methods, which is beyond the scope this paper. The matrices M, D, and K often have particular properties such as symmetry, skew-symmetry, and positive (semi-)definiteness. We do not exploit nor assume any of such properties. We only assume that K is invertible. If this would not be the case, we assume there is an $s_0 \in \mathcal{R}$ so that $s_0^2 M + s_0 D + K$ is nonsingular.

2 Second-order system and dimension reduction

The second-order system Σ_N of the form (1) is the representation of Σ_N in the time domain, or the state space. Equivalently, one can also represent the system in the frequency domain via the Laplace transform. Under the assumption of the initial conditions $q(0) = q_0 = 0$ and $\dot{q}(0) = \dot{q}_0 = 0$ and $u(0) = 0$. Then the input $U(s)$ and output $Y(s)$ in the frequency domain are related by the *transfer function*

$$H(s) = l^T(s^2 M + sD + K)^{-1} f, \tag{2}$$

where physically meaningful values of the complex variable s are $s = \mathtt{i}\omega$, $\omega \geq 0$ is referred to as the *frequency*. The power series expansion of $H(s)$ is formally given by

$$H(s) = m_0 + m_1 s + m_2 s^2 + \cdots = \sum_{\ell=0}^{\infty} m_\ell s^\ell,$$

where m_ℓ for $\ell \geq 0$ are called *moments*. The moment m_ℓ can be expressed as the inner product of the vectors l and r_ℓ:

$$m_\ell = l^T r_\ell \quad \text{for} \quad \ell \geq 0, \tag{3}$$

where the vector sequence $\{r_\ell\}$ is defined by the following linear homogeneous second-order recurrence relation

$$\begin{aligned} r_0 &= K^{-1} b \\ r_1 &= -K^{-1} D r_0 \\ r_\ell &= -K^{-1}(D r_{\ell-1} + M r_{\ell-2}) \quad \text{for} \quad \ell = 2, 3, \ldots \end{aligned} \tag{4}$$

As mentioned above, we assume that K is nonsingular, otherwise, see the discussion in section 5. The vector sequence $\{r_\ell\}$ is called a *second-order Krylov vector sequence*. Correspondingly, the subspace spanned by the vector sequence $\{r_\ell\}$ is called a *second-order Krylov subspace*:

$$\mathcal{G}_n(A, B; r_0) = \text{span}\{r_0, r_1, r_2, \ldots r_{n-1}\}, \tag{5}$$

where $A = -K^{-1}D$ and $B = -K^{-1}M$. When the matrices A and B, i.e., the matrices M, D and K, and r_0 are known from the context, we will drop them in our notation, and simply write $\mathcal{G}_n$.

Let Q_n be an orthonormal basis of $\mathcal{G}_n$, i.e.,

$$\mathcal{G}_n = \text{span}\{Q_n\} \text{ and } Q_n^T Q_n = I.$$

An orthogonal projection technique of dimension reduction onto the subspace $\mathcal{G}_n$ seeks an approximation of $q(t)$, constrained to stay in the subspace spanned by the columns of Q_n, namely

$$q(t) \approx Q_n z(t) \ .$$

This is often referred to as the *change-of-state coordinates*. Then by imposing the so-called Galerkin condition:

$$M Q_n \ddot{z}(t) + D Q_n \dot{z}(t) + K Q_n z(t) - f\, u(t) \ \perp \ \mathcal{G}_n,$$

we obtain the following reduced-order system:

$$\Sigma_n : \ \begin{cases} M_n \ddot{z}_n(t) + D_n \dot{z}_n(t) + K_n z(t) = f_n\, u(t) \\ \tilde{y}(t) = l_n^T z(t) \end{cases}, \tag{6}$$

where $M_n = Q_n^T M Q_n$, $D_n = Q_n^T D Q_n$, $K_n = Q_n^T K Q_n$, $f_n = Q_n^T f$ and $l_n = Q_n^T l$. We note that by explicitly formulating the matrices M_n, D_n and K_n in Σ_n, essential structures of M, D and K are preserved. For example, if M is symmetric positive definite, so is M_n. As a result, we can preserve the stability, symmetry and physical meaning of the original second-order system Σ_N. This is in the same spirit of the widely used PRIMA algorithm for passive reduced-order modeling of linear dynamical systems arising from interconnect analysis in circuit simulations [OCP98].

The use of the second-order Krylov subspace $\mathcal{G}_n$ for structure-preserving dimension reduction of the second-order system Σ_N has been studied by Su and Craig back to 1991 [SCJ91], although the subspace $\mathcal{G}_n$ is not explicitly defined and exploited as presented here. It has been revisited in recent years [RW00, Bai02, Slo02, BS04a, SL04, MR03]. It has been applied to very large second-order systems from structural analysis and MEMS simulations. The work of Meyer and Srinivasan [MS96] is an extension of balancing truncation methods for the second-order system. Recent such effort includes [CLM+02]. Another structure-preserving model reduction technique is recently presented in [GCFP03]. Those two approaches focus on the application of moderate size second-order systems.

The transfer function $h_n(s)$ and moments $m_\ell^{(n)}$ of the reduced second-order system Σ_n in (6) are defined similar to the ones of the original system Σ_N, namely,

$$h_n(s) = l_n^T (s^2 M_n + s D_n + K_n)^{-1} f_n$$

and

$$m_\ell^{(n)} = l_n^T r_\ell^{(n)} \quad \text{for} \quad \ell \geq 0 \ ,$$

where $r_\ell^{(n)}$ are the second-order Krylov vectors as defined in (4) associated with the matrices M_n, D_n and K_n.

One way to assess the quality of the approximation is by comparing the number of moments matched between the original system Σ_N and the reduced-order system Σ_n. The following theorem shows that the structure-preserving reduced system Σ_n matches as many moments as the linearization approach (see section 3). A rigorous proof of the theorem can be found in [BS04a].

Moment-matching Theorem. *The first n moments of the original system Σ_N in (1) and the reduced system Σ_n in (6) are matched, i.e., $m_\ell = m_\ell^{(n)}$ for $\ell = 0, 1, 2, \ldots, n-1$. Hence $h_n(s)$ is an n-th Padé-type approximant of the transfer function $h(s)$:*

$$h(s) = h_n(s) + \mathcal{O}(s^n).$$

Furthermore, if the original system Σ_N is symmetric, i.e., M, D and K are symmetric and $f = l$, then the first $2n$ moments of $h(s)$ and $h_n(s)$ are equal and $h_n(s)$ is an n-th Padé approximant of $h(s)$:

$$h(s) = h_n(s) + \mathcal{O}(s^{2n}).$$

The gist of structure-preserving dimension reduction of the second-order system Σ_N is now on how to efficiently compute an orthonormal basis Q_n of the second-order Krylov subspace $\mathcal{G}_n$. In section 4, we will discuss recently developed Arnoldi-like procedures for computing such an orthonormal basis.

3 Linearization method

In this section, we review the Arnoldi-based linearization approach for the dimension reduction of Σ_N. By exploiting the underlying second-order structure of this approach, it leads to the recently proposed structure-preserving methods to be discussed in the following sections.

It is easy to see that the original second-order system Σ_N is mathematically equivalent to the following linear system:

$$\Sigma_N^L : \begin{cases} C\dot{x}(t) + Gx(t) = \widehat{f}\,u(t) \\ y(t) = \widehat{l}^T x(t) \end{cases}, \tag{7}$$

where

$$x(t) = \begin{bmatrix} q(t) \\ \dot{q}(t) \end{bmatrix}, \; C = \begin{bmatrix} D & M \\ -Z & 0 \end{bmatrix}, \; G = \begin{bmatrix} K & 0 \\ 0 & Z \end{bmatrix}, \; \widehat{f} = \begin{bmatrix} f \\ 0 \end{bmatrix}, \; \widehat{l} = \begin{bmatrix} l \\ 0 \end{bmatrix}. \tag{8}$$

Z is an arbitrary $N \times N$ nonsingular matrix.

An alternative linear system can be defined by the following system matrices

$$x(t) = \begin{bmatrix} q(t) \\ \dot{q}(t) \end{bmatrix}, \; C = \begin{bmatrix} 0 & M \\ -Z & 0 \end{bmatrix}, \; G = \begin{bmatrix} K & D \\ 0 & Z \end{bmatrix}, \; \widehat{f} = \begin{bmatrix} f \\ 0 \end{bmatrix}, \; \widehat{l} = \begin{bmatrix} l \\ 0 \end{bmatrix}. \tag{9}$$

Various linearizations have been proposed in the literature, see [TM01] for a survey. We consider the above two, since they can be used in the methods we discuss. The linearization discussed by [MW01] does not fit in this framework.

Note that both linearizations produce

$$-G^{-1}C = \begin{bmatrix} -K^{-1}D & K^{-1}M \\ I & 0 \end{bmatrix}. \tag{10}$$

The zero block in (10) is very important for Arnoldi-like methods discussed in this paper.

Let $\mathcal{K}_n(-G^{-1}C; \widehat{r}_0)$ denote the Krylov subspace based on the matrix $-G^{-1}C$ and the starting vector $\widehat{r}_0 = G^{-1}\widehat{f}$:

$$\mathcal{K}_n(-G^{-1}C; \widehat{r}_0) = \text{span}\{\widehat{r}_0, (-G^{-1}C)\widehat{r}_0, \ldots, (-G^{-1}C)^{n-1}\widehat{r}_0\}.$$

The following Arnoldi procedure is a popular numerically stable procedure to generate an orthonormal basis V_n of the Krylov subspace $\mathcal{K}_n(-G^{-1}C; \widehat{r}_0) \subseteq \mathcal{R}^{2N}$, namely,

$$\text{span}\{V_n\} = \mathcal{K}_n(-G^{-1}C; \widehat{r}_0)$$

and $V_n^T V_n = I$.

Algorithm 1 *Arnoldi procedure*

Input: $C, G, \widehat{f}, n$
Output: V_n
1. $v_1 = G^{-1}\widehat{f}/\|G^{-1}\widehat{f}\|_2$
2. *for* $j = 1, 2, \ldots, n$ *do*
3. $\quad r = -G^{-1}Cv_j$
4. $\quad h_j = V_j^T r$
5. $\quad r = r - V_j h_j$
6. $\quad h_{j+1,j} = \|r\|_2$
7. $\quad$ *stop if* $h_{j+1,j} = 0$
8. $\quad v_{j+1} = r/h_{j+1,j}$
9. *end for*

The governing equation of the Arnoldi procedure is

$$(-G^{-1}C)\, V_n = V_{n+1}\widehat{H}_n, \tag{11}$$

where $\widehat{H}_n = (h_{ij})$ is an $(n+1) \times n$ upper Hessenberg matrix and $V_{n+1} = [V_n\ v_{n+1}]$ is a $2N \times (n+1)$ matrix with orthonormal columns. By making the use of the orthonormality of the columns of V_{n+1}, it follows that

$$V_n^T(-G^{-1}C)\, V_n = H_n$$

where H_n is the $n \times n$ leading principal submatrix of $\widehat{H}_n$.

By the framework of an orthogonal projection dimension reduction technique, one seeks an approximation of $x(t)$, constrained to the subspace spanned by the columns of V_n, namely

$$x(t) \approx V_n z(t).$$

Then by imposing the so-called Galerkin condition:

$$G^{-1}CV_n\dot{z}(t) + V_n z(t) - G^{-1}\widehat{f}\,u(t) \ \perp\ \text{span}\{V_n\},$$

we obtain the following reduced-order system in linear form:

$$\Sigma_n^L : \begin{cases} C_n\dot{z}(t) + G_n z(t) = \widehat{f}_n\, u(t) \\ \tilde{y}(t) = \widehat{l}_n^T z(t) \end{cases} \tag{12}$$

where $C_n = -H_n$, $G_n = I_n$, $\widehat{f}_n = e_1\|G^{-1}\widehat{f}\|_2$, and $\widehat{l}_n = V_n^T\widehat{l}$.

It can be shown that the reduced linear system Σ_n^L matches the first n moments of the original linear system Σ_N^L, which are equal to the first n moments of the original second-order system Σ_N. In finite precision arithmetic,

reorthogonalization may lead to a smaller order for the same precision, see [Mee03]. The major disadvantages of this method include doubling the storage requirement, and the loss of the second-order structure for the reduced-order model.

We note that the Arnoldi procedure breaks down when $h_{j+1,j} = 0$ at iteration j. This happens if and only if the starting vector $\widehat{r}_0$ is a linear combination of j eigenvectors of $-G^{-1}C$. In addition, $\mathcal{K}_j(-G^{-1}C; \widehat{r}_0)$ is an invariant subspace and $\mathcal{K}_k(-G^{-1}C; \widehat{r}_0) = \mathcal{K}_j(-G^{-1}C; \widehat{r}_0)$ for all $k \geq j$. It can be shown that at the breakdown, the moments of the reduced-order system are identical to those of the original system, i.e., $h(s) \equiv h_j(s)$. Therefore, the breakdown is considered as a rare but lucky situation.

4 Modified Arnoldi procedures

Define the Krylov matrix K_n by

$$K_n = [\, \widehat{r}_0,\ (-G^{-1}C)\widehat{r}_0,\ (-G^{-1}C)^2\widehat{r}_0,\ \ldots,\ (-G^{-1}C)^{n-1}\widehat{r}_0\,].$$

It is easy to see that the Krylov matrix K_n can be rewritten in the following form:

$$K_n = \begin{bmatrix} r_0 & r_1 & r_2 & \cdots & r_{n-1} \\ 0 & r_0 & r_1 & \cdots & r_{n-2} \end{bmatrix}, \tag{13}$$

where the vectors $\{r_0, r_1, r_2, \ldots, r_{n-1}\}$ are defined by the second-order recurrences (4). It is well-known, for example see [Ste01, section 5.1], that the orthonormal basis V_n, generated by the Arnoldi procedure (Algorithm 1), is the orthogonal Q-factor of the QR factorization of the Krylov matrix K_n:

$$K_n = V_n R_n, \tag{14}$$

where R_n is some $n \times n$ upper triangular matrix. Partition V_n into the 2×1 block matrix

$$V_n = \begin{bmatrix} U_n \\ W_n \end{bmatrix},$$

then equation (14) can be written in the form

$$\begin{bmatrix} r_0 & r_1 & r_2 & \cdots & r_{n-1} \\ 0 & r_0 & r_1 & \cdots & r_{n-2} \end{bmatrix} = \begin{bmatrix} U_n \\ W_n \end{bmatrix} R_n.$$

It shows that we can generate an orthonormal basis Q_n of $\mathcal{G}_n$ by orthonormalizing the U-block vectors or the W-block vectors. The leads to the Q-Arnoldi method to be described in §4.1. The SOAR in §4.2 is a procedure to compute the orthonormal basis Q_n directly, without computing the U- or W-block first.

Before we present these procedures, we note that one can show that the Krylov subspace $\mathcal{K}_n(-G^{-1}C; \widehat{r}_0)$ can be *embedded* in the second-order Krylov subspace $\mathcal{G}_n(A, B; r_0)$, namely

$$\text{span}\{V_n\} \subseteq \text{span}\left\{ \begin{bmatrix} Q_n & 0 \\ 0 & Q_n \end{bmatrix} \right\}.$$

This is a very useful observation and can be applied to a number of cases, for example, to prove the moment-matching theorem. See [BS04a] for details.

4.1 Q-Arnoldi procedure

Recall from (10) that

$$-G^{-1}C = \begin{bmatrix} -K^{-1}D & -K^{-1}M \\ I & 0 \end{bmatrix}.$$

From the second block row of the governing equation (11) of the Arnoldi procedure, we have

$$U_n = W_{n+1}\widehat{H}_n. \tag{15}$$

We can exploit this relation to avoid the storage of the U-vectors with a slight increase of the computational cost. All products with U_n are to be replaced by the products of W_{n+1} and $\widehat{H}_n$. This observation has been made in [MR03] for the solution of the quadratic eigenvalue problem and parametrized equations. With the motivation of constructing an orthonormal basis of the second-order Krylov subspace $\mathcal{G}_n$, we derive the following algorithm.

Algorithm 2 *Q-Arnoldi procedure (W-version)*

Input: M, D, K, r_0, n
Output: Q_n
1. $u = r_0/\|r_0\|_2$ *and* $w_1 = 0$
2. *for* $j = 1, 2, \ldots, n$ *do*
3. $\quad r = -K^{-1}(Du + Mw_j)$
4. $\quad t = u$
5. $\quad h_j = \begin{bmatrix} \widehat{H}_{j-1}^T(W_j^T r) + W_{j-1}^T t \\ u^T r + w_j^T t \end{bmatrix}$
6. $\quad r = r - \begin{bmatrix} W_j & u \end{bmatrix} \left(\begin{bmatrix} \widehat{H}_{j-1} & 0 \\ 0 & 1 \end{bmatrix} h_j \right)$
7. $\quad t = t - W_j h_j$
8. $\quad h_{j+1,j} = (\|r\|_2^2 + \|t\|_2^2)^{1/2}$
9. $\quad$ *stop if* $h_{j+1,j} = 0$
10. $\quad u = r/h_{j+1,j}$
11. $\quad w_{j+1} = t/h_{j+1,j}$
12. *end for*
13. $Q_{n+1} = \texttt{orth}([W_{n+1} \quad u])$ $\quad$ *% orthogonalization*

We note that the function $\texttt{orth}(X)$ in step 13 stands for the modified Gram-Schmidt process or QR decomposition for generating an orthonormal basis for the range of X.

An alternative approach of the Q-Arnoldi method is to avoid the storage of the W-vectors. By equation (15) and noting that $w_1 = 0$, we have

$$W_{n+1}(:, 2:n+1) = U_n \widehat{H}(2:n+1, 1:n)^{-1} \ . \tag{16}$$

Operations with W_n can then use the expression (16). We obtain another modified Arnoldi procedure.

Algorithm 3 *Q-Arnoldi procedure (U-version)*

Input: M, D, K, r_0, n
Output: Q_n
1. $u_1 = r_0/\|r_0\|_2$ *and* $w = 0$
2. *for* $j = 1, 2, \ldots, n$ *do*
3. $\quad r = -K^{-1}(Du_j + Mw)$
4. $\quad t = u_j$
5. $\quad h_j = U_j^T r + \begin{bmatrix} 0 \\ \widehat{H}(2:j, 1:j-1)^{-T} U_{j-1}^T \end{bmatrix} t$
6. $\quad r = r - U_j h_j$
7. $\quad t = t - \begin{bmatrix} 0 \ U_{j-1} \widehat{H}(2:j, 1:j-1)^{-1} \end{bmatrix} h_j$
8. $\quad h_{j+1,j} = (\|r\|_2^2 + \|t\|_2^2)^{1/2}$
9. $\quad$ *stop if* $h_{j+1,j} = 0$
10. $\quad u_{j+1} = r/h_{j+1,j}$
11. $\quad w = t/h_{j+1,j}$
12. *end for*
13. $Q_{n+1} = \texttt{orth}(U_{n+1})$ $\quad$ *% orthogonalization*

Note that both modified Arnoldi procedures 2 and 3 produce the same $\widehat{H}_n$ as the Arnoldi procedure in exact arithmetic. If we would compute the U block using (15) after the execution of Algorithm 2, we would obtain exactly the same U block as the one produced by Algorithm 3. The breakdown of both Q-Arnoldi procedures happens in the same situation as the standard Arnoldi procedure.

4.2 Second-order Arnoldi procedure

The Second-Order ARnoldi (SOAR) procedure computes an orthonormal basis of the second-order Krylov subspace $\mathcal{G}_n$ directly, without first computing the U- or W-block. It is based on the observation that the elements of the upper Hessenberg matrix $\widehat{H}_n$ in the governing equation (11) of the Arnoldi procedure can be chosen to enforce the orthonormality of the U-vectors directly. The procedure is first proposed by Su and Craig [SCJ91], and further improved in the recent work of Bai and Su [BS04b]. The simplest version of the procedure is as follows.

Algorithm 4 *SOAR procedure*

Inputs: M, D, K, r_0, n
Output: Q_n
1. $q_1 = r_0/\|r_0\|$
2. $w = 0$
3. *for* $j = 1, 2, \ldots, n$ *do*
4. $\quad r = -K^{-1}(Dq_j + Mw)$
5. $\quad h_j = Q_j^T r$
6. $\quad r := r - Q_j h_j$
7. $\quad h_{j+1\,j} = \|r\|_2$
8. $\quad$ *stop if* $h_{j+1\,j} = 0$,
9. $\quad q_{j+1} = r/h_{j+1\,j}$
10. $\quad$ *solve* $\widehat{H}_j(2 : j+1, 1 : j)g = e_j$ *for* g
11. $\quad w = Q_j g$
12. *end for*

Special attention needs to be paid to the case of breakdown for the SOAR procedure. This occurs when $h_{j+1\,j} = 0$ at iteration j. There are two possible cases. One is that the vector sequence $\{r_i\}_{i=0}^{j-1}$ is linearly dependent, but the double length vector sequence $\{[r_i^T\ r_{i-1}^T]^T\}_{i=0}^{j-1}$ is linearly independent. We call this situation *deflation*. With a proper treatment, the SOAR procedure can continue. Deflation is regarded as an advantage of the SOAR procedure. A modified SOAR procedure with the treatment of deflation is presented in [BS04b]. Another possible case is that both vector sequences $\{r_i\}_{i=0}^{j-1}$ and $\{[r_i^T\ r_{i-1}^T]^T\}_{i=0}^{j-1}$ are linearly dependent, respectively. In this case, the SOAR procedure terminates. We call this *breakdown*. At the breakdown of the SOAR, one can prove that the transfer functions $h(s)$ and $h_j(s)$ of the original system Σ_N and the reduced system Σ_j are identical, the same as in the linearization method [BS04a].

4.3 Complexity

Table 1 summarizes the memory requirements and computational costs of the Arnoldi and modified procedures discussed in this section.

Table 1. Complexity of Arnoldi procedure and modifications

Procedure	memory	flops
Arnoldi	$2(n+1)N$	$2Nn(n+3)$
Q-Arnoldi (W-version)	$(n+1)N$	$2Nn(n+1)$
Q-Arnoldi (U-version)	$(n+2)N$	$2Nn(n+3)$
SOAR	$(n+2)N$	$(3/2)Nn(n+4/3)$

We only consider the storage of the Arnoldi vectors, since this is the dominant factor. The storage of Q_{n+1} in W-version of the Q-Arnoldi procedure

(Algorithm 2) uses the same locations as W_{n+1} and in U-version procedure (Algorithm 3) the same locations as U_{n+1}. The storage of w_1 is not required since it is zero. This explains the slightly lower cost for the W-version of Q-Arnoldi procedure.

For the computational costs, first note that the matrix-vector products involving matrices M, D and K are typically far more expensive than the other operations. All three procedure use the same number of matrix-vector products. The remaining cost is dominated by the orthogonalization procedures. For the Q-Arnoldi procedures, the cost is dominated by the inner products with W_j and U_j respectively. The cost of the U-version is slightly higher, because w_1 is zero. For SOAR, we assume that there are no zero columns in Q_{n+1}. These costs do not include the computation of Q_{n+1} in Step 13 of the Q-Arnoldi procedures 2 and 3. This cost is of the order of Nn^2.

5 Structure-preserving dimension reduction algorithm

We now present the Q-Arnoldi or SOAR-based method for structure-preserving dimension reduction of the second-order system Σ_N.

In practice, we are often interested in the approximation of the original system Σ_N around a prescribed expansion point $s_0 \neq 0$. In this case, the transfer function $h(s)$ of Σ_N can be written in the form:

$$\begin{aligned} h(s) &= l^T(s^2M + sD + K)^{-1}f \\ &= l^T((s-s_0)^2M + (s-s_0)\widetilde{D} + \widetilde{K})^{-1}f, \end{aligned}$$

where

$$\widetilde{D} = 2s_0M + D \quad \text{and} \quad \widetilde{K} = s_0^2M + s_0D + K.$$

Note that s_0 can be an arbitrary, but fixed value such that the matrix $\widetilde{K}$ is nonsingular. The moments of $h(s)$ about s_0 can be defined in a similar way as in (3).

By applying the Q-Arnoldi or SOAR procedure, we can generate an orthonormal basis Q_n of the second-order Krylov subspace $\mathcal{G}_n(A, B; r_0)$:

$$\text{span}\{Q_n\} = \mathcal{G}_n(A, B; r_0)$$

with

$$A = -\widetilde{K}^{-1}\widetilde{D},\ B = -\widetilde{K}^{-1}M \text{ and } r_0 = \widetilde{K}^{-1}f.$$

Following the orthogonal projection technique as discussed in section 2, the subspace spanned by the columns of Q_n can be used as the projection subspace, and subsequently, to define a reduced system Σ_n as in (6). The transfer function $h_n(s)$ of Σ_n about the expansion point s_0 is given by

$$h_n(s) = l_n^T((s-s_0)^2M_n + (s-s_0)\widetilde{D}_n + \widetilde{K}_n)^{-1}f_n,$$

where $M_n = Q_n^T M Q_n$, $\widetilde{D}_n = Q_n^T \widetilde{D} Q_n$, $\widetilde{K}_n = Q_n^T \widetilde{K} Q_n$ and $l_n^T = Q_n^T l$ and $f_n^T = Q_n^T f$. By a straightforward algebraic manipulation, $h_n(s)$ can be simply expressed as

$$h_n(s) = l_n^T (s^2 M_n + s D_n + K_n)^{-1} f_n, \tag{17}$$

where

$$M_n = Q_n^T M Q_n,\ D_n = Q_n^T D Q_n,\ K_n = Q_n^T K Q_n,\ l_n = Q_n^T l,\ f_n = Q_n^T f.$$

In other words, the transformed matrix triplet $(M, \widetilde{D}, \widetilde{K})$ is used to generate an orthonormal basis Q_n of the projection subspace $\mathcal{G}_n$, but the original matrix triplet (M, D, K) is directly projected onto the subspace $\mathcal{G}_n$ to define a reduced system Σ_n about the selected expansion point s_0.

The moment-matching theorem in section 2 is still applied here. We can show that the first n moments about the expansion point s_0 of $h(s)$ and $h_n(s)$ are the same. Therefore, $h_n(s)$ is an n-th Padé-type approximant of $h(s)$ about s_0. Furthermore, if Σ_N is a symmetric second-order system, then the first $2n$ moments about s_0 of $h(s)$ and $h_n(s)$ are the same, which implies that $h_n(s)$ is an n-th Padé approximant of $h(s)$ about s_0.

The following algorithm is a high-level description of the second-order structure-preserving dimension reduction algorithm based on Q-Arnoldi or SOAR procedure.

Algorithm 5 *Structure-preserving dimension reduction algorithm*

1. *Select an order n for the reduced system, and an expansion point s_0.*
2. *Run n steps of Q-Arnoldi or SOAR procedure to generate an orthonormal basis Q_n of $\mathcal{G}_n(A, B; r_0)$, where $A = -\widetilde{K}^{-1}\widetilde{D}$, $B = -\widetilde{K}^{-1}M$ and $r_0 = \widetilde{K}^{-1} f$.*
3. *Compute $M_n = Q_n^T M Q_n$, $D_n = Q_n^T D Q_n$, $K_n = Q_n^T K Q_n$, $l_n = Q_n^T l$, and $f_n = Q_n^T f$. This defines a reduced system Σ_n as in (6) about the selected expansion point s_0.*

As we have noticed, by the definitions of the matrices M_n, D_n and K_n in the reduced system Σ_n, essential properties of the matrices M, D and K of the original system Σ_N are preserved. For example, if M is symmetric positive definite, so is M_n. Consequently, we can preserve stability, possible symmetry and the physical meaning of the original second-order system Σ_N.

The explicit formulation of the matrices M_n, D_n and K_n is done by using first matrix-vector product operations Mq, Dq and Kq for an arbitrary vector q and vector inner products. This is an overhead compared to the linearization method discussed in section 3. In the linearization method as described in section 3, the matrix $C_n = -H_n$ and $G_n = I$ in the reduced system Σ_n^L is obtained as a by-product of the Arnoldi procedure without additional cost. However, we believe that the preservation of the structure of the underlying problem outweighs the extra cost of floating point operations in a modern computing environment. In fact, we observed that this step takes only a small

fraction of the total work, due to extreme sparsity of the matrices M and D and K in practical problems we encountered. The bottleneck of the computational costs is often associated with the matrix-vector product operations involving $\widetilde{K}^{-1}$.

6 Numerical examples

In this section, we report our numerical experiments on the performance of the structure-preserving dimension reduction algorithm based on Q-Arnoldi and SOAR procedures. The superior numerical properties of the SOAR-based method over the linearization approach as described in section 3 have been reported in [BS04a] for examples from structural dynamics and MEMS systems. In this section, we focus on the performance of the Q-Arnoldi-based and SOAR-based structure-preserving dimension reduction methods. All numerical examples do not use reorthogonalization.

Example 1. This example is from the simulation of a linear-drive multi-mode resonator structure [CZP98]. This is a nonsymmetric second-order system. The mass and damping matrices M and D are singular. The stiffness matrix K is ill-conditioned due to the multi-scale of the physical units used to define the elements of K, such as the beam's length and cross sectional area, and its moment of inertia and modulus of elasticity. For this numerical experiment, the order of 1-norm condition number of K is at $\mathcal{O}(10^{15})$. We use the expansion point s_0 to approximate the bode plot of interest, the same as in [CZP98]. The condition number of the transformed stiffness matrix $\widetilde{K} = s_0^2 M + s_0 D + K$ is is slightly improved to $\mathcal{O}(10^{13})$. In Figure 1, the Bode plots of frequency responses of the original second-order system Σ_N of order $N = 63$, and the reduced-order systems of orders $n = 10$ via the Q-Arnoldi (W-version) and SOAR methods are reported. The corresponding relative errors are also shown over the frequency range of interest. From the relative errors, we see that the SOAR-based method is slightly more accurate than the Q-Arnoldi-based method.

Example 2. This is an example from an acoustic radiation problem discussed in [PA91]. Consider a circular piston subtending a polar angle $0 < \theta < \theta_p$ on a submerged massless and rigid sphere of radius δ. The piston vibrates harmonically with a uniform radial acceleration. The surrounding acoustic domain is unbounded and is characterized by its density ρ and sound speed c.

We denote by p and a_r the prescribed pressure and normal acceleration respectively. In order to have a steady state solution $\tilde{p}(r, \theta, t)$ verifying

$$\tilde{p}(r, \theta, t) = \mathcal{R}\mathrm{e}\left(p(r, \theta) e^{i\omega t}\right),$$

the transient boundary condition is chosen as:

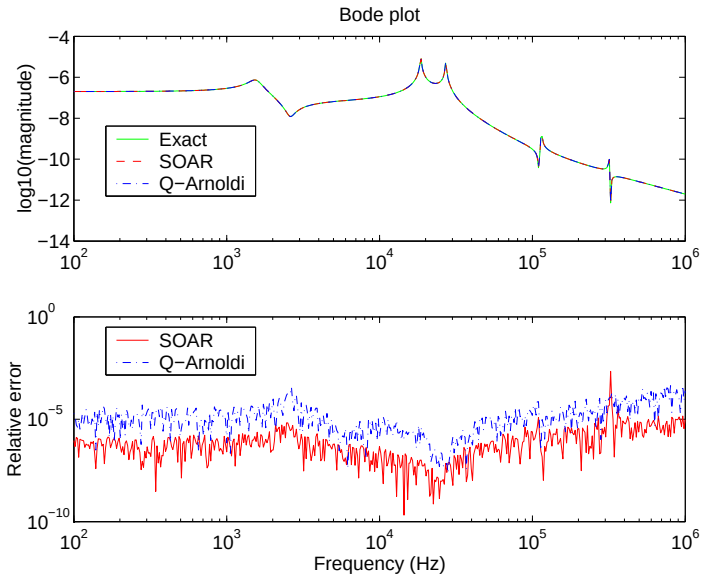

Fig. 1. Bode plots of $h(\mathrm{j}\omega)$ of the resonator, approximations by Q-Arnoldi and SOAR, and relative errors.

$$a_r = \frac{-1}{\rho}\frac{\partial p(r,\theta)}{\partial r}\bigg|_{r=a} = \begin{cases} a_0 \sin(\omega t), & 0 \le \theta \le \theta_p, \\ 0, & \theta > \theta_p. \end{cases}$$

The axisymmetric discrete finite-infinite element model relies on a mesh of linear quadrangle finite elements for the inner domain (region between spherical surfaces $r = \delta$ and $r = 1.5\delta$). The numbers of divisions along radial and circumferential directions are 5 and 80, respectively. The outer domain relies on conjugated infinite elements of order 5. For this example we used $\delta = 1(\mathrm{m})$, $\rho = 1.225(\mathrm{kg/m^3})$, $c = 340(\mathrm{m/s})$, $a_0 = 0.001(\mathrm{m/s^2})$ and $\omega = 1000(\mathrm{rad/s})$.

The matrices K, D, M and the right-hand side f are computed by ACTRAN [Fre03]. The dimension of the second-order system is $N = 2025$. For numerical tests, an expansion point $s_0 = 2 \times 10^2\pi$ is used. Figure 2 shows the magnitudes (in log of base 10) of the exact transfer function $h(s)$ and approximate ones computed by the Q-Arnoldi (W-version) and SOAR-based methods with the reduced dimension $n = 100$. For this example, the accuracy of two methods are essentially the same.

7 Conclusions

In this paper, using a unified style, we discussed the recent progress in the development of Arnoldi-like methods for structure-preserving dimension reduction of a second-order dynamical system Σ_N. The reduced second-order

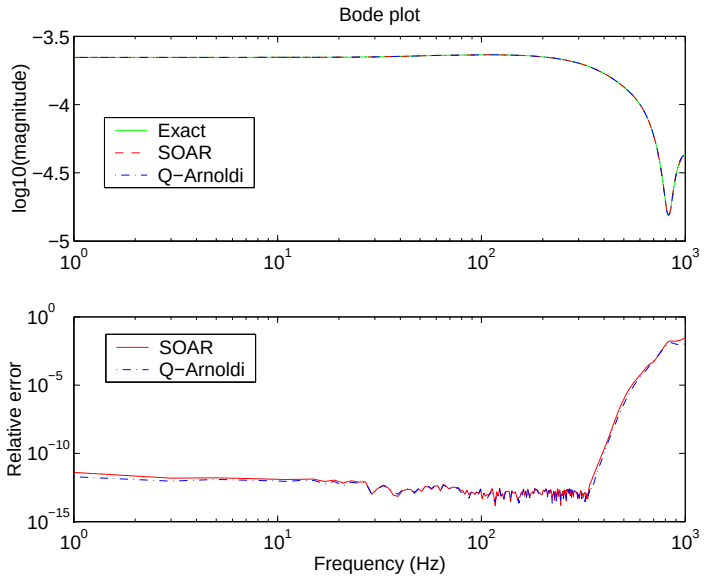

Fig. 2. Bode plot of $h(\mathrm{j}\omega)$ of ACTRAN2025, approximations by Q-Arnoldi and SOAR, and relative errors.

system Σ_n enjoys the same moment-matching properties as the Arnoldi-based algorithm via linearization. The major difference between the Q-Arnoldi and SOAR procedures lies in the orthogonalization.

We only focused on the basic schemes and the associated properties of structure-preserving algorithms. There are a number of interesting research issues for further study, such as numerical stability and the effect of reorthogonalization.

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