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Brief paper

Krylov projection framework for Fourier model reduction ☆

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Abstract

This paper analyzes the Fourier model reduction (FMR) method from a rational Krylov projection framework and shows how the FMR reduced model, which has guaranteed stability and a global error bound, can be computed in a numerically efficient and robust manner. By monitoring the rank of the Krylov subspace that underlies the FMR model, the projection framework also provides an improved criterion for determining the number of Fourier coefficients that are needed, and hence the size of the resulting reduced-order model. The advantages of applying FMR in the rational Krylov projection framework are demonstrated on a simple example.

Keywords: Model reduction; System order reduction; Approximation; Interpolation; Discrete Fourier transform

1. Introduction

Model reduction entails the systematic generation of cost-efficient representations of large-scale systems that result, for example, from discretization of partial differential equations. Reduction methods have been successfully applied in different settings, including simulation, optimization, and control of large-scale systems arising in applications such as fluid dynamics, structural dynamics, and circuit design (Antoulas, 2005). In the case of control, model reduction is essential since many control design techniques, such as LQG and $\mathscr{H}_\infty$ methods, lead to controllers of complexity comparable to that of the original system; hence, large-scale plants lead to large-scale controllers. In real-time applications, high-order controllers are undesirable due to factors such as a need for complex hardware and degraded computational speed.

Optimal Hankel model reduction (Adamjan, Arov, & Krein, 1971; Glover, 1984), balanced truncation (Moore, 1981; Mullis & Roberts, 1976), and singular perturbation approximation (Liu & Anderson, 1989) methods have rigorous guarantees of quality and global error bounds on the resulting reduced models. Despite their appealing theoretical properties, the computational requirements associated with these methods make them impractical for application to large-scale systems of order 10^5 or higher. Several other methods have been developed that are applicable to large-scale systems, including Krylov-based methods (Gallivan, Grimme, & Van Dooren, 1994; Grimme, 1997), approximate balanced truncation (Gugercin, Sorensen, & Antoulas, 2003; Gugercin & Antoulas, 2004; Li & White, 2002), and proper orthogonal decomposition (Holmes, Lumley, & Berkooz, 1996; Kunisch & Volkwein, 1999; Sirovich, 1987). In many cases, this latter group of methods trades computational efficiency for a lack of rigorous guarantees and global error bounds.

In this paper, we investigate the Fourier model reduction (FMR) method (Willcox & Megretski, 2005). FMR preserves stability by performing a bilinear transformation and applying reduction in the discrete-frequency domain via a truncated Fourier expansion. Despite its theoretical properties such as guaranteed stability and a global error bound, the underlying projection framework and Krylov-based (interpolation) features of FMR have gone unnoticed. This paper analyzes FMR from a projection framework and shows the underlying rational Krylov projection. Through this analysis, we illustrate the interpolation

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and restricted optimal $\mathscr{H}_2$ properties of FMR; and show how the FMR reduced model can be computed in a numerically efficient and robust manner in a Krylov-based model reduction setting. Moreover, a new, more robust stopping criterion for FMR is proposed.

2. Model reduction via projection

Consider a single-input/single-output (SISO) dynamical system $\mathbf{G}(s)$ with transfer function

$$\mathbf{G}(s) = \mathbf{h}(s\mathbf{I} - \mathbf{F})^{-1}\mathbf{g} + \mathbf{J}, \tag{1}$$

where $\mathbf{F} \in \mathbb{R}^{n\times n}$, $\mathbf{g}, \mathbf{h}^{\mathrm{T}} \in \mathbb{R}^n$, and $\mathbf{J} \in \mathbb{R}$. The goal of model reduction, in this setting, is to produce a much smaller order system $\mathbf{G}_r(s)$ with transfer function

$$\mathbf{G}_r(s) = \mathbf{h}_r(s\mathbf{I}_r - \mathbf{F}_r)^{-1}\mathbf{g}_r + \mathbf{J}_r, \tag{2}$$

where $\mathbf{F}_r \in \mathbb{R}^{r\times r}$, $\mathbf{g}, \mathbf{h}^{\mathrm{T}} \in \mathbb{R}^r$, and $\mathbf{J}_r \in \mathbb{R}$, such that the reduced system $\mathbf{G}_r(s)$ approximates $\mathbf{G}(s)$ well. In *model reduction via projection*, $\mathbf{G}_r(s)$ in (2) is obtained as

$$\mathbf{F}_r = \mathbf{W}^{\mathrm{T}}\mathbf{F}\mathbf{V}, \quad \mathbf{g}_r = \mathbf{W}^{\mathrm{T}}\mathbf{g}, \quad \mathbf{h}_r = \mathbf{h}\mathbf{V} \quad \text{and} \quad \mathbf{J}_r = \mathbf{J}, \tag{3}$$

where $\mathbf{V} \in \mathbb{R}^{n\times r}$ and $\mathbf{W} \in \mathbb{R}^{n\times r}$ with $\mathbf{W}^{\mathrm{T}}\mathbf{V} = \mathbf{I}_r$. The corresponding oblique projector is given by $\mathbf{V}\mathbf{W}^{\mathrm{T}}$. Since $\mathbf{J}_r = \mathbf{J}$, without loss of generality, we assume that $\mathbf{J} = 0$.

2.1. Rational Krylov-based model reduction

In model reduction by rational Krylov projection, the goal is to find a reduced model $\mathbf{G}_r(s)$ as in (2) and (3) that interpolates $\mathbf{G}(s)$ and a certain number of its derivatives (called moments) at selected points s_k in the complex plane. In other words, the goal is to find the reduced system matrices $\mathbf{F}_r$, $\mathbf{g}_r$, and $\mathbf{h}_r$ so that

$$\begin{aligned}\frac{(-1)^j}{j!}\frac{\mathrm{d}^j\mathbf{G}(s)}{\mathrm{d}s^j}\bigg|_{s=s_k} &= \mathbf{h}(s_k\mathbf{I}_n - \mathbf{J})^{-(j+1)}\mathbf{g} \\ &= \mathbf{h}_r(s_k\mathbf{I}_r - \mathbf{F}_r)^{-(j+1)}\mathbf{g}_r \\ &= \frac{(-1)^j}{j!}\frac{\mathrm{d}^j\mathbf{G}_r(s)}{\mathrm{d}s^j}\bigg|_{s=s_k}\end{aligned} \tag{4}$$

for $k = 1, \ldots, K$ and for $j = 1, \ldots, J$, where K and J denote, respectively, the number of interpolation points s_k and the number of moments to be matched at each s_k. The quantity $\mathbf{h}(s_k\mathbf{I}_n - \mathbf{F})^{-(j+1)}\mathbf{g}$ is the jth moment of $\mathbf{G}(s)$ at s_k. If $s_k = \infty$, the moments are called Markov parameters and are given by $\mathbf{h}\mathbf{F}^j\mathbf{g}$ for $j = 0, 1, 2, \ldots$. Since the moments are extremely ill-conditioned to compute, the goal in rational Krylov-based model reduction is to find $\mathbf{G}_r(s)$ that satisfies (4) *without computing the moments explicitly*. De Villemagne and Skelton (1987) showed that the matrices $\mathbf{V}$ and $\mathbf{W}$ chosen so that

$$\begin{aligned}\mathrm{Ran}(\mathbf{V}) = \mathrm{Im}\{&(s_1\mathbf{I} - \mathbf{F})^{-1}\mathbf{g}, \ldots, (s_1\mathbf{I} - \mathbf{F})^{-K_1}\mathbf{g}, \\ &\ldots, (s_J\mathbf{I} - \mathbf{F})^{-1}\mathbf{g}, \ldots, (s_J\mathbf{I} - \mathbf{F})^{-K_J}\mathbf{g}\},\end{aligned}$$

$$\begin{aligned}\mathrm{Ran}(\mathbf{W}) = \mathrm{Im}\{&(\overline{s_1}\mathbf{I} - \mathbf{F}^{\mathrm{T}})^{-1}\mathbf{h}^{\mathrm{T}}, \ldots, (\overline{s_1}\mathbf{I} - \mathbf{H}^{\mathrm{T}})^{-K_1}\mathbf{h}^{\mathrm{T}}, \\ &\ldots, (\overline{s_J}\mathbf{I} - \mathbf{F}^{\mathrm{T}})^{-1}\mathbf{h}^{\mathrm{T}}, \ldots, (\overline{s_J}\mathbf{I} - \mathbf{F}^{\mathrm{T}})^{-K_J}\mathbf{h}^{\mathrm{T}}\},\end{aligned}$$

produce reduced-order models $\mathbf{G}_r(s)$ via (3) matching $2K_i$ moments of $\mathbf{G}(s)$ at the interpolation points s_i for $i = 1, \ldots, J$, i.e. $\mathbf{G}_r(s)$ interpolates $\mathbf{G}(s)$ and its first $2K_i - 1$ derivatives at each s_i; hence matching the moments without ever computing them. Grimme (1997) showed how one can obtain the required matrices $\mathbf{V}$ and $\mathbf{W}$ as above in a numerically efficient way using the rational Krylov method, and hence showed how to solve the moment matching problem using *Krylov projection* methods in an effective way.

3. Fourier model reduction

Given $\mathbf{G}(s)$ as in (1), let the nth-order discrete-time system $\mathbf{H}(z) = \mathbf{c}(z\mathbf{I} - \mathbf{A})^{-1}\mathbf{b} + \mathbf{d}$ be obtained from $\mathbf{G}(s)$ via a bilinear transformation, i.e.

$$\mathbf{A} = (\omega_0\mathbf{I} + \mathbf{F})(\omega_0\mathbf{I} - \mathbf{F})^{-1}, \quad \mathbf{b} = \sqrt{2\omega_0}(\omega_0\mathbf{I} - \mathbf{F})^{-1}\mathbf{g},$$

$$\mathbf{c} = \sqrt{2\omega_0}\mathbf{h}(\omega_0\mathbf{I} - \mathbf{F})^{-1}, \quad \mathbf{d} = \mathbf{J} + \mathbf{h}(\omega_0\mathbf{I} - \mathbf{F})^{-1}\mathbf{g},$$

where $\omega_0 > 0$. It is well known that

$$\mathbf{G}(s) = \mathbf{H}\left(\frac{\omega_0 + s}{\omega_0 - s}\right) \quad \text{or} \quad \mathbf{G}\left(\omega_0\frac{z-1}{z+1}\right) = \mathbf{H}(z). \tag{5}$$

Let η_i denote the Markov parameters of the discrete-time system $\mathbf{H}(z)$, i.e. $\eta_0 = \mathbf{d}$, and $\eta_i = \mathbf{c}\mathbf{A}^{i-1}\mathbf{b}$, $i \geqslant 1$.

FMR was proposed in Willcox and Megretski (2005) as an efficient method to compute reduced models with guaranteed stability and a rigorous error bound. FMR uses discrete-time Fourier coefficients to compute an intermediate discrete-time reduced model, to which balanced truncation can be subsequently applied using explicit formulae. The rth-order intermediate reduced model $\mathbf{H}_r(z) = \mathbf{c}_r(z\mathbf{I}_r - \mathbf{A}_r)^{-1}\mathbf{b}_r + \mathbf{d}$ is defined by

$$\mathbf{H}_r(z) = \sum_{k=0}^{r}\eta_k z^{-k}, \tag{6}$$

and has the form

$$\mathbf{A}_r = [\mathbf{e}_2, \mathbf{e}_3, \ldots, \mathbf{e}_r, \mathbf{0}], \quad \mathbf{b}_r = \mathbf{e}_1,$$

$$\mathbf{c}_r = [\eta_1, \eta_2, \ldots, \eta_r] \quad \text{and} \quad \mathbf{d}_r = \eta_0, \tag{7}$$

where $\mathbf{e}_i$ denotes the ith unit vector and $\mathbf{0}$ is a vector of zeroes. If desired, a continuous-time reduced model $\mathbf{G}_r(s)$ can be obtained from $\mathbf{H}_r(z)$ by an inverse bilinear transformation. As shown in Willcox and Megretski (2005), both the intermediate discrete-time model $\mathbf{H}_r(z)$ and the final continuous-time

reduced model $\mathbf{G}(s)$ are stable. Moreover, let $\mathbf{E}(z) := \mathbf{H}(z) - \mathbf{H}_r(z)$ be the discrete-time error system. Then,

$$\|\mathbf{E}(z)\|^2_{\mathscr{H}_\infty} \leqslant \frac{r^{1-2q}}{2\pi(2q-1)} \int_{-\pi}^{\pi} |\mathbf{H}^{(q)}(\mathrm{e}^{\jmath\theta})|^2 \,\mathrm{d}\theta, \tag{8}$$

where $\mathbf{H}^{(q)}$ is the qth derivative of $\mathbf{H}(\mathrm{e}^{\jmath\theta})$ with respect to θ.

For the rest of the paper, $\mathbf{H}(z)$ denotes the discrete-time system in (5) obtained via bilinear transformation of $\mathbf{G}(s)$. $\mathbf{H}_r(z)$ denotes the intermediate reduced-order model as in (6) and (7) obtained from $\mathbf{H}(z)$ via FMR. Finally, $\mathbf{G}_r(s)$ is the final continuous-time reduced system obtained via inverse bilinear transformation of $\mathbf{H}_r(z)$.

4. Interpolation and optimality properties of FMR and $\mathscr{H}_2/\mathscr{H}_\infty$ error bounds

It follows from the construction of $\mathbf{H}_r(z)$ in (6) and (7) that $\mathbf{H}_r(z)$ matches the first r Markov parameters of $\mathbf{H}(z)$. Hence, $\mathbf{G}_r(s)$ interpolates the first r moments of $\mathbf{G}(s)$ at $s = \omega_0$. To present the optimality properties of FMR, we recall the following theorem slightly modified from Gaier (1987) and Meier and Luenberger (1967):

Theorem 1 (*Gaier, 1987; Meier and Luenberger, 1967*). *Given a stable discrete-time dynamical system* $\mathbf{H}(z)=\mathbf{c}(z\mathbf{I}-\mathbf{A})^{-1}+\mathbf{d}$, *and a fixed stable pole* α, *define*

$$\widehat{\mathbf{H}}_r(z) := \mathbf{d} + \frac{\beta_0 + \beta_1 z + \cdots + \beta_{r-1} z^{r-1}}{(z-\alpha)^r}.$$

Then $\|\mathbf{H} - \widehat{\mathbf{H}}_r\|_{\mathscr{H}_2}$ *is minimized if and only if*

$$\frac{\mathrm{d}^j \mathbf{H}(z)}{\mathrm{d}z^j} = \frac{\mathrm{d}^j \widehat{\mathbf{H}}_r(z)}{\mathrm{d}z^j} \quad \text{at } z = \frac{1}{\alpha} \text{ for } j = 0, \ldots, r-1. \tag{9}$$

Due to (7), $\mathbf{H}_r(z)$ has all of its poles located at $z = 0$. As stated in the beginning of this section, $\mathbf{H}_r(z)$ interpolates first r moments of $\mathbf{H}(z)$ at $z = \infty$ (i.e. the first r Markov parameters). Hence due to Theorem 1, $\mathbf{H}_r(z)$ is the rth-order optimal $\mathscr{H}_2$ approximation to $\mathbf{H}(z)$ among all models having all r poles located at $z = 0$. In other words, if we define

$$\widetilde{\mathbf{H}}(z) = \mathbf{d} + \frac{\beta_1 z^{r-1} + \beta_2 z^{r-2} + \cdots + \beta_{r-1} z^{r-1}}{z^r} = \mathbf{d} + \frac{\mathbf{n}(z)}{z^r},$$

then, $\mathbf{H}_r(z) = \arg\min_{\mathbf{n}(z)} \|\mathbf{H} - \widetilde{\mathbf{H}}\|_{\mathscr{H}_2}$.

Lemma 2. *Given the above set-up,*

$$\|\mathbf{H}(z) - \mathbf{H}_r(z)\|_{\mathscr{H}_2} = \sum_{i=r+1}^{\infty} |\eta_i|^2. \tag{10}$$

Moreover, let $\mathbf{A}$ *be diagonalizable and let* $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{-1}$ *be the eigenvalue decomposition with* $\mathbf{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. *Define* $\kappa_{\mathbf{A}} = \|\mathbf{U}\|\|\mathbf{U}^{-1}\|$ *and* $\rho_{\mathbf{A}} = \max_i |\lambda_i|$. *Then*

$$\|\mathbf{H}(z) - \mathbf{H}_r(z)\|_{\mathscr{H}_2} \leqslant \|\mathbf{c}\|^2 \|\mathbf{b}\|^2 \kappa_{\mathbf{A}}^2 \frac{\rho_{\mathbf{A}}^{2r}}{1-\rho_{\mathbf{A}}^2}. \tag{11}$$

Proof. Eq. (10) follows from the fact that by definition of $\mathbf{H}_r(z)$ in (6), $\mathbf{H}(z) - \mathbf{H}_r(z) = \sum_{k=r+1}^{\infty} \eta_k z^{-k}$. To prove (11), first use the definition of $\eta_i = \mathbf{c}\mathbf{A}^{i-1}\mathbf{b}$ in (6) and note that $|\eta_i|^2 \leqslant \|\mathbf{c}\|^2\|\mathbf{b}\|^2\|\mathbf{A}^{i-1}\|^2$. Plugging $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{-1}$ into the last inequality and using $\|\mathbf{A}\| \leqslant \|\mathbf{U}\|\|\mathbf{\Lambda}\|\|\mathbf{U}^{-1}\|$ leads to the desired formula (11) after realizing $\|\mathbf{\Lambda}\| = \rho_{\mathbf{A}} < 1$. □

Remark 3. Note that (10) is a global error expression, and does not involve reduced-order matrices. Since $\rho(\mathbf{A}) < 1$, for sufficiently large values of i, η_i^2 will decrease quickly. We note that even though (10) contains an infinite sum, since $\eta_i = \mathbf{c}\mathbf{A}^{i-1}\mathbf{b}$ and $\rho_{\mathbf{A}} < 1$, it is always bounded as shown in (11). This behavior is similar to the decay of Hankel singular values and the error bound (10) has a similar structure to that in the balanced truncation framework. On the other hand, (11) gives an a priori global error bound, which can be easily computable for small-to-medium scale problems.

Remark 4. In the case that $\mathbf{A}$ is not diagonalizable, one could use the Schur decomposition of $\mathbf{A}$ instead of the eigenvalue decomposition. Let $\mathbf{A} = \mathbf{Y}(\mathit{\Lambda} + \mathbf{N})\mathbf{Y}^{\mathrm{T}}$ be the Schur decomposition of $\mathbf{A}$, where $\mathbf{Y}\mathbf{Y}^{\mathrm{T}} = \mathbf{I}$, $\mathit{\Lambda}$ is diagonal, and $\mathbf{N}$ is strictly upper triangular. Then in (11), $\rho_{\mathbf{A}}$ should be replaced by $\rho_{\mathbf{A}} + \varepsilon$, where $\varepsilon > 0$ with $\rho_{\mathbf{A}} + \varepsilon < 1$, and $\kappa_{\mathbf{A}}$ should be replaced by $\kappa_\varepsilon = (\|\mathbf{N}\|_F/\varepsilon)^{2(n-1)}$, where $\|\mathbf{N}\|_F$ denotes the Frobenius norm of $\mathbf{N}$. Note that such an ε always exists (Gugercin et al., 2003).

Corollary 5. *For* $q = 1, 2, \ldots,$

$$\|\mathbf{G}(s) - \mathbf{G}_r(s)\|^2_{\mathscr{H}_\infty} \leqslant \frac{r^{1-2q}}{2\pi(2q-1)} \int_{-\pi}^{\pi} |\mathbf{H}^{(q)}(\mathrm{e}^{\jmath\theta})|^2 \,\mathrm{d}\theta,$$

where $\mathbf{H}^{(q)}$ *is the qth derivative of* $\mathbf{H}(\mathrm{e}^{\jmath\theta})$ *with respect to* θ.

Proof. The result follows from combining (8) with the fact that bilinear transformation preserves the $\mathscr{H}_\infty$ norm. □

Remark 6. If the derivatives $\mathbf{H}^{(q)}$ can be computed using some quadrature rule, then Corollary 5 provides a computable $\mathscr{H}_\infty$ error bound for the continuous-time error system.

5. Rational Krylov projection framework for FMR

In this section, we analyze FMR from a (rational Krylov) projection framework and derive an algorithm that constructs $\mathbf{H}_r(z)$ in (7) from $\mathbf{H}(z)$ using a Krylov-based algorithm without directly computing the Markov parameters η_i. The motivation for this analysis is twofold. First, in the case where the spectral radius of $\mathbf{A}$ is close to unity, the Krylov-based approach provides a numerically more robust way to compute the FMR reduced model. Second, in Willcox and Megretski (2005) it was proposed that magnitudes of the Markov parameters should be used as a guidance to select r, the size of the FMR reduced model. We will show that the Krylov approach provides a better way to determine an appropriate value of r.

5.1. Projection matrices

To derive the rational Krylov framework for FMR, we must construct matrices $\mathbf{V}$ and $\mathbf{W}$, where $\mathbf{V}$ and/or $\mathbf{W}$ span a Krylov subspace with $\mathbf{W}^{\mathrm{T}}\mathbf{V} = \mathbf{I}_r$ such that the projections

$$\mathbf{A}_r = \mathbf{W}^{\mathrm{T}}\mathbf{A}\mathbf{V}, \quad \mathbf{b}_r = \mathbf{W}^{\mathrm{T}}\mathbf{b}, \quad \mathbf{c}_r = \mathbf{c}\mathbf{V} \tag{12}$$

yield the matrices in (7). Since $\mathbf{H}_r(z)$ matches the first r Markov parameters of $\mathbf{H}(z)$, it follows that the matrix $\mathbf{V}$ is given by

$$\mathbf{V} = [\mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \ldots, \mathbf{A}^{r-1}\mathbf{b}]. \tag{13}$$

Eq. (13) shows that $\mathbf{V}$ spans a regular Krylov subspace, hence reflecting the underlying Krylov projection framework for FMR. Next, we need to determine $\mathbf{W}$. Let $\mathbf{W}^{\mathrm{T}}$ be *any* left inverse of $\mathbf{V}$. Since $\mathbf{W}^{\mathrm{T}}\mathbf{V} = \mathbf{I}_r$, one has

$$[\mathbf{W}^{\mathrm{T}}\mathbf{b}, \mathbf{W}^{\mathrm{T}}\mathbf{A}\mathbf{b}, \mathbf{W}^{\mathrm{T}}\mathbf{A}^2\mathbf{b}, \ldots, \mathbf{W}^{\mathrm{T}}\mathbf{A}^{r-1}\mathbf{b}] = \mathbf{I}_r,$$

or equivalently $\mathbf{W}^{\mathrm{T}}\mathbf{A}^{i-1}\mathbf{b} = \mathbf{e}_i$, $i = 1, \ldots, r$. For this selection of $\mathbf{W}$, the resulting reduced system matrices are given by

$$\begin{aligned}\mathbf{A}_r &= \mathbf{W}^{\mathrm{T}}\mathbf{A}\mathbf{V} = \mathbf{W}^{\mathrm{T}}[\mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \ldots, \mathbf{A}^r\mathbf{b}] \\ &= [\mathbf{e}_2, \mathbf{e}_3, \ldots, \mathbf{e}_r, \mathbf{W}^{\mathrm{T}}\mathbf{A}^r\mathbf{b}],\end{aligned} \tag{14}$$

$$\mathbf{b}_r = \mathbf{W}^{\mathrm{T}}\mathbf{b} = \mathbf{e}_1 \quad \text{and} \quad \mathbf{c}_r = \mathbf{c}\mathbf{V} = [\eta_1, \eta_2, \ldots, \eta_r]. \tag{15}$$

As can be seen from (15), $\mathbf{b}_r$ and $\mathbf{c}_r$ are already in the desired form (7) for *any* left inverse $\mathbf{W}^{\mathrm{T}}$ of $\mathbf{V}$. Also, (14) shows that the first $r-1$ columns of $\mathbf{A}_r$ have the desired form. In order to achieve the appropriate last column of $\mathbf{A}_r$ as in (7), we require $\mathbf{W}$ to satisfy $\mathbf{W}^{\mathrm{T}}\mathbf{V} = \mathbf{I}_r$ and $\mathbf{W}^{\mathrm{T}}\mathbf{A}^r\mathbf{b} = \mathbf{0}$. The following lemma specifies this selection of $\mathbf{W}$:

Lemma 7. *Let* $\mathbf{V}$ *be as given in* (13). *Moreover, let*

$$[\mathbf{V} \;\; \mathbf{A}^r\mathbf{b}] = [\mathbf{Q}_1 \;\; \mathbf{q}_2]\begin{bmatrix}\mathbf{R}_1 & \mathbf{x} \\ \mathbf{0} & \alpha\end{bmatrix} \tag{16}$$

be the QR-decomposition of $[\mathbf{V} \;\; \mathbf{A}^r\mathbf{b}]$, *i.e.* $\mathbf{Q}_1^{\mathrm{T}}\mathbf{Q}_1 = \mathbf{I}_r$, $\mathbf{q}_2^{\mathrm{T}}\mathbf{q}_2 = 1$, $\mathbf{Q}_1^{\mathrm{T}}\mathbf{q}_2 = \mathbf{0}$, $\mathbf{R}_1 \in \mathbb{R}^{r\times r}$ *is an upper-triangular matrix,* $\mathbf{x} \in \mathbb{R}^r$, *and* α *is a scalar. Then, using*

$$\mathbf{W} = \left(\mathbf{Q}_1 - \frac{1}{\alpha}\mathbf{q}_2\mathbf{x}^{\mathrm{T}}\right)(\mathbf{R}_1^{-1})^{\mathrm{T}} \tag{17}$$

together with $\mathbf{V}$ *in the projection* (12) *yields the desired reduced-order matrices in* (7), *and thus an equivalent projection framework for FMR.*

Proof. If we only required $\mathbf{W}^{\mathrm{T}}$ to be a left inverse of $\mathbf{V}$, a straightforward choice would be $\mathbf{W}^{\mathrm{T}} = \mathbf{R}_1^{-1}\mathbf{Q}_1^{\mathrm{T}}$. However, to force the additional constraint $\mathbf{W}^{\mathrm{T}}\mathbf{A}^r\mathbf{b} = \mathbf{0}$, this selection must be modified so that the left inverse property still holds with the additional property that $\mathbf{A}^r\mathbf{b}$ is in the kernel of $\mathbf{W}^{\mathrm{T}}$. To achieve this, one needs to use the QR-decomposition of the appended matrix $[\mathbf{V} \;\; \mathbf{A}^r\mathbf{b}]$. From (16), a potential selection is of the form

$$\mathbf{W}^{\mathrm{T}} = \mathbf{R}_1^{-1}(\mathbf{Q}_1^{\mathrm{T}} + \mathbf{z}\mathbf{q}_2^{\mathrm{T}}). \tag{18}$$

We observe that this selection still satisfies $\mathbf{W}^{\mathrm{T}}\mathbf{V} = \mathbf{0}$. So, what is left is to find the appropriate $\mathbf{z}$ so that $\mathbf{W}^{\mathrm{T}}\mathbf{A}^r\mathbf{b} = \mathbf{0}$. It follows from (16) that $\mathbf{A}^r\mathbf{b} = \mathbf{Q}_1\mathbf{x} + \mathbf{q}_2\alpha$. Plugging this expression, together with $\mathbf{W}^{\mathrm{T}}$ as in (18), into the equation $\mathbf{W}^{\mathrm{T}}\mathbf{A}^r\mathbf{b} = \mathbf{0}$ and solving for $\mathbf{z}$ yields the solution $\mathbf{z} = -(1/\alpha)\mathbf{x}$. Finally, using this selection of $\mathbf{z}$ in (18) completes the proof. □

Remark 8. The formulation in Lemma 7 puts FMR into a rational Krylov projection framework: one simply uses an Arnoldi-type algorithm to compute an orthogonal basis for $[\mathbf{V} \;\; \mathbf{A}^r\mathbf{b}] = [\mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \ldots, \mathbf{A}^r\mathbf{b}]$, which spans a Krylov subspace. Even though the required subspace is a regular Krylov subspace in terms of the discrete-time matrices, it is a rational Krylov subspace in terms of the original continuous-time matrices. However, only one shift has been used, and hence only one sparse decomposition is required. Hence, this formulation of FMR can be implemented in a numerically effective way. As noted above, direct computation of the Markov parameters is avoided.

Remark 9. In a systems theoretical setting, going from $\mathbf{H}(z)$ to $\mathbf{H}_r(z)$ amounts to direct truncation of the controllable canonical form of $\mathbf{H}(z)$. Let $\mathcal{Q}$ be the full controllability matrix for $\mathbf{H}(z)$, i.e. $\mathcal{Q} = [\mathbf{b}, \mathbf{A}\mathbf{b}, \ldots, \mathbf{A}^{n-1}\mathbf{b}]$. Then, the projection (12) amounts to choosing $\mathbf{V}$ as the first r columns of $\mathcal{Q}$ and $\mathbf{W}^{\mathrm{T}}$ as the first r rows of $\mathcal{Q}^{-1}$.

5.2. Computational implementation

Even though the above analysis puts FMR into Krylov projection framework, it uses the power basis $\mathbf{V}$ explicitly, which is numerically ill-conditioned. Here, we will resolve this issue and show how to avoid explicit computation of $\mathbf{V}$ while still obtaining the quantities $\mathbf{R}_1$, $\mathbf{x}$ and α that result from the QR-decomposition of $\mathbf{V}$ as defined in (16).

One can show that

$$\mathbf{A}[\mathbf{V} \;\; \mathbf{A}^r\mathbf{b}] = [\mathbf{V} \;\; \mathbf{A}^r\mathbf{b}][\mathbf{e}_2, \mathbf{e}_3, \ldots, \mathbf{e}_{r+1}, \mathbf{h}_{r+1}] + \mathbf{f}\mathbf{e}_{r+1}^{\mathrm{T}}, \tag{19}$$

where $\mathbf{h}_{r+1}$ and $\mathbf{f}$ are vectors of appropriate size. Based on (16) and (19), we make the following definitions:

$$\mathbf{Q} := [\mathbf{Q}_1 \;\; \mathbf{q}_2], \quad \mathbf{R} := \begin{bmatrix}\mathbf{R}_1 & \mathbf{x} \\ \mathbf{0} & \alpha\end{bmatrix},$$

$$\mathbf{H} := [\mathbf{e}_2, \mathbf{e}_3, \ldots, \mathbf{e}_{r+1}, \mathbf{h}_{r+1}]. \tag{20}$$

Therefore, (19) becomes $\mathbf{A}\mathbf{Q}\mathbf{R} = \mathbf{Q}\mathbf{R}\mathbf{H} + \mathbf{f}\mathbf{e}_{r+1}^{\mathrm{T}}$. Multiplying this expression by $\mathbf{R}^{-1}$ from right, we obtain

$$\mathbf{A}\mathbf{Q} = \mathbf{Q}\underbrace{\mathbf{R}\mathbf{H}\mathbf{R}^{-1}}_{:=\hat{\mathbf{H}}} + \underbrace{\mathbf{f}\mathbf{e}_{r+1}^{\mathrm{T}}\mathbf{R}^{-1}}_{:=\hat{\mathbf{f}}\mathbf{e}_{r+1}^{\mathrm{T}}}, \tag{21}$$

i.e.

$$\mathbf{A}\mathbf{Q} = \mathbf{Q}\hat{\mathbf{H}} + \hat{\mathbf{f}}\mathbf{e}_{r+1}^{\mathrm{T}}. \tag{22}$$

Eq. (22) is precisely what one would obtain if $r+1$ steps of the Arnoldi algorithm were run on $\mathbf{A}$ and $\mathbf{b}$. This is done without explicitly forming the powers of $\mathbf{A}$. However, to obtain the desired matrix $\mathbf{W}$ in (17), we need to *extract* $\mathbf{R}$ from $\hat{\mathbf{H}}$. Because

of the specific upper Hessenberg structures of $\mathbf{H}$ and $\hat{\mathbf{H}}$, this can be done as follows. Note that, by definition, $\hat{\mathbf{H}}\mathbf{R} = \mathbf{R}\mathbf{H}$. Let $\hat{h}_{ij}$ and ρ_{ij} denote the (i, j)th entry of $\hat{\mathbf{H}}$ and $\mathbf{R}$, respectively. Also, let $\hat{\mathbf{h}}_j$ and $\mathbf{r}_j$ denote, respectively, the jth columns of $\hat{\mathbf{H}}$ and $\mathbf{R}$. $\mathbf{r}_1$ is explicitly known: $\mathbf{r}_1 = \|\mathbf{b}\|\mathbf{e}_1$ (hence, $\rho_{11} = \|\mathbf{b}\|$). Multiplying $\hat{\mathbf{H}}\mathbf{R} = \mathbf{R}\mathbf{H}$ with $\mathbf{e}_1$ from the left yields $\rho_{11}\hat{\mathbf{h}}_1 = \mathbf{r}_2$; hence, the second column of $\mathbf{R}$ is obtained. Then, similarly, multiplication by $\mathbf{e}_2$ yields $\mathbf{r}_3$, and so on. Continuing in this way, one *extracts* $\mathbf{R}$ from $\hat{\mathbf{H}}$ iteratively *without forming* $\mathbf{V}$ as desired. This approach of obtaining $\mathbf{R}$ is numerically efficient since it only requires r matrix–vector multiplications with the small matrix $\hat{\mathbf{H}} \in \mathbb{R}^{(r+1)\times(r+1)}$. Moreover, the vector multiplying the matrix $\hat{\mathbf{H}}$ at the kth step has only k non-zero entries. Upon completion of the iterative process, one can construct the required reduced model by re-defining $\mathbf{V}$ and $\mathbf{W}$ as

$$\mathbf{V} = \mathbf{Q}_1 \quad \text{and} \quad \mathbf{W} = \mathbf{Q}_1 - \frac{1}{\alpha}\mathbf{q}_2\mathbf{x}^{\mathrm{T}}, \tag{23}$$

without forming the power basis. The resulting reduced model will have the same transfer function $\mathbf{H}_r(z)$ as in (6) as desired and be only a similarity transformation away from the state-space matrices in (7). Eq. (23) completes the effective numerical computation of FMR through rational Krylov projection. As explained above, this is achieved by first running $r + 1$ steps of Arnoldi algorithm on $\mathbf{A}$ and $\mathbf{b}$, then extracting $\mathbf{R}$ from the Arnoldi basis and finally reducing the system via projection using $\mathbf{V}$ and $\mathbf{W}$ in (23).

5.3. A stopping criterion for FMR

Willcox and Megretski (2005) proposed that magnitudes of the Markov parameters should be used as a guidance to select r, the size of the FMR reduced model. Even though this approach works effectively for the cases where the magnitudes of the Markov parameters η_i decrease rapidly, it might lead to unnecessarily large reduced-order dimension r when the η_i decrease very slowly. This can be explained by observing that even if the magnitudes of the Markov parameters are not decreasing, the Krylov subspace $\mathbf{V}$ underlying FMR will *not* necessarily carry new information with the addition of another column; in other words, even though the η_i are not decreasing, it is possible that the Krylov subspace $\mathbf{V}$ is almost rank deficient and another column does *not* bring any new information.

The new Krylov-based formulation of FMR provides an easy and more effective way to determine an appropriate value of r. We will simply monitor the rank of $\mathbf{V}$ and will use this information as a stopping criterion *without computing* $\mathbf{V}$. There are two possible ways to achieve this goal. The first one is simply to use the diagonal entries of $\mathbf{R}$ as a measure for the rank deficiency of $\mathbf{V}$. Note that $\mathbf{R}$ is obtained iteratively at each step. Once the ratio $\mathbf{R}(1, 1)/\mathbf{R}(k, k)$ drops below certain tolerance, one can deduce that $\mathbf{V}$ is rank deficient and the reduced model will not be improved with an additional step since no new information will be added to $\mathbf{V}$. The second way is to monitor the condition number of $\mathbf{V}$, which is equal to the condition number of $\mathbf{R}$, by computing the singular value decomposition of $\mathbf{R}$ and examining the ratio $\sigma_1(\mathbf{R})/\sigma_k(\mathbf{R})$. Once this number is below a tolerance value, one can terminate the algorithm. We note that at the kth step, $\mathbf{R}$ has dimension $k \times k$, where k is small; hence SVD of $\mathbf{R}$ is cheap. However, one still does not need to re-compute the SVD of $\mathbf{R}$ at each step. The SVD of $\mathbf{R}$ at the $(k + 1)$th step can be effectively updated using the SVD of $\mathbf{R}$ from the kth step since each step corresponds adding one column to $\mathbf{R}$; see, for example, Gugercin et al. (2003).

6. Numerical example

In this section, we illustrate the concepts of Section 5 by a numerical example. The full-order model we use describes the dynamics between the lens actuator and the radial arm position of a portable CD player; it has 120 states, i.e. $n = 120$, with a single input and a single output. The goal is to create a reduced model in order to control the arm position dynamics. For more details on this system, see Grimme (1997).

We apply the original formulation of FMR and the new rational Krylov formulation, denoted by RK-FMR, with the frequency $\omega_0 = 300\,\mathrm{rad/s}$ and reduce the order to $k = 1 : 20$. The results are shown in Figs. 1(a) and (b). Fig. 1(a) depicts how the two ratios $\mathbf{R}(1, 1)/\mathbf{R}(k, k)$ and $\sigma_1(\mathbf{V})/\sigma_k(\mathbf{V})$ evolve as k increases. The figure reveals that the ratio $\mathbf{R}(1, 1)/\mathbf{R}(k, k)$ follows the behavior of the true condition number quite well. Moreover, even for $k = 20$, the Krylov subspace $\mathbf{V}$ is full-rank, which, in turn, implies that every iteration step brings in new information. This can also be seen in Fig. 1(b) which shows that the $\mathscr{H}_\infty$ error is reduced after each step, i.e. the reduced model is improved at each step. On the other hand, as Fig. 1(b) illustrates, RK-FMR produces the same result as FMR *without explicit moment computation*.

For the second case, we apply FMR and RK-FMR with the frequency $\omega_0 = 1.5\,\mathrm{rad/s}$ and reduce the order to $k = 1 : 20$ as above. The evolution of $\mathbf{R}(1, 1)/\mathbf{R}(k, k)$ and $\sigma_1(\mathbf{V})/\sigma_k(\mathbf{V})$, and the relative $\mathscr{H}_\infty$ error are depicted in Figs. 2(a) and (b), respectively. As Fig. 2(a) illustrates, for this choice of ω_0, the Krylov subspace $\mathbf{V}$ becomes numerically rank deficient after a small number of iterations. Once more, the ratio $\mathbf{R}(1, 1)/\mathbf{R}(k, k)$ predicts the behavior of true condition number well. We set a tolerance value as $\varepsilon = 10^{-10}$ and terminate RK-FMR once $\mathbf{R}(1, 1)/\mathbf{R}(k, k)$ is below ε; this is the reason why the graph of $\mathbf{R}(1, 1)/\mathbf{R}(k, k)$ stays constant after $k = 9$ (since no more steps are taken in RK-FMR). However, as Fig. 2(b) reveals there is almost no loss of accuracy in terms of the $\mathscr{H}_\infty$ norm of the error. Since $\mathbf{V}$ becomes almost rank-deficient, running FMR after $k = 9$ barely improves the quality of the resulting error system. As can be seen from Fig. 2(b), with $k = 9$, RK-FMR yields a relative $\mathscr{H}_\infty$ error of 0.9997, while FMR with $k = 20$ results in 0.9995. This indicates that, as expected from the conditioning of the Krylov subspace $\mathbf{V}$, almost no improvement has occurred despite increasing the reduced model size from $k = 9$ to 20.

Finally, we examine if the behavior of $\mathbf{V}$ for the second case, i.e. for $\omega_0 = 1.5$, can be recovered from inspecting the Markov parameters η_i of $\mathbf{H}(z)$; in other words, we examine if magnitudes of η_i would be a reasonable stopping criterion. Fig. 3 plots the Markov parameters η_i of $\mathbf{H}(z)$ for $\omega_0 = 1.5$ and shows that the η_i do not decay at all; on the contrary, they

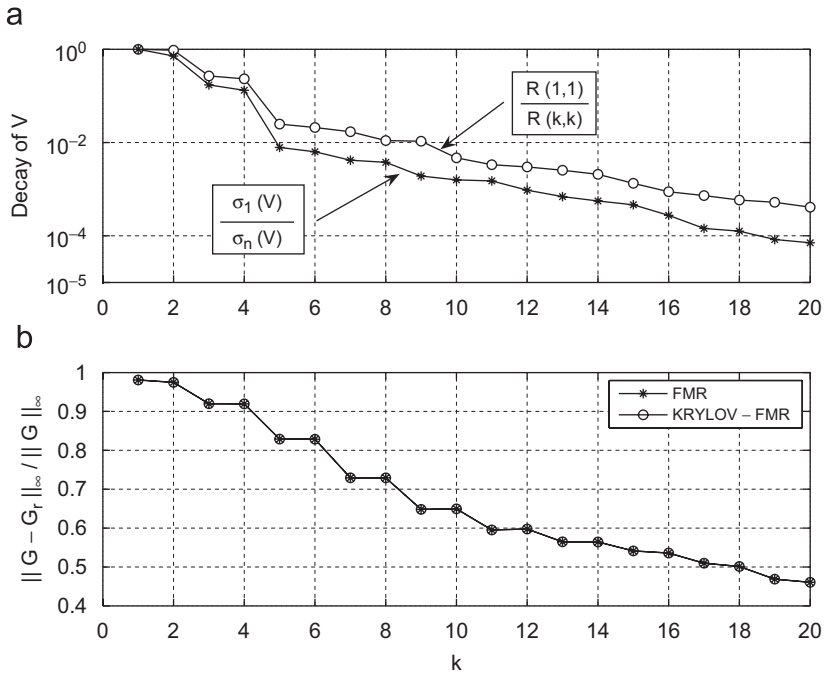

Fig. 1. FMR vs. RK-FMR for $\omega_0 = 300$ (a) – Numerical rank of V, (b) – Relative H_∞ error.

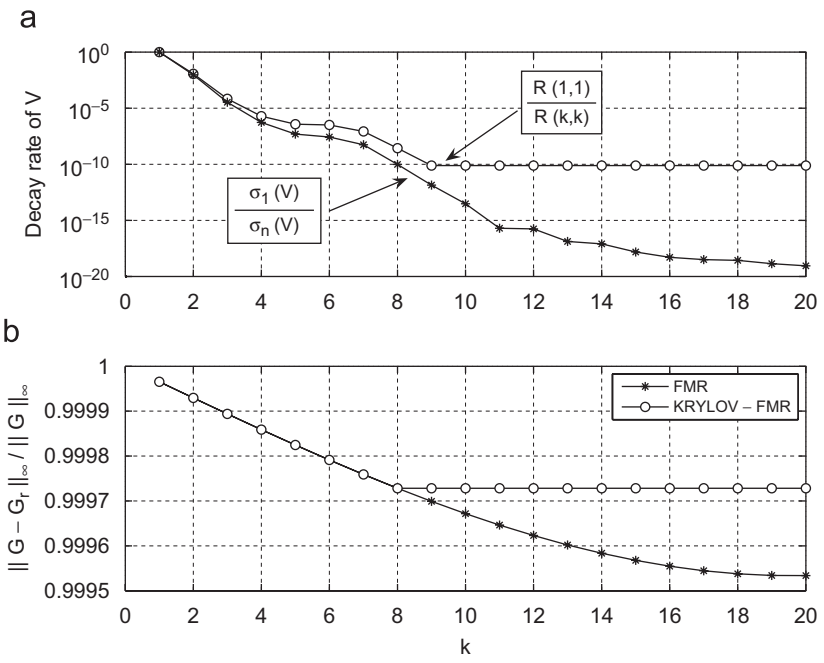

Fig. 2. FMR vs. Krylov-FMR for $\omega_0 = 1.5$ (a) – Numerical rank of V, (b) – Relative H_∞ error.

grow even until $k = 40$. This means that a stopping criterion based on the decay of η_i will yield unnecessarily large reduced order, even though this does not improve the quality of the reduced-order model as shown in Fig. 2(b). Hence, the Krylov-based stopping criterion is more appropriate and numerically effective for FMR. Moreover, monitoring the rank of $\mathbf{V}$ as done in RK-FMR can also be used to determine if the choice of ω_0 is poor at a much earlier stage. In this case, simply looking at the $\mathscr{H}_\infty$ error behavior in Fig. 2(b) and the decay of η_i in Fig. 3, one might decide to continue the FMR steps expecting that the error will decay. However, monitoring $\sigma_1(\mathbf{V})/\sigma_k(\mathbf{V})$ as in Fig. 2(a) reveals that the subspace has become rank-deficient, and that the next step will not bring in new information; hence one should choose a different frequency ω_0.

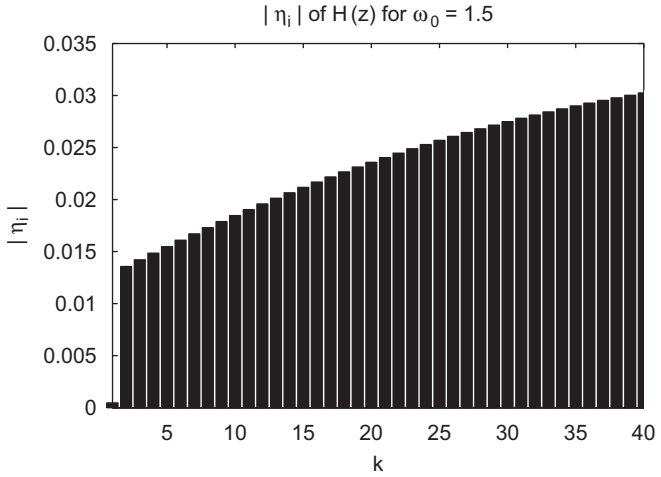

Fig. 3. FMR vs. Krylov-FMR for $\omega_0 = 1.5$.

7. Conclusions

In this note, we have developed the rational Krylov projection framework for FMR, and introduced its interpolation and optimality properties. A numerically efficient Krylov-based setting has been illustrated to perform FMR and a new, more robust stopping criterion has been proposed.

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