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DIMENSION REDUCTION OF LARGE-SCALE SECOND-ORDER DYNAMICAL SYSTEMS VIA A SECOND-ORDER ARNOLDI METHOD*

ZHAOJUN BAI† AND YANGFENG SU‡

Abstract. A structure-preserving dimension reduction algorithm for large-scale second-order dynamical systems is presented. It is a projection method based on a second-order Krylov subspace. A second-order Arnoldi (SOAR) method is used to generate an orthonormal basis of the projection subspace. The reduced system not only preserves the second-order structure but also has the same order of approximation as the standard Arnoldi-based Krylov subspace method via linearization. The superior numerical properties of the SOAR-based method are demonstrated by examples from structural dynamics and microelectromechanical systems.

Key words. dimension reduction, reduced-order modeling, dynamical systems, second-order Krylov subspace, second-order Arnoldi procedure

AMS subject classifications. 65F15, 65F30, 65P99

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1. Introduction.

A continuous time-invariant single-input single-output second-order system is described by

$$\Sigma_N : \begin{cases} \mathbf{M}\ddot{\mathbf{q}}(t) + \mathbf{D}\dot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) = \mathbf{b}\, u(t), \\ \qquad\qquad\qquad\qquad\quad y(t) = \mathbf{l}^{\mathrm{T}}\mathbf{q}(t) \end{cases} \tag{1.1}$$

with initial conditions $\mathbf{q}(0) = \mathbf{q}_0$ and $\dot{\mathbf{q}}(0) = \dot{\mathbf{q}}_0$. Here t is the time variable. $\mathbf{q}(t) \in \mathcal{R}^N$ 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. $\mathbf{M}$, $\mathbf{D}$, $\mathbf{K} \in \mathcal{R}^{N\times N}$ are system matrices, such as mass, damping, and stiffness as known in structural dynamics. $\mathbf{b}, \mathbf{l} \in \mathcal{R}^N$ are input distribution and output measurement vectors, respectively.

Second-order systems Σ_N arise in the study of many types of physical systems, with common examples being electrical, mechanical, and structural systems, electromagnetics, and microelectromechanical systems (MEMS) [11, 6, 9, 3, 23, 25, 26, 29]. The state-space dimension N of the system Σ_N arising from those applications is often very large and it can be formidable to use for many practical analysis and design tasks within a reasonable computing resource. Therefore, it is necessary to obtain a reduced-order model which retains important properties of the original system and yet is efficient for practical use. In this paper, we discuss a computational technique for dimension reduction of the second-order system Σ_N. Specifically, for the given second-order system Σ_N, we show how to construct another system Σ_n of the same second-order form but with a smaller state-space dimension, such that it accurately

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†Department of Computer Science and Department of Mathematics, University of California, Davis, CA 95616 (bai@cs.ucdavis.edu). The research of this author was supported in part by the National Science Foundation under grant 0220104.

‡Department of Mathematics, Fudan University, Shanghai 200433, China (yfsu@fudan.edu.cn). The research of this author was supported in part by NSFC research project 10001009 and NSFC research key project 90307017.

captures the input-output behaviors while retaining essential properties of the original system Σ_N. An accurate and effective reduced system thus replaces the original one and can be efficiently applied for a variety of types of analyses to significantly reduce design and simulation time.

The most common approach to the dimension reduction of the second-order system Σ_N is based on a mathematically equivalent linearized formulation of the second-order system. Different dimension reduction methods of linear systems have been studied in various fields. Most of these methods can be classified into the families of balancing truncation methods and moment-matching methods; see [14, 2, 1] and references therein. However, the linearization approach has a number of disadvantages. It ignores the physical meaning of the original system matrices, and the reduced-order system is no longer in a second-order form. For engineering design and control of such a system, it is highly desirable to have a reduced-order model preserving the second-order form and the essential properties, such as stability and passivity.

Over the years, there have been a number of efforts toward structure-preserving dimension reduction of a second-order system. Su and Craig proposed a structure-preserving method with moment-match property in 1991 [28]. This has been revisited in recent years [23, 2, 25, 26]. It has been applied to very large second-order systems. The work of Meyer and Srinivasan [20] is an extension of balancing truncation methods for the second-order system. Recent such effort includes [7]. Another structure-preserving model reduction technique was presented in [15]. Those two approaches focus on the application of moderate-size second-order systems.

The method presented in this paper is a further study of the work by Su and Craig [28]. We pursue a structure-preserving dimension reduction algorithm for large-scale second-order systems. The algorithm is developed under the framework of projection. We use a second-order Krylov subspace as the projection subspace. Subsequently, a second-order Arnoldi (SOAR) method is used to generate an orthonormal basis of the projection subspace. The resulting reduced system not only preserves the second-order structure but also has the same order of approximation of a reduced linear system obtained by the standard Arnoldi-based Krylov subspace projection method via linearization. We demonstrate the considerable superior numerical properties of this new approach with examples from structural dynamics and MEMS simulations.

The remainder of the paper is organized as follows. In section 2, we review the definitions of transfer function and moment of the second-order system Σ_N and specify the goals of dimension reduction. In section 3, we discuss the projection subspace and present a SOAR procedure to generate an orthonormal basis of the projection subspace. In section 4, we present the dimension reduction algorithm via the SOAR method and prove its moment-matching properties. In section 5, we discuss a practical algorithm and review the standard Arnoldi-based dimension reduction for the second-order system with linearization. In section 6, we present results of numerical experiments for examples from different areas of applications. Concluding remarks are in section 7.

Throughout the paper, we follow the notational convention commonly used in matrix computation literature. Specifically, we use boldface letters to denote vectors (lower cases) and matrices (upper cases), $\mathbf{I}$ for the identity matrix, $\mathbf{e}_j$ for the jth column of the identity matrix $\mathbf{I}$, and $\mathbf{0}$ for zero vectors and matrices. The dimensions of these vectors and matrices are conformed with dimensions used in the context. $\cdot^{\mathrm{T}}$ denotes the transpose. N denotes the order of the original system (1.1).

span$\{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n\}$ and span$\{\mathbf{Q}\}$ denote the space spanned the vector sequence $\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n$ and the columns of the matrix $\mathbf{Q}$, respectively. $\|\cdot\|_1$ and $\|\cdot\|_2$ denote 1-norm and 2-norm, respectively, for vector or matrix.

2. Second-order system and dimension reduction. In this section, we first review the definitions of transfer function and moment of the second-order dynamical system Σ_N, and then we formally state the goals of dimension reduction. For simplicity, we assume that we have zero initial conditions $\mathbf{q}(0) = \mathbf{0}$, $\dot{\mathbf{q}}(0) = \mathbf{0}$, and $\mathbf{u}(0) = \mathbf{0}$ in (1.1). Taking the Laplace transform of Σ_N, we have

$$\begin{cases} s^2\mathbf{M}\tilde{\mathbf{q}}(s) + s\mathbf{D}\tilde{\mathbf{q}}(s) + \mathbf{K}\tilde{\mathbf{q}}(s) = \mathbf{b}\,\tilde{u}(s), \\ \tilde{y}(s) = \mathbf{l}^{\mathrm{T}}\tilde{\mathbf{q}}(s). \end{cases} \tag{2.1}$$

Here $\tilde{\mathbf{q}}(s)$, $\tilde{y}(s)$, and $\tilde{u}(s)$ represent the Laplace transform of $\mathbf{q}(t)$, $y(t)$, and $u(t)$, respectively. Eliminating $\tilde{\mathbf{q}}(s)$ in (2.1) results in the frequency domain input-output relation $\tilde{y}(s) = h(s)\tilde{u}(s)$, where $h(s)$ is the *transfer function*:

$$h(s) = \mathbf{l}^{\mathrm{T}} \left(s^2\mathbf{M} + s\mathbf{D} + \mathbf{K}\right)^{-1} \mathbf{b}. \tag{2.2}$$

The physically meaningful values of the complex variables s are $s = \mathtt{j}\omega$, where $\omega \geq 0$ is referred to as the frequency, $\mathtt{j} = \sqrt{-1}$. The following lemma shows that the transfer function $h(s)$ can be rewritten in linear form of the variable s.

LEMMA 2.1. *Let* 2×2 *block matrices* $\mathbf{C}$ *and* $\mathbf{G}$ *and the block vectors* $\widehat{\mathbf{b}}$ *and* $\widehat{\mathbf{l}}$ *be defined as*

$$\mathbf{C} = \begin{bmatrix} \mathbf{D} & \mathbf{M} \\ -\mathbf{W} & \mathbf{0} \end{bmatrix}, \qquad \mathbf{G} = \begin{bmatrix} \mathbf{K} & \mathbf{0} \\ \mathbf{0} & \mathbf{W} \end{bmatrix}, \qquad \widehat{\mathbf{b}} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}, \qquad \widehat{\mathbf{l}} = \begin{bmatrix} \mathbf{l} \\ \mathbf{0} \end{bmatrix}, \tag{2.3}$$

where $\mathbf{W}$ *is an arbitrary* $N \times N$ *nonsingular matrix. Then the transfer function* $h(s)$ *as defined in* (2.2) *can be written as*

$$h(s) = \widehat{\mathbf{l}}^{\mathrm{T}}(s\mathbf{C} + \mathbf{G})^{-1}\widehat{\mathbf{b}}. \tag{2.4}$$

Proof. The lemma is proved by the following identity of the inverse of the 2×2 block matrix $s\mathbf{C} + \mathbf{G}$:

$$(s\mathbf{C} + \mathbf{G})^{-1} = \begin{bmatrix} s\mathbf{D} + \mathbf{K} & s\mathbf{M} \\ -s\mathbf{W} & \mathbf{W} \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{P}(s)^{-1} & -\mathbf{P}(s)^{-1}s\mathbf{M}\mathbf{W}^{-1} \\ s\mathbf{P}(s)^{-1} & \mathbf{P}(s)^{-1}(s\mathbf{D} + \mathbf{K})\mathbf{W}^{-1} \end{bmatrix},$$

where $\mathbf{P}(s) = s^2\mathbf{M} + s\mathbf{D} + \mathbf{K}$. $\square$

A common choice of $\mathbf{W}$ is to be the identity matrix, $\mathbf{W} = \mathbf{I}$, as it is used throughout this paper. If $\mathbf{M}$, $\mathbf{D}$, and $\mathbf{K}$ are all symmetric and $\mathbf{M}$ is nonsingular, we can choose $\mathbf{W} = -\mathbf{M}$. The result is that $\mathbf{C}$ and $\mathbf{G}$ are symmetric matrices.

The power series expansion of $h(s)$ is formally given by

$$h(s) = m_0 + m_1 s + m_2 s^2 + \cdots = \sum_{\ell=0}^{\infty} m_\ell s^\ell, \tag{2.5}$$

where m_ℓ for $\ell \geq 0$ are called (low-frequency) moments. By Lemma 2.1 and the assumption that $\mathbf{K}$ is invertible, moments m_ℓ can be compactly expressed as $m_\ell = \widehat{\mathbf{l}}^{\mathrm{T}}(-\mathbf{G}^{-1}\mathbf{C})^\ell(\mathbf{G}^{-1}\widehat{\mathbf{b}})$ for $\ell \geq 0$. If $\mathbf{K}$ is singular, we can consider the Taylor series expansion of $h(s)$ about a selected expansion point $s_0 \neq 0$. This will be discussed in section 5.

The desiderata for a moment-matching dimension reduction method are to construct a reduced system of the *same* second-order form but with many fewer states and meanwhile to match the moments of the transfer functions of the original system and the reduced system as much as possible. Specifically, for the given second-order system Σ_N in (1.1), we want to find a reduced second-order system of the *same* form

$$\Sigma_n : \begin{cases} \mathbf{M}_n\ddot{\mathbf{z}}(t) + \mathbf{D}_n\dot{\mathbf{z}}(t) + \mathbf{K}_n\mathbf{z}(t) = \mathbf{b}_n u(t), \\ \widehat{y}(t) = \mathbf{l}_n^{\mathbf{T}}\mathbf{z}(t), \end{cases} \tag{2.6}$$

where the state vector $\mathbf{z}(t)$ is of dimension n, $n < N$, and in most cases, $n \ll N$. $\mathbf{M}_n$, $\mathbf{D}_n$, and $\mathbf{K}_n$ are $n \times n$ matrices, and $\mathbf{b}_n$ and $\mathbf{l}_n$ are vectors of length n. The corresponding transfer function $h_n(s)$ of the reduced system Σ_n is given by

$$h_n(s) = \mathbf{l}_n^{\mathrm{T}} \left(s^2\mathbf{M}_n + s\mathbf{D}_n + \mathbf{K}_n\right)^{-1} \mathbf{b}_n = \widehat{\mathbf{l}}_n^{\mathrm{T}} \left(s\mathbf{C}_n + \mathbf{G}_n\right)^{-1} \widehat{\mathbf{b}}_n,$$

where

$$\mathbf{C}_n = \begin{bmatrix} \mathbf{D}_n & \mathbf{M}_n \\ -\mathbf{I} & \mathbf{0} \end{bmatrix}, \qquad \mathbf{G}_n = \begin{bmatrix} \mathbf{K}_n & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \qquad \widehat{\mathbf{b}}_n = \begin{bmatrix} \mathbf{b}_n \\ \mathbf{0} \end{bmatrix}, \qquad \widehat{\mathbf{l}}_n = \begin{bmatrix} \mathbf{l}_n \\ \mathbf{0} \end{bmatrix}.$$

The moments of Σ_n are $m_\ell^{(n)} = \widehat{\mathbf{l}}_n^{\mathrm{T}}(-\mathbf{G}_n^{-1}\mathbf{C}_n)^\ell(\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n)$ for $\ell \geq 0$. It is desired that for the largest q possible, the first q moments of two systems Σ_N and Σ_n are matched, i.e.,

$$m_\ell = m_\ell^{(n)} \quad \text{for } \ell = 0, 1, 2, \ldots, q-1. \tag{2.7}$$

This implies that $h_n(s)$ is a qth-order Padé-type approximant of $h(s)$:

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

In section 4, we will show how to construct such a reduced system so that $h_n(s)$ is an nth Padé-type approximant of $h(s)$, i.e., $q = n$. Furthermore, if Σ_N is symmetric, namely, $\mathbf{M}$, $\mathbf{D}$, and $\mathbf{K}$ are symmetric and $\mathbf{b} = \mathbf{l}$, then $h_n(s)$ is an nth Padé approximant of $h(s)$, i.e., $q = 2n$.

3. Second-order Krylov subspace and SOAR procedure. We will use the framework of a subspace projection technique to derive a reduced system (2.6) with the moment-matching property (2.7). The gist of the projection technique is on the choice of a subspace which the full-order system is to be projected onto. If the transfer function $h(s)$ is written in the linear form (2.4) in terms of the matrices $\mathbf{C}$ and $\mathbf{G}$, then it can be cast using only one matrix:

$$h(s) = \widehat{\mathbf{l}}^{\mathrm{T}}(\mathbf{I} + s\mathbf{G}^{-1}\mathbf{C})^{-1}\mathbf{G}^{-1}\widehat{\mathbf{b}} = \widehat{\mathbf{l}}^{\mathrm{T}}(\mathbf{I} - s\mathbf{H})^{-1}\widehat{\mathbf{b}}_0,$$

where $\mathbf{H} = -\mathbf{G}^{-1}\mathbf{C}$ and $\widehat{\mathbf{b}}_0 = \mathbf{G}^{-1}\widehat{\mathbf{b}}$. Then it is natural to consider the following Krylov subspace as the projection subspace for the dimension reduction:

$$\mathcal{K}_n(\mathbf{H}, \widehat{\mathbf{b}}_0) = \mathrm{span}\{\widehat{\mathbf{b}}_0, \mathbf{H}\,\widehat{\mathbf{b}}_0, \mathbf{H}^2\,\widehat{\mathbf{b}}_0, \mathbf{H}^3\,\widehat{\mathbf{b}}_0, \ldots, \mathbf{H}^{n-1}\,\widehat{\mathbf{b}}_0\}.$$

However, in this paper, we will use a second-order Krylov subspace as the projection subspace. We will show that by using this second-order Krylov subspace, the reduced system not only has the same order of approximation as the one derived based on the projection onto the Krylov subspace $\mathcal{K}_n$ but also preserves the second-order form of the original system Σ_N.

We note that

$$\mathbf{H} = -\mathbf{G}^{-1}\mathbf{C} = \begin{bmatrix} -\mathbf{K}^{-1}\mathbf{D} & -\mathbf{K}^{-1}\mathbf{M} \\ \mathbf{I} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{I} & \mathbf{0} \end{bmatrix} \quad \text{and} \quad \widehat{\mathbf{b}}_0 = \begin{bmatrix} \mathbf{K}^{-1}\mathbf{b} \\ \mathbf{0} \end{bmatrix},$$

where $\mathbf{A} = -\mathbf{K}^{-1}\mathbf{D}$ and $\mathbf{B} = -\mathbf{K}^{-1}\mathbf{M}$. Let

$$\begin{aligned} \mathbf{r}_0 &= \mathbf{K}^{-1}\mathbf{b}, \\ \mathbf{r}_1 &= \mathbf{A}\mathbf{r}_0, \\ \mathbf{r}_\ell &= \mathbf{A}\mathbf{r}_{\ell-1} + \mathbf{B}\mathbf{r}_{\ell-2} \quad \text{for } \ell \geq 2. \end{aligned}$$

Then one can easily derive that the vectors $\{\mathbf{r}_\ell\}$ of length N and the Krylov vectors $\{\mathbf{H}^\ell \widehat{\mathbf{b}}_0\}$ of length $2N$ are related as the following:

$$\begin{bmatrix} \mathbf{r}_\ell \\ \mathbf{r}_{\ell-1} \end{bmatrix} = \mathbf{H}^\ell \widehat{\mathbf{b}}_0 \quad \text{for } \ell \geq 1. \tag{3.1}$$

In other words, the vector sequence $\{\mathbf{r}_\ell\}$, in principle, *defines* the entire Krylov sequence $\{\mathbf{H}^j \widehat{\mathbf{b}}_0\}$. It indicates that the projection subspace spanned by $\{\mathbf{r}_\ell\}$ of $\mathcal{R}^N$ should be able to provide sufficient information for dimension reduction as does the Krylov subspace $\mathcal{K}_n(\mathbf{H}; \widehat{\mathbf{b}}_0)$ of $\mathcal{R}^{2N}$. This essential idea is first proposed in [28], although it is not in the form we present here. In [4], such a subspace is called a *second-order Krylov subspace* since the vector $\mathbf{r}_\ell$ is generated by a linear homogeneous recurrence relation of degree 2. Formally, an nth second-order Krylov subspace with matrices $\mathbf{A}$ and $\mathbf{B}$ and the starting vector $\mathbf{r}_0$ is defined by

$$\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0) = \operatorname{span}\{\mathbf{r}_0, \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{n-1}\}.$$

A SOAR method was proposed in [4] for generating an orthonormal basis of $\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0)$. The following is a pseudocode of the SOAR procedure.

ALGORITHM 1. *SOAR procedure.*

```
q_1 = u/||u||_2
f = 0
for j = 1, 2, ..., n do
    r = A q_j + B f
    for i = 1, 2, ..., j do
        t_ij = q_i^T r
        r := r - q_i t_ij
    end for
    t_{j+1,j} = ||r||_2
    if t_{j+1,j} ≠ 0,
        q_{j+1} := r / t_{j+1,j}
        f = Q_j T̂(2 : j+1, 1 : j)^{-1} e_j
    else
        reset t_{j+1,j} = 1
        q_{j+1} = 0
        f = Q_j T̂(2 : j+1, 1 : j)^{-1} e_j
        save f
```

```
18.         if f belongs to the subspace spanned by previously saved f,
              then stop (breakdown)
19.      end if
20.   end for
```

Note that at line 18 of the algorithm, if $\mathbf{f}$ belongs to the subspace spanned by previously saved $\mathbf{f}$ vectors, then the algorithm encounters a breakdown and terminates. Otherwise, there is a deflation at step j. After setting $t_{j+1,j}$ to 1 or any nonzero constant and $\mathbf{q}_{j+1} = \mathbf{0}$, the algorithm continues. To check whether $\mathbf{f}$ is in the subspace spanned by the previously saved $\mathbf{f}$, we can use a modified Gram–Schmidt procedure [27]. Note that it is not necessary to use extra storage to save those $\mathbf{f}$ vectors. They can be stored at the columns of $\mathbf{Q}_n$ where the corresponding $\mathbf{q}_j = \mathbf{0}$.

At the return of the SOAR procedure, it computes a basis $\mathbf{Q}_n$ of the second-order Krylov subspace:

$$\operatorname{span}\{\mathbf{Q}_n\} = \mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0).$$

Furthermore, the nonzero columns of $\mathbf{Q}_n$ form an orthonormal basis. The dimension of the second-order subspace $\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0)$ equals the number of nonzero columns of $\mathbf{Q}_n$, which could be less than n when deflation occurs. To simplify the presentation, we will still use $\mathbf{Q}_n$ to denote such an orthonormal basis. If the SOAR procedure breaks down at the n_0th step, then it indicates that

$$\operatorname{span}\{\mathbf{Q}_{n_0}\} = \mathcal{G}_\infty(\mathbf{A}, \mathbf{B}; \mathbf{r}_0) = \operatorname{span}\{\mathbf{r}_0, \mathbf{r}_1, \mathbf{r}_2, \ldots\}.$$

Before we proceed to the use of the projection subspace $\operatorname{span}\{\mathbf{Q}_n\}$ for dimension reduction, we present the following theorem, which shows the relationship between the standard Krylov subspace $\mathcal{K}_n(\mathbf{H}; \widehat{\mathbf{b}}_0)$ and the second-order Krylov subspace $\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0)$. This is the essential observation leading to moment-matching and approximation properties of the reduced system to be discussed in section 4.

THEOREM 3.1. *Let $\mathbf{Q}_n$ be an orthonormal basis of the second-order Krylov subspace $\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0)$. Let $\mathbf{Q}_{[n]}$ denote the following 2×2 block diagonal matrix:*

$$\mathbf{Q}_{[n]} = \begin{bmatrix} \mathbf{Q}_n & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_n \end{bmatrix}. \tag{3.2}$$

Then $\mathbf{H}^\ell \widehat{\mathbf{b}}_0 \in \operatorname{span}\{\mathbf{Q}_{[n]}\}$ for $\ell = 0, 1, 2, \ldots, n-1$. This means that

$$\mathcal{K}_n(\mathbf{H}; \widehat{\mathbf{b}}_0) \subseteq \operatorname{span}\{\mathbf{Q}_{[n]}\}.$$

We say that the standard Krylov subspace $\mathcal{K}_n(\mathbf{H}; \widehat{\mathbf{b}}_0)$ is embedded *into the second-order Krylov subspace $\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0)$.*

Proof. By the fact that the SOAR procedure generates an orthonormal basis of the second-order Krylov subspace [4], we have that for any $\ell \geq 0$,

$$\begin{bmatrix} \mathbf{r}_0 & \mathbf{r}_1 & \cdots & \mathbf{r}_{\ell-1} \end{bmatrix} = \mathbf{Q}_\ell \mathbf{R}_\ell,$$

where $\operatorname{span}\{\mathbf{Q}_\ell\} = \mathcal{G}_\ell(\mathbf{A}, \mathbf{B}; \mathbf{r}_0)$ and $\mathbf{Q}_\ell^{\mathrm{T}} \mathbf{Q}_\ell = \mathbf{I}$. $\mathbf{R}_\ell$ is an $\ell \times \ell$ nonsingular upper triangular matrix. Hence we have

$$\begin{bmatrix} \mathbf{r}_0 & \mathbf{r}_1 & \cdots & \mathbf{r}_{n-1} \\ \mathbf{0} & \mathbf{r}_0 & \cdots & \mathbf{r}_{n-2} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_n & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_n \end{bmatrix} \left[\begin{array}{cc} \multicolumn{2}{c}{\mathbf{R}_n} \\ \hline \mathbf{0} & \mathbf{R}_{n-1} \\ \mathbf{0} & 0 \end{array} \right].$$

The theorem is then proved by the preceding expression and (3.1). ∎

To conclude this section, we note that the work in computing an orthonormal basis $\mathbf{Q}_n$ of the second-order Krylov subspace $\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0)$ is divided between the computation of the matrix-vector products $\mathbf{Aq}$ and $\mathbf{Bf}$ and the orthogonalization. The cost of the former varies depending on the sparsity and structures of the matrices $\mathbf{A}$ and $\mathbf{B}$. The cost of the orthogonalization is about $3n^2N$ flops. The main advantage of the SOAR procedure is on the memory requirement. It takes $(n+1)N$ and is a half of the memory requirement of the Arnoldi procedure (see, for example, [16, 13, 27]) for generating an orthonormal basis of the Krylov subspace $\mathcal{K}_n(\mathbf{H}; \widehat{\mathbf{b}}_0)$.

4. Dimension reduction based on the SOAR procedure. We now derive a reduced second-order system using the framework of a projection technique developed for linear systems; for example, see [12]. The idea of projection can be viewed as to approximate the state vector $\mathbf{q}(t)$ of the original system Σ_N by another state vector $\mathbf{z}(t)$ constrained to the subspace $\mathcal{G}_n$ spanned by $\mathbf{Q}_n$. This can be simply expressed by the change-of-state variables

$$\mathbf{q}(t) \approx \mathbf{Q}_n \mathbf{z}(t), \tag{4.1}$$

where $\mathbf{z}(t)$ is a vector of dimension n. Substituting (4.1) into (1.1) and multiplying the first equation of (1.1) with $\mathbf{Q}_n^{\mathrm{T}}$ from the left yield the system

$$\Sigma_n : \begin{cases} \mathbf{M}_n \ddot{\mathbf{z}}(t) + \mathbf{D}_n \dot{\mathbf{z}}(t) + \mathbf{K}_n \mathbf{z}(t) = \mathbf{b}_n u(t), \\ \qquad\qquad\qquad\qquad\qquad \widetilde{y}(t) = \mathbf{l}_n^{\mathbf{T}} \mathbf{z}(t), \end{cases} \tag{4.2}$$

where $\mathbf{M}_n$, $\mathbf{D}_n$, and $\mathbf{K}_n$ are $n \times n$ matrices such that $\mathbf{M}_n = \mathbf{Q}_n^{\mathbf{T}} \mathbf{M} \mathbf{Q}_n$, $\mathbf{D}_n = \mathbf{Q}_n^{\mathrm{T}} \mathbf{D} \mathbf{Q}_n$, and $\mathbf{K}_n = \mathbf{Q}_n^{\mathrm{T}} \mathbf{K} \mathbf{Q}_n$. $\mathbf{b}_n$ and $\mathbf{l}_n$ are $n \times 1$ vectors such that $\mathbf{b}_n = \mathbf{Q}_n^{\mathrm{T}} \mathbf{b}$ and $\mathbf{l}_n = \mathbf{Q}_n^{\mathrm{T}} \mathbf{l}$. The second-order system (4.2) is called a reduced-order system Σ_n of the original system Σ_N.

We note that by explicitly formulating the matrices $\mathbf{M}_n$, $\mathbf{D}_n$, and $\mathbf{K}_n$ in Σ_n, essential structures of $\mathbf{M}$, $\mathbf{D}$, and $\mathbf{K}$ are preserved. For example, if $\mathbf{M}$ is symmetric positive definite, so is $\mathbf{M}_n$. As a result, we can preserve the stability, symmetry, and physical meanings of the original second-order system Σ_N. This is in the same spirit of the widely used PRIMA algorithm for the passive reduced-order modeling of linear dynamical systems arising from interconnect analysis in circuit simulations [22].

The transfer function of the reduced second-order system Σ_n in (4.2) is given by

$$h_n(s) = \mathbf{l}_n^{\mathrm{T}} (s^2 \mathbf{M}_n + s \mathbf{D}_n + \mathbf{K}_n)^{-1} \mathbf{b}_n. \tag{4.3}$$

By Lemma 2.1, $h_n(s)$ can be equivalently expressed as

$$h_n(s) = \widehat{\mathbf{l}}_n^{\mathrm{T}} \left(s\mathbf{C}_n + \mathbf{G}_n \right)^{-1} \widehat{\mathbf{b}}_n,$$

where

$$\widehat{\mathbf{l}}_n = \mathbf{Q}_{[n]}^{\mathrm{T}} \widehat{\mathbf{l}}, \qquad \widehat{\mathbf{b}}_n = \mathbf{Q}_{[n]}^{\mathrm{T}} \widehat{\mathbf{b}}, \qquad \mathbf{C}_n = \begin{bmatrix} \mathbf{D}_n & \mathbf{M}_n \\ -\mathbf{I} & \mathbf{0} \end{bmatrix}, \qquad \mathbf{G}_n = \begin{bmatrix} \mathbf{K}_n & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}. \tag{4.4}$$

Furthermore, by the definition of the 2×2 block diagonal matrix $\mathbf{Q}_{[n]}$ in (3.2), $\mathbf{C}_n$ and $\mathbf{G}_n$ can be expressed as $\mathbf{C}_n = \mathbf{Q}_{[n]}^{\mathrm{T}} \mathbf{C} \mathbf{Q}_{[n]}$ and $\mathbf{G}_n = \mathbf{Q}_{[n]}^{\mathrm{T}} \mathbf{G} \mathbf{Q}_{[n]}$. The moments $m_\ell^{(n)}$ of Σ_n can be compactly expressed as $m_\ell^{(n)} = \widehat{\mathbf{l}}_n^{\mathrm{T}} (-\mathbf{G}_n^{-1} \mathbf{C}_n)^\ell (\mathbf{G}_n^{-1} \widehat{\mathbf{b}}_n)$ for $\ell \geq 0$.

We now discuss the moment-matching properties between the original system Σ_N in (1.1) and the reduced system Σ_n in (4.2). We first show that for the general second-order system Σ_N in (1.1), the first n moments of $h(s)$ and $h_n(s)$ are matched. Then we show that for a symmetric second-order system, the first $2n$ moments of $h(s)$ and $h_n(s)$ are matched. These results are still true in the presence of deflations. Furthermore, if the SOAR procedure breaks down at the n_0th step, then the transfer function $h_{n_0}(s)$ of the reduced-order system Σ_{n_0} is identical to the transfer function $h(s)$ of the original system Σ_N, i.e., $h_{n_0}(s) \equiv h(s)$. Therefore, we may regard this as a lucky breakdown.

THEOREM 4.1. *The first n moments of the original system Σ_N in* (1.1) *and the reduced system Σ_n in* (4.2) *are matched, i.e., $m_\ell = m_\ell^{(n)}$ for $\ell = 0, 1, 2, \ldots, n-1$. Hence $h_n(s)$ is an nth Padé-type approximant of the transfer function $h(s)$:*

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

The result of Theorem 4.1 is from a combination of the subspace embedding Theorem 3.1 and a theorem on the Krylov subspace-based moment-matching property presented in [17, Theorem 3.1]. For the sake of completeness, we present a proof here. We first prove a couple of lemmas. These lemmas will also be used later.

LEMMA 4.2. *For $\ell = 0, 1, \ldots, n-1$, $\mathbf{Q}_{[n]}\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{H}^\ell\,\widehat{\mathbf{b}}_0 = \mathbf{H}^\ell\,\widehat{\mathbf{b}}_0$.*

Proof. From Theorem 3.1, $\mathbf{H}^\ell\widehat{\mathbf{b}}_0 \in \operatorname{span}\{\mathbf{Q}_{[n]}\}$ for $\ell \geq 0$. Since $\mathbf{Q}_{[n]}\mathbf{Q}_{[n]}^{\mathrm{T}}$ is the orthogonal projector onto $\operatorname{span}\{\mathbf{Q}_{[n]}\}$, the lemma follows immediately. ∎

LEMMA 4.3. *For $\ell = 0, 1, 2, \ldots, n-1$, $(-\mathbf{G}_n^{-1}\mathbf{C}_n)^\ell\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n = \mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{H}^\ell\widehat{\mathbf{b}}_0$.*

Proof. We prove by induction on ℓ. As the base case, for $\ell = 0$, by the definition of $\widehat{\mathbf{b}}_0$ and Lemma 4.2, it gives that $\widehat{\mathbf{b}} = \mathbf{G}\mathbf{Q}_{[n]}\mathbf{Q}_{[n]}^{\mathrm{T}}\widehat{\mathbf{b}}_0$. Then we have

$$\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n = \mathbf{G}_n^{-1}\mathbf{Q}_{[n]}^{\mathrm{T}}\widehat{\mathbf{b}} = \mathbf{G}_n^{-1}\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{G}\mathbf{Q}_{[n]}\mathbf{Q}_{[n]}^{\mathrm{T}}\widehat{\mathbf{b}}_0 = \mathbf{Q}_{[n]}^{\mathrm{T}}\widehat{\mathbf{b}}_0.$$

This proves that the lemma is true for $\ell = 0$. Suppose that the lemma is true for $\ell - 1$. For $\ell\,(< n)$, by the hypothesis $\mathbf{C}_n = \mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{C}\mathbf{Q}_{[n]}$ and Lemma 4.2, it yields that

$$\begin{aligned}
\left(-\mathbf{G}_n^{-1}\mathbf{C}_n\right)^\ell \mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n &= \left(-\mathbf{G}_n^{-1}\mathbf{C}_n\right)\left(-\mathbf{G}_n^{-1}\mathbf{C}_n\right)^{\ell-1}\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n \\
&= \left(-\mathbf{G}_n^{-1}\mathbf{C}_n\right)\cdot\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{H}^{\ell-1}\widehat{\mathbf{b}}_0 \\
&= -\mathbf{G}_n^{-1}\cdot\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{C}\mathbf{Q}_{[n]}\cdot\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{H}^{\ell-1}\widehat{\mathbf{b}}_0 \\
&= -\mathbf{G}_n^{-1}\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{C}\cdot\mathbf{H}^{\ell-1}\widehat{\mathbf{b}}_0.
\end{aligned}$$

Inserting $\mathbf{I} = \mathbf{G}\mathbf{G}^{-1}$ in the middle of the right-hand side of the preceding expression, we obtain

$$\left(-\mathbf{G}_n^{-1}\mathbf{C}_n\right)^\ell \mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n = -\mathbf{G}_n^{-1}\mathbf{Q}_{[n]}^{\mathrm{T}}\cdot\mathbf{G}\mathbf{G}^{-1}\cdot\mathbf{C}\mathbf{H}^{\ell-1}\widehat{\mathbf{b}}_0 = \mathbf{G}_n^{-1}\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{G}\cdot\mathbf{H}^\ell\widehat{\mathbf{b}}_0.$$

Finally, by Lemma 4.2 again, we have

$$\left(-\mathbf{G}_n^{-1}\mathbf{C}_n\right)^\ell \mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n = \mathbf{G}_n^{-1}\cdot\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{G}\cdot\mathbf{Q}_{[n]}\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{H}^\ell\widehat{\mathbf{b}}_0 = \mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{H}^\ell\widehat{\mathbf{b}}_0.$$

This finishes the induction argument, which completes the proof of the lemma. ∎

Proof of Theorem 4.1. For any $\ell < n$, by the definition of $m_\ell^{(n)}$ and Lemma 4.3, we have

$$m_\ell^{(n)} = \widehat{\mathbf{l}}_n^{\mathrm{T}}(-\mathbf{G}_n^{-1}\mathbf{C}_n)^\ell\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n = \widehat{\mathbf{l}}_n^{\mathrm{T}}\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{H}^\ell\widehat{\mathbf{b}}_0.$$

Next, by the definition of $\widehat{\mathbf{l}}_n^{\mathrm{T}}$ and Lemma 4.2, we have

$$m_\ell^{(n)} = \widehat{\mathbf{l}}^{\,\mathrm{T}}\mathbf{Q}_{[n]}\mathbf{Q}_{[n]}^{\mathrm{T}}\mathbf{H}^\ell\widehat{\mathbf{b}}_0 = \widehat{\mathbf{l}}^{\,\mathrm{T}}\mathbf{H}^\ell\widehat{\mathbf{b}}_0 = m_\ell.$$

This proves that the first n moments of $h(s)$ and $h_n(s)$ are equal. □

The following theorem concerns the property of the reduced system Σ_n at the breakdown of the SOAR procedure.

THEOREM 4.4. *If the SOAR procedure breaks down at step n_0, i.e.,* $\mathrm{span}\{\mathbf{Q}_{n_0}\} = \mathcal{G}_\infty(\mathbf{A},\mathbf{B};\mathbf{r}_0)$*, then the transfer function $h_{n_0}(s)$ of the reduced system Σ_{n_0} is identical to the transfer function $h(s)$ of the original system Σ_N, i.e., $h_{n_0}(s) \equiv h(s)$.*

Proof. As we discussed in section 3, when the SOAR procedure breaks down at step n_0, we know that $\mathbf{r}_\ell \in \mathrm{span}\{\mathbf{Q}_{n_0}\} = \mathcal{G}_\infty(\mathbf{A},\mathbf{B};\mathbf{r}_0)$ for all $\ell \geq 0$. By Theorem 3.1, this indicates that $\mathbf{H}^\ell\widehat{\mathbf{b}}_0 \in \mathrm{span}\{\mathbf{Q}_{[n_0]}\}$ for all $\ell \geq 0$, which implies that

$$\mathcal{K}_\infty\big(\mathbf{H};\widehat{\mathbf{b}}_0\big) \subseteq \mathrm{span}\{\mathbf{Q}_{[n_0]}\}.$$

On the other hand, by the Cayley–Hamilton theorem (for example, see [18, p. 86]), there is a polynomial $p(t)$ of degree at most $N-1$ such that $(\mathbf{I}-s\mathbf{H})^{-1} = p(\mathbf{I}-s\mathbf{H})$. It gives that

$$(\mathbf{I}-s\mathbf{H})^{-1}\widehat{\mathbf{b}}_0 \in \mathrm{span}\{\mathbf{Q}_{[n_0]}\}. \tag{4.5}$$

Thus there exists a vector $\mathbf{f}$ such that

$$(\mathbf{I}-s\mathbf{H})^{-1}\widehat{\mathbf{b}}_0 = \mathbf{Q}_{[n_0]}\mathbf{f}. \tag{4.6}$$

Substituting the definition of $\widehat{\mathbf{b}}_0 = \mathbf{G}^{-1}\widehat{\mathbf{b}}$ into (4.6) and reordering the expression yields that

$$\mathbf{Q}_{[n_0]}^{\mathrm{T}}\widehat{\mathbf{b}} = \mathbf{Q}_{[n_0]}^{\mathrm{T}}\mathbf{G}(\mathbf{I}-s\mathbf{H})\mathbf{Q}_{[n_0]}\mathbf{f} = \mathbf{Q}_{[n_0]}^{\mathrm{T}}(\mathbf{G}+s\mathbf{C})\mathbf{Q}_{[n_0]}\mathbf{f} = (\mathbf{G}_{n_0}+s\mathbf{C}_{n_0})\,\mathbf{f}.$$

Next multiplying $(\mathbf{G}_{n_0}+s\mathbf{C}_{n_0})^{-1}$ from the left of the preceding equation and by (4.6) and the orthonormality of $\mathbf{Q}_{[n_0]}$, we have

$$(\mathbf{G}_{n_0}+s\mathbf{C}_{n_0})^{-1}\,\mathbf{Q}_{[n_0]}^{\mathrm{T}}\widehat{\mathbf{b}} = \mathbf{f} = \mathbf{Q}_{[n_0]}^{\mathrm{T}}(\mathbf{I}-s\mathbf{H})^{-1}\mathbf{G}^{-1}\widehat{\mathbf{b}} = \mathbf{Q}_{[n_0]}^{\mathrm{T}}(\mathbf{G}+s\mathbf{C})^{-1}\widehat{\mathbf{b}}. \tag{4.7}$$

Now recall that the transfer function h_{n_0} of Σ_{n_0} can be written as

$$h_{n_0}(s) = \mathbf{l}_{n_0}^{\mathrm{T}}\left(s^2\mathbf{M}_{n_0}+s\mathbf{D}_{n_0}+\mathbf{K}_{n_0}\right)^{-1}\mathbf{b}_{n_0} = \widehat{\mathbf{l}}^{\,\mathrm{T}}\mathbf{Q}_{[n_0]}\left(s\mathbf{C}_{n_0}+\mathbf{G}_{n_0}\right)^{-1}\mathbf{Q}_{[n_0]}^{\mathrm{T}}\widehat{\mathbf{b}}.$$

Hence, by (4.7), we have

$$h_{n_0}(s) = \widehat{\mathbf{l}}^{\,\mathrm{T}}\mathbf{Q}_{[n_0]}\mathbf{Q}_{[n_0]}^{\mathrm{T}}(\mathbf{G}+s\mathbf{C})^{-1}\widehat{\mathbf{b}}^{\mathrm{T}}.$$

Using (4.5) and Lemma 4.2, we get

$$h_{n_0}(s) = \widehat{\mathbf{l}}^{\,\mathrm{T}}(\mathbf{G}+s\mathbf{C})^{-1}\widehat{\mathbf{b}}^{\mathrm{T}} = h(s).$$

This completes the proof. □

We now consider the moment-matching property for a symmetric second-order system Σ_N^{S}, namely, matrices $\mathbf{M}$, $\mathbf{D}$, and $\mathbf{K}$ are symmetric and $\mathbf{b} = \mathbf{l}$. The transfer function of Σ_N^{S} is given by

$$h^{(\mathrm{S})}(s) = \mathbf{b}^{\mathrm{T}}\left(s^2\mathbf{M}+s\mathbf{D}+\mathbf{K}\right)^{-1}\mathbf{b}.$$

Correspondingly, the transfer function of the reduced symmetric second-order system Σ_n^{S} is of the form

$$h_n^{(\mathrm{s})}(s) = \mathbf{b}_n^{\mathrm{T}} \left(s^2\mathbf{M}_n + s\mathbf{D}_n + \mathbf{K}_n\right)^{-1} \mathbf{b}_n,$$

where matrices $\mathbf{M}_n$, $\mathbf{D}_n$, and $\mathbf{K}_n$ and the vector $\mathbf{b}_n$ are defined as in (4.2).

THEOREM 4.5. *For the symmetric second-order system Σ_N^{S} and its reduced system Σ_n^{S}, the first $2n$ moments of $h^{(s)}(s)$ and $h_n^{(s)}(s)$ are equal, i.e., $m_\ell = m_\ell^{(n)}$ for $\ell = 0, 1, 2, \ldots, 2n-1$. Hence $h_n^{(s)}(s)$ is an nth Padé approximant of $h^{(s)}(s)$:*

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

The theorem is a consequence of Theorem 4.1 with a careful exploitation of symmetry. We provide only a sketch of the proof.

Sketch of proof. First, by induction, we can show that the following two identities hold:

$$\widehat{\mathbf{b}}^{\mathrm{T}}\mathbf{G}^{-1}\left(-\mathbf{C}\mathbf{G}^{-1}\right)^{\ell} = \widehat{\mathbf{b}}^{\mathrm{T}}\mathbf{G}^{-1}\left(-\mathbf{C}^{\mathrm{T}}\mathbf{G}^{-1}\right)^{\ell} \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{M} \end{bmatrix} \quad \text{for } \ell \geq 0 \tag{4.8}$$

and

$$\widehat{\mathbf{b}}_n^{\mathrm{T}}\mathbf{G}_n^{-1}\left(-\mathbf{C}_n\mathbf{G}_n^{-1}\right)^{\ell} = \widehat{\mathbf{b}}_n^{\mathrm{T}}\mathbf{G}_n^{-1}\left(-\mathbf{C}_n^{\mathrm{T}}\mathbf{G}_n^{-1}\right)^{\ell} \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{M}_n \end{bmatrix} \quad \text{for } \ell \geq 0. \tag{4.9}$$

Then, we note that for any $\ell \leq 2n-1$, the moment $m_\ell^{(n)}$ can be written in the form

$$\begin{aligned} m_\ell^{(n)} &= \widehat{\mathbf{b}}_n^{\mathrm{T}}(-\mathbf{G}_n^{-1}\mathbf{C}_n)^{i+j+1}(\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n) \\ &= -\widehat{\mathbf{b}}_n^{\mathrm{T}}\mathbf{G}_n^{-1}(-\mathbf{C}_n\mathbf{G}_n^{-1})^{i}\mathbf{C}_n(-\mathbf{G}_n^{-1}\mathbf{C}_n)^{j}(\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n), \end{aligned}$$

where $\ell = i+j+1$ and $0 \leq i,\ j < n$. By (4.9), we get

$$m_\ell^{(n)} = -((-\mathbf{G}_n^{-1}\mathbf{C}_n)^{i}\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n)^{\mathrm{T}} \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{M}_n \end{bmatrix} \mathbf{C}_n(-\mathbf{G}_n^{-1}\mathbf{C}_n)^{j}(\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n).$$

By the definitions of $\mathbf{M}_n$ and $\mathbf{C}_n$, the above expression can be written as

$$m_\ell^{(n)} = -((-\mathbf{G}_n^{-1}\mathbf{C}_n)^{i}\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n)^{\mathrm{T}}\mathbf{Q}_{[n]}^{\mathrm{T}} \begin{bmatrix} \mathbf{D} & \mathbf{M} \\ \mathbf{M} & \mathbf{0} \end{bmatrix} \mathbf{Q}_{[n]}(-\mathbf{G}_n^{-1}\mathbf{C}_n)^{j}(\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n). \tag{4.10}$$

On the other hand, by applying Lemma 4.3 and then Lemma 4.2, we have

$$\begin{aligned} \mathbf{Q}_{[n]}(-\mathbf{G}_n^{-1}\mathbf{C}_n)^{j}(\mathbf{G}_n^{-1}\widehat{\mathbf{b}}_n) &= \mathbf{Q}_{[n]}\mathbf{Q}_{[n]}^{\mathrm{T}}(-\mathbf{G}^{-1}\mathbf{C})^{j}(\mathbf{G}^{-1}\widehat{\mathbf{b}}) \\ &= (-\mathbf{G}^{-1}\mathbf{C})^{j}(\mathbf{G}^{-1}\widehat{\mathbf{b}}). \end{aligned} \tag{4.11}$$

Substituting (4.11) into (4.10), we have

$$\begin{aligned} m_\ell^{(n)} &= -((-\mathbf{G}^{-1}\mathbf{C})^{i}\mathbf{G}^{-1}\widehat{\mathbf{b}})^{\mathrm{T}} \begin{bmatrix} \mathbf{D} & \mathbf{M} \\ \mathbf{M} & \mathbf{0} \end{bmatrix} (-\mathbf{G}^{-1}\mathbf{C})^{j}(\mathbf{G}^{-1}\widehat{\mathbf{b}}) \\ &= -\widehat{\mathbf{b}}^{\mathrm{T}}\mathbf{G}^{-1}(-\mathbf{C}^{\mathrm{T}}\mathbf{G}^{-1})^{i} \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{M} \end{bmatrix} \mathbf{C}(-\mathbf{G}^{-1}\mathbf{C})^{j}(\mathbf{G}^{-1}\widehat{\mathbf{b}}). \end{aligned}$$

Finally, by (4.8), we deduce that for $\ell \leq 2n-1$,

$$\begin{aligned} m_\ell^{(n)} &= -\widehat{\mathbf{b}}^{\mathrm{T}}\mathbf{G}^{-1}(-\mathbf{C}\mathbf{G}^{-1})^{i}\mathbf{C}(-\mathbf{G}^{-1}\mathbf{C})^{j}(\mathbf{G}^{-1}\widehat{\mathbf{b}}) \\ &= \widehat{\mathbf{b}}^{\mathrm{T}}(-\mathbf{G}^{-1}\mathbf{C})^{i+j+1}(\mathbf{G}^{-1}\widehat{\mathbf{b}}) = m_\ell. \end{aligned}$$

This completes the sketch of proof. ∎

5. Algorithms. In this section, we continue the discussion of the SOAR-based method for dimension reduction of the second-order system Σ_N described in section 4. For the purpose of comparisons, we include the standard Arnoldi-based algorithm for the dimension reduction of Σ_N via linearization.

In practice, often an approximant of the transfer function $h(s)$ of the original system Σ_N around a selected expansion point $s_0 \neq 0$ is interested. In this case, $h(s)$ can be written in the form

$$h(s) = \mathbf{l}^{\mathrm{T}}((s-s_0)^2\mathbf{M} + (s-s_0)\widetilde{\mathbf{D}} + \widetilde{\mathbf{K}})^{-1}\mathbf{b},$$

where $\widetilde{\mathbf{D}} = 2s_0\mathbf{M} + \mathbf{D}$ and $\widetilde{\mathbf{K}} = s_0^2\mathbf{M} + s_0\mathbf{D} + \mathbf{K}$. s_0 is an arbitrary but of fixed value such that the matrix $\widetilde{\mathbf{K}}$ is nonsingular. Correspondingly, the moments of $h(s)$ about s_0 can be defined in a way similar to (2.5).

By applying the SOAR procedure (Algorithm 1), we can generate an orthonormal basis $\mathbf{Q}_n$ of the second-order Krylov subspace $\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0)$ with matrices $\mathbf{A} = -\widetilde{\mathbf{K}}^{-1}\widetilde{\mathbf{D}}$ and $\mathbf{B} = -\widetilde{\mathbf{K}}^{-1}\mathbf{M}$ and the starting vector $\mathbf{r}_0 = \widetilde{\mathbf{K}}^{-1}\mathbf{b}$. The subspace spanned by the nonzero columns of $\mathbf{Q}_n$ is used as the projection subspace for defining a reduced system Σ_n. Subsequently, the transfer function $h_n(s)$ of the reduced system Σ_n about the expansion point s_0 is given by

$$h_n(s) = \mathbf{l}_n^{\mathrm{T}}((s-s_0)^2\mathbf{M}_n + (s-s_0)\widetilde{\mathbf{D}}_n + \widetilde{\mathbf{K}}_n)^{-1}\mathbf{b}_n,$$

where $\mathbf{M}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{M}\mathbf{Q}_n$, $\widetilde{\mathbf{D}}_n = \mathbf{Q}_n^{\mathrm{T}}\widetilde{\mathbf{D}}\mathbf{Q}_n$, $\widetilde{\mathbf{K}}_n = \mathbf{Q}_n^{\mathrm{T}}\widetilde{\mathbf{K}}\mathbf{Q}_n$, $\mathbf{l}_n^{\mathrm{T}} = \mathbf{Q}_n^{\mathrm{T}}\mathbf{l}$, and $\mathbf{b}_n^{\mathrm{T}} = \mathbf{Q}_n^{\mathrm{T}}\mathbf{b}$. By a straightforward algebraic manipulation, $h_n(s)$ can be simply expressed as

$$h_n(s) = \mathbf{l}_n^{\mathrm{T}}\left(s^2\mathbf{M}_n + \mathbf{D}_n + \mathbf{K}_n\right)^{-1}\mathbf{b}_n, \tag{5.1}$$

where $\mathbf{M}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{M}\mathbf{Q}_n$, $\mathbf{D}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{D}\mathbf{Q}_n$, $\mathbf{K}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{K}\mathbf{Q}_n$, $\mathbf{l}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{l}$, and $\mathbf{b}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{b}$. In other words, the transformed matrix triplet $(\mathbf{M}, \widetilde{\mathbf{D}}, \widetilde{\mathbf{K}})$ is used to generate an orthonormal basis $\mathbf{Q}_n$ of the projection subspace $\mathcal{G}_n$, but the original matrix triplet $(\mathbf{M}, \mathbf{D}, \mathbf{K})$ is directly projected onto the subspace $\mathcal{G}_n$ to define a reduced system Σ_n.

By an equivalent argument as presented in section 4, 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 nth Padé-type approximant of $h(s)$ about s_0, i.e.,

$$h(s) = h_n(s) + \mathcal{O}\left((s-s_0)^n\right).$$

Furthermore, if Σ_N is a symmetric second-order system, Σ_N^{S}, then the first $2n$ moments about s_0 of $h^{(\mathrm{S})}(s)$ and $h_n^{(\mathrm{S})}(s)$ are the same, which implies that $h_n^{(\mathrm{S})}(s)$ is an nth Padé approximant of $h(s)$ about s_0, i.e.,

$$h^{(\mathrm{S})}(s) = h_n^{(\mathrm{S})}(s) + \mathcal{O}\left((s-s_0)^{2n}\right).$$

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

ALGORITHM 2. *Second-order 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 the SOAR procedure (Algorithm 1) to generate an orthonormal basis $\mathbf{Q}_n$ of $\mathcal{G}_n(\mathbf{A}, \mathbf{B}; \mathbf{r}_0)$, where $\mathbf{A} = -\widetilde{\mathbf{K}}^{-1}\widetilde{\mathbf{D}}$, $\mathbf{B} = -\widetilde{\mathbf{K}}^{-1}\mathbf{M}$, and $\mathbf{r}_0 = \widetilde{\mathbf{K}}^{-1}\mathbf{b}$. $\widetilde{\mathbf{D}} = 2s_0\mathbf{M} + \mathbf{D}$ and $\widetilde{\mathbf{K}} = s_0^2\mathbf{M} + s_0\mathbf{D} + \mathbf{K}$.*

3. *Compute* $\mathbf{M}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{M}\mathbf{Q}_n$, $\mathbf{D}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{D}\mathbf{Q}_n$, $\mathbf{K}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{K}\mathbf{Q}_n$, $\mathbf{l}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{l}$, *and* $\mathbf{b}_n = \mathbf{Q}_n^{\mathrm{T}}\mathbf{b}$. *This defines a reduced system* Σ_n *as in* (4.2) *about the selected expansion point* s_0.

As we have noticed, by the definitions of the matrices $\mathbf{M}_n$, $\mathbf{D}_n$, and $\mathbf{K}_n$ in the reduced system Σ_n, essential properties of the matrices $\mathbf{M}$, $\mathbf{D}$, and $\mathbf{K}$ of the original system Σ_N are preserved. For example, if $\mathbf{M}$ is symmetric positive definite, so is $\mathbf{M}_n$. Consequently, we can preserve the stability, symmetric, and physical meaning of the original second-order system Σ_N.

The explicit formulation of the matrices $\mathbf{M}_n$, $\mathbf{D}_n$, and $\mathbf{K}_n$ is done by using matrix-vector product operations $\mathbf{Mq}$, $\mathbf{Dq}$, and $\mathbf{Kq}$ for an arbitrary vector $\mathbf{q}$. Later in this section, we will see that this is an overhead comparing to the method based on the Arnoldi procedure, in which the projection of the matrix is obtained as a by-product without any additional cost. However, we believe this is a numerically better way to use the computed orthonormal basis $\mathbf{Q}_n$ for the second-order system. The preservation of structure of the underlying problem outweighs the extra cost of floating point operations in 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 $\mathbf{M}$ and $\mathbf{D}$ and $\mathbf{K}$ in practical problems we encountered. The bottleneck of computational costs is often associated with the matrix-vector multiplication operations involving $\widetilde{\mathbf{K}}^{-1}$ at step 2 of the algorithm.

In the rest of this section, we give a short review on the basic Arnoldi-based Krylov subspace projection method for the dimension reduction of the second-order system Σ_N via linearization. By denoting $\mathbf{x}(t) = [\mathbf{q}(t)^{\mathrm{T}}, \dot{\mathbf{q}}(t)^{\mathrm{T}}]^{\mathrm{T}}$, the second-order system Σ_N can be written in an equivalent linear form:

$$\Sigma_N^{\mathrm{L}} : \begin{cases} \mathbf{C}\dot{\mathbf{x}}(t) + \mathbf{G}\mathbf{x}(t) = \widehat{\mathbf{b}}u(t), \\ y(t) = \widehat{\mathbf{l}}^{\mathrm{T}}\mathbf{x}(t), \end{cases} \tag{5.2}$$

where $\mathbf{C}$, $\mathbf{G}$, $\widehat{\mathbf{b}}$, and $\widehat{\mathbf{l}}$ are as defined in Lemma 2.1. The transfer function of Σ_N^{L} and its Taylor series expansion about a selected expansion point s_0 are given by

$$h(s) = \widehat{\mathbf{l}}^{\mathrm{T}}(s\mathbf{C} + \mathbf{G})^{-1}\widehat{\mathbf{b}} = \widehat{\mathbf{l}}^{\mathrm{T}}(\mathbf{I} - (s - s_0)\mathbf{H}^{(\mathrm{L})})^{-1}\widehat{\mathbf{r}} = \sum_{\ell=0}^{\infty} m_\ell \, (s - s_0)^\ell,$$

where $\mathbf{H}^{(\mathrm{L})} = -(\mathbf{G} + s_0\mathbf{C})^{-1}\mathbf{C}$ and $\widehat{\mathbf{r}} = (\mathbf{G} + s_0\mathbf{C})^{-1}\widehat{\mathbf{b}}$. s_0 is an arbitrary but fixed value such that the matrkx $\mathbf{G} + s_0\mathbf{C}$ is invertible. The moments of $h(s)$ are $m_\ell = \widehat{\mathbf{l}}^{\mathrm{T}}(\mathbf{H}^{(\mathrm{L})})^\ell\widehat{\mathbf{r}}$ for $\ell \geq 0$.

Let $\mathbf{V}_n$ be an orthonormal basis of the Krylov subspace $\mathcal{K}_n(\mathbf{H}^{(\mathrm{L})}; \widehat{\mathbf{r}})$ generated by the standard Arnoldi process; see, for example, [16, 13, 27]. Then by approximating the state vector $\mathbf{x}(t)$ of the linear system Σ_N^{L} by another state vector $\mathbf{x}_n(t)$ constrained to the subspace spanned by $\mathbf{V}_n$, namely, $\mathbf{x}(t) \approx \mathbf{V}_n\mathbf{x}_n(t)$, where $\mathbf{x}_n(t)$ is an $n \times 1$ vector, we obtain a reduced linear system

$$\Sigma_n^{\mathrm{L}} : \begin{cases} \mathbf{C}_n^{(\mathrm{L})}\dot{\mathbf{x}}_n(t) + \mathbf{G}_n^{(\mathrm{L})}\mathbf{x}_n(t) = \widehat{\mathbf{b}}_n u(t), \\ \widetilde{y}(t) = \widehat{\mathbf{l}}_n^{\mathrm{T}}\mathbf{x}_n(t), \end{cases} \tag{5.3}$$

where $\mathbf{C}_n^{(\mathrm{L})} = -\mathbf{H}_n^{(\mathrm{L})}$, $\mathbf{G}_n^{(\mathrm{L})} = \mathbf{I} + s_0\mathbf{H}_n^{(\mathrm{L})}$, $\widehat{\mathbf{b}}_n = \mathbf{V}_n^{\mathrm{T}}\widehat{\mathbf{r}}$, and $\widehat{\mathbf{l}}_n = \mathbf{V}_n^{\mathrm{T}}\widehat{\mathbf{l}}$. $\mathbf{H}_n^{(\mathrm{L})} = \mathbf{V}_n^{\mathrm{T}}\mathbf{H}^{(\mathrm{L})}\mathbf{V}_n$ is an $n \times n$ upper Hessenberg matrix and generated as a by-product of the Arnoldi procedure. Note that $\widehat{\mathbf{r}}$ is the first vector in $\mathcal{K}_n(\mathbf{H}^{(\mathrm{L})}; \widehat{\mathbf{r}})$. Therefore, the vector $\widehat{\mathbf{b}}_n$ can be rewritten as $\widehat{\mathbf{b}}_n = \|\widehat{\mathbf{r}}\|_2 \mathbf{e}_1$, where $\mathbf{e}_1$ is the first unit vector. The transfer function of the reduced system $\Sigma_n^{\rm L}$ is given by

$$h_n^{(\rm L)}(s) = \widehat{\mathbf{l}}_n^{\rm T}(s\mathbf{C}_n^{(\rm L)} + \mathbf{G}_n^{(\rm L)})^{-1}\widehat{\mathbf{b}}_n = \|\widehat{\mathbf{r}}\|_2 \cdot \widehat{\mathbf{l}}_n^{\rm T}(\mathbf{I} - (s-s_0)\mathbf{H}_n^{(\rm L)})^{-1}\mathbf{e}_1.$$

This Arnoldi-based method for the dimension reduction of the second-order system Σ_N via linearization is outlined as follows.

Algorithm 3. *Arnoldi-based method for dimension reduction of second-order system via linearization.*

1. *Select an order n for the reduced system, and an expansion point s_0.*
2. *Run n steps of the Arnoldi procedure to compute an orthonormal basis $\mathbf{V}_n$ of Krylov subspace $\mathcal{K}_n(\mathbf{H}^{(\rm L)}, \widehat{\mathbf{r}})$, where $\mathbf{H}^{(\rm L)} = -(\mathbf{G}+s_0\mathbf{C})^{-1}\mathbf{C}$ and $\widehat{\mathbf{r}} = (\mathbf{G}+s_0\mathbf{C})^{-1}\widehat{\mathbf{b}}$.*
3. *Let $\mathbf{C}_n^{(\rm L)} = -\mathbf{H}_n^{(\rm L)}$, $\mathbf{G}_n^{(\rm L)} = \mathbf{I} + s_0\mathbf{H}_n^{(\rm L)}$, $\widehat{\mathbf{b}}_n = \|\widehat{\mathbf{r}}\|_2\mathbf{e}_1$, and $\widehat{\mathbf{l}}_n = \mathbf{V}_n^{\rm T}\widehat{\mathbf{l}}$. Then a reduced system $\Sigma_n^{\rm L}$ of Σ_N is defined by* (5.3).

It is well known that the first n moments about the expansion point s_0 of $h(s)$ and $h_n^{(\rm L)}(s)$ are the same. Therefore, $h_n^{(\rm L)}(s)$ is an nth Padé-type approximant of $h(s)$ about s_0, i.e.,

$$h(s) = h_n^{(\rm L)}(s) + \mathcal{O}\left((s-s_0)^n\right).$$

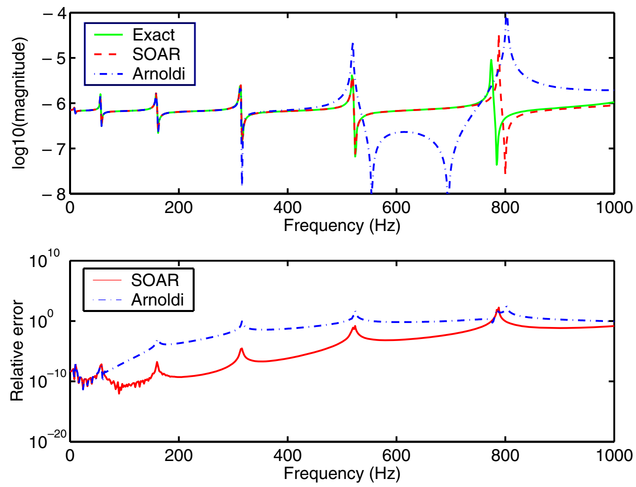
Furthermore, if Σ_N is a symmetric second-order system and a symmetric linearization is utilized, then the first $2n$ moments about the expansion point s_0 of $h(s)$ and $h_n^{(\rm L)}(s)$ are the same. As a result, $h_n^{(\rm L)}(s)$ is an nth Padé approximant of $h(s)$ about s_0,

$$h(s) = h_n^{(\rm L)}(s) + \mathcal{O}\left((s-s_0)^{2n}\right).$$

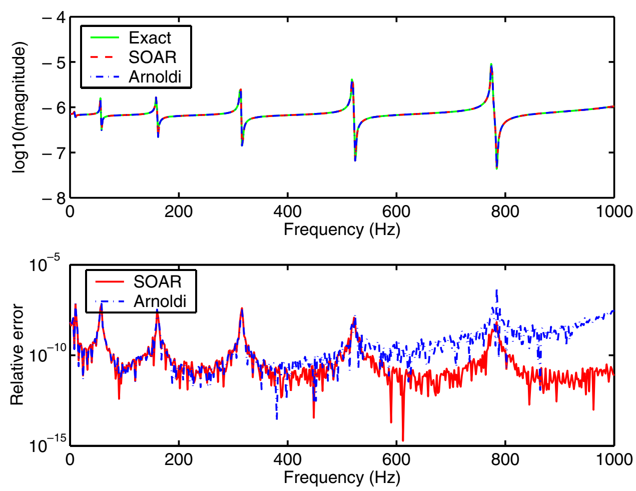
Hence the reduced systems Σ_n (2.6) and $\Sigma_n^{(\rm L)}$ (5.3) have the same orders of approximations of transfer function $h(s)$. However, only the reduced system Σ_n preserves the second-order form of the original system Σ_N.

6. Numerical examples. In this section, we present three numerical examples to compare the accuracy of dimension reduction methods of Σ_N based on the SOAR procedure (Algorithm 2) and on the standard Arnoldi procedure (Algorithm 3). Under the scope of this work, we are concerned only with the basic properties and behaviors of the new SOAR-based method. It is implemented in a straightforward way, as outlined in Algorithm 2. Therefore, we will compare the SOAR method with a straightforward implementation of the Arnoldi method as described in Algorithm 3. All numerical experiments were run in MATLAB on a Sun Ultra 10 workstation.

Example 1. This is an example for the frequency response analysis of a second-order system of order $N = 400$, which comes from a finite element model of a shaft on bearing supports with a damper. The data were extracted from MSC/NASTRAN [19]. This is a symmetric second-order system, where $\mathbf{M}$ and $\mathbf{D}$ are symmetric but not positive definite, and $\mathbf{K}$ is symmetric positive definite with 1-norm condition number about $\mathcal{O}(10^9)$. There is no shift, i.e., $s_0 = 0$. Figure 6.1(a) shows the magnitudes (in log of base 10) of the exact transfer function $h(s)$ and approximate ones by the SOAR method (Algorithm 2) at $n = 15$. The relative errors $|h(\mathrm{j}\omega) - h_n(\mathrm{j}\omega)|/|h(\mathrm{j}\omega)|$ and $|h(\mathrm{j}\omega) - h_n^{(\rm L)}(\mathrm{j}\omega)|/|h(\mathrm{j}\omega)|$ are shown at the second plot of Figure 6.1(a). Figure 6.1(b) shows the results for $n = 30$. This example shows that the SOAR method not only preserves the symmetry and second-order structure but also results in a more accurate approximation. We note that this example was also reported in the previous work [2],



(a) $n = 15$

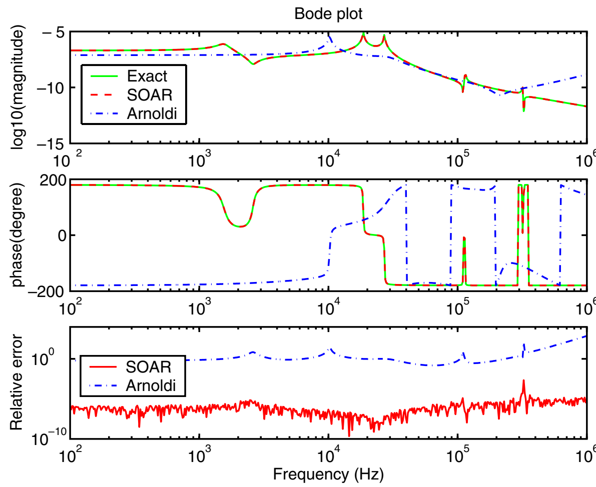


(b) $n = 30$

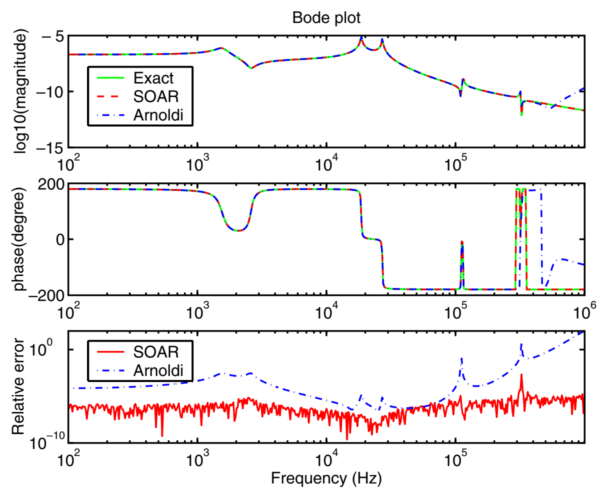
FIG. 6.1. *Magnitudes of* $h(\mathrm{j}\omega)$ *for the shaft on bearing support with a damper and its approximations* $h_n(\mathrm{j}\omega)$ *obtained by the SOAR-based method and* $h_n^{(\mathrm{L})}(\mathrm{j}\omega)$ *by the Arnoldi-based method and relative errors.*

which implements Su and Craig's algorithm [28]. The SOAR-based method uses a much smaller reduced-order system and produces a better approximation of $h(s)$.

Example 2. In this example, we report the numerical results for the simulation of a linear-drive multimode resonator structure [10]. This is a nonsymmetric second-order system. The mass and damping matrices $\mathbf{M}$ and $\mathbf{D}$ are singular, and the stiffness matrix $\mathbf{K}$ is very ill-conditioned with 1-norm condition number at $\mathcal{O}(10^{15})$. An expansion point $s_0 = 2 \times 10^5\pi$ is used, the same as in [10]. The 1-norm condition number of the transformed stiffness matrix $\widetilde{\mathbf{K}} = s_0^2\mathbf{M} + s_0\mathbf{D} + \mathbf{K}$ is slightly improved to $\mathcal{O}(10^{13})$. No further attempt is made to improve the condition number of $\widetilde{\mathbf{K}}$. In Figure 6.2, 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 $n = 10$ and $n = 20$ via



(a) $n = 10$



(b) $n = 20$

FIG. 6.2. *Bode plots of $h(\mathrm{j}\omega)$ of the resonator, its approximations $h_n(\mathrm{j}\omega)$ by the SOAR procedure and $h_n^{(\mathrm{L})}(\mathrm{j}\omega)$ by the Arnoldi procedure, and relative errors.*

the SOAR and Arnoldi methods are reported. The corresponding relative errors are also shown over the frequency range of interest. The results clearly indicate that the SOAR-based method is considerably superior to the Arnoldi-based method.

Example 3. This example is from the frequency response simulation of a torsional micromirror described in [8]. Using a lumped finite element analysis results in a second-order system Σ_N of state-space dimension $N = 846$. Mass and damping matrices $\mathbf{M}$ and $\mathbf{D}$ are symmetric with small elements: $\|\mathbf{M}\|_1 = \mathcal{O}(10^{-8})$ and $\|\mathbf{D}\|_1 = \mathcal{O}(10^{-6})$. In contrast, stiffness matrix $\mathbf{K}$ is nonsymmetric with large elements: $\|\mathbf{K}\|_1 = \mathcal{O}(10^9)$. All matrices are ill-conditioned with 1-norm condition number about $\mathcal{O}(10^{18})$. An expansion point $s_0 = 2 \times 10^4\pi$ is selected. The 1-norm condition number of the transformed stiffness matrix $\widetilde{\mathbf{K}} = s_0^2\mathbf{M} + s_0\mathbf{D} + \mathbf{K}$ is still

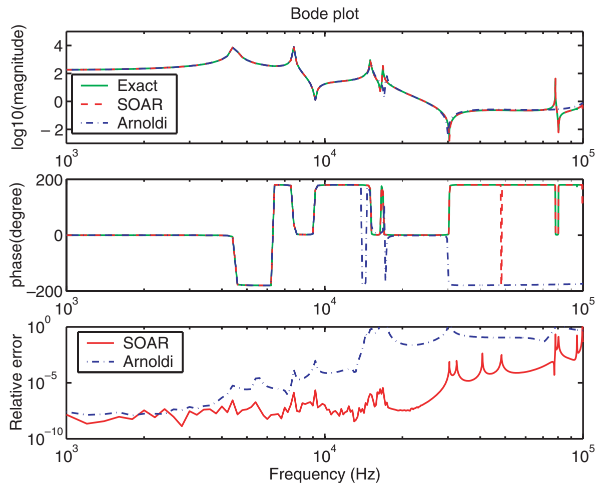


FIG. 6.3. *Bode and phase of the micromirror between* $1 - 100\,kHz$ *(top two graphs) and the corresponding relative errors (bottom).*

ill-conditioned. No attempt is made to improve the condition number of $\widetilde{\mathbf{K}}$. Applying the SOAR-based method to the system, we find that a reduced second system of order $n = 20$ is sufficient for the desired accuracy. Bode plots of $h(\mathtt{j}\omega)$ are shown in Figure 6.3. In Figure 6.3, the transfer function $h_n(\mathtt{j}\omega)$ obtained by the SOAR-based method is superimposed on $h(\mathtt{j}\omega)$. These results demonstrate again that the SOAR-based method not only preserves the second-order structure but also generates a significantly better approximation than the Arnoldi-based method.

7. Concluding remarks. We presented a structure-preserving dimension reduction algorithm for a second-order dynamical system Σ_N. The reduced second-order system Σ_n in (4.2) enjoys the same moment-matching properties as the existing Arnoldi-based Krylov subspace algorithm via linearization. This new approach has considerable superior numerical accuracy.

There are a number of interesting research issues for further study. One is about error estimation and adaptive selection of the dimension n of the reduced system, such as the work presented in [5, 21] for dimension reduction of linear systems. Another issue is about the numerical impact of SOAR-based algorithm in the presence of finite precision arithmetic. Another important extension of this work is about the dimension reduction of multi-input, multioutput second-order systems, particularly by taking into the account of deflations in a block second-order Krylov subspace. Applications of this method to the RCS circuit simulation and for comparing to the ENOR and SMOR algorithms [24, 30] used in the circuit simulation community are the subjects of further study.

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