Presented as late breaking results contribution
21st IFAC World Congress (Virtual)
Berlin, Germany, July 12-17, 2020

Modeling in the Loewner framework: from linear dynamics to quadratic nonlinearities

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Abstract: In this contribution, we address an extension of the Loewner framework for modeling quadratic systems from data.

Keywords: Modeling nonlinear systems, Frequency domain identification, Complex systems.

1. INTRODUCTION

With the ever-increasing availability of measured data in many engineering fields, the need for incorporating measurements in the modeling process has steadily grown over the last decades. The main challenge is how to use the available data effectively in order to construct models that can accurately represent the dynamics of the underlying dynamical process. Sometimes, in order to satisfy accuracy requirements, the fitted models might have large dimension and hence are not suitable for fast numerical simulation. That is why it is of great interest to come up with reliable reduced-order surrogate models instead.

Model reduction is commonly viewed as a methodology used for reducing the computational complexity of large scale complex models in numerical simulations. The goal is to construct a smaller system with the same structure and similar response characteristics as the original. For an overview of model reduction methods, we refer the reader to the books Antoulas [2005], Benner et al. [2017], Antoulas et al. [2020].

In this work, we assume that the nonlinear systems to be modeled contains quadratic nonlinearities. This class of systems is of interest since most smooth nonlinear systems can be reformulated, without any approximation, as quadratic or quadratic-bilinear (QB) systems (provided that the nonlinearities are analytical). Model order reduction (MOR) methods specifically tailored for reducing QB systems have been already proposed in Benner and Breiten [2015], Benner and Goyal [2017], Benner et al. [2018]. For a general overview on system theoretical nonlinear MOR approaches, see Baur et al. [2014].

The MOR method that is in the center of the current study is the Loewner Framework (LF). It is a data-driven model identification and reduction technique that was originally introduced in Mayo and Antoulas [2007]. Using only measured data, it constructs surrogate models directly, and with basically no computational effort. For a tutorial paper on LF for linear systems, we refer the reader to Antoulas et al. [2017]. For an extension that uses time-domain data, see Peherstorfer et al. [2017]. The Loewner framework has been recently extended to certain classes of nonlinear systems, such as bilinear systems in Antoulas et al. [2016], and quadratic-bilinear (QB) systems in Gosea and Antoulas [2018].

In this study, we will analyze the later extension. By means of using time-domain data (output trajectories when the input is an oscillating signal, i.e. a sine/cosine), we compute transfer function values of the quadratic system. We apply this procedure to nonlinear examples such as the Lorenz system and the van der Pol oscillator.

2. QUADRATIC SYSTEMS

Consider quadratic systems that are characterized by the following equations

$$\begin{aligned} \mathbf{E}\dot{\mathbf{x}}(t) &= \mathbf{A}\mathbf{x}(t) + \mathbf{Q}\left(\mathbf{x}(t) \otimes \mathbf{x}(t)\right) + \mathbf{B}\mathbf{u}(t), \\ \mathbf{y}(t) &= \mathbf{C}\mathbf{x}(t). \end{aligned} \tag{1}$$

where $\mathbf{E}, \mathbf{A} \in \mathbb{R}^{n \times n}, \mathbf{B}, \mathbf{C}^T \in \mathbb{R}^n$ and $\mathbf{Q} \in \mathbb{R}^{n \times n^2}$. The Kronecker product is used, i.e.

$$\mathbf{x} \otimes \mathbf{x} = [x_1^2 \;\; x_1x_2 \;\; \ldots \;\; x_1x_n \;\; \ldots \;\; x_n^2]^T \in \mathbb{R}^{n^2}.$$

For such class of systems, one can explicitly compute generalized transfer functions in the frequency domain. This will be done through Volterra series theory. In general, the Volterra series describes the relationship between the control input and the observed output of a dynamical system whose dynamics is characterized by nonlinear behavior. For more details, see Rugh [1981].

An explicit formulation of input-output mappings in the time domain is provided by means of the Volterra kernels. The frequency domain equivalent of these kernels is represented by the generalized transfer functions (which are multi-variate rational functions). Such functions can be derived from time-domain data by applying generalized Fourier or Laplace transformations.

A method for deriving analytical expressions of generalized transfer functions is the harmonic input probing method in Bedrosian and Rice [1971]. It is based on the fact that a harmonic input must result in a harmonic output. For simplicity, we use a single harmonic function to identify explicit formulas for the generalized transfer functions in the case of quadratic systems.

Consider the input signal to be purely oscillatory, i.e. $\mathbf{u}(t) = \alpha e^{j\omega t}$, where $j = \sqrt{-1}$ and $\omega, \alpha > 0$. Begin by making the following assumption for the solution of (1)

$$\mathbf{x}(t) = \sum_{\ell=1}^{\infty} \mathbf{G}_\ell(j\omega)\alpha^\ell e^{\ell j\omega t}, \tag{2}$$

where $\mathbf{G}_\ell : \mathbb{C} \to \mathbb{C}^n$. Substitute the formulation of $\mathbf{x}(t)$ from (2) into the original differential equation in (1), and equate the coefficient of the term $e^{\ell j\omega t}$, $\forall \ell \geqslant 1$ from both left and right sides of the equation. In this way, one can find explicit formulas for functions $\mathbf{G}_\ell$ in (2). Then, the transfer functions $\mathbf{H}_\ell : \mathbb{C} \to \mathbb{C}$ are written as follows $\mathbf{H}_\ell(j\omega) = \mathbf{C}\mathbf{G}_\ell(j\omega)$, $\forall \ell \geq 1$.

The first transfer function is $\mathbf{H}_1(j\omega) = \mathbf{C}\mathbf{G}_1(j\omega)$ and can be written in terms of the system's matrices as

$$\mathbf{H}_1(j\omega) = \mathbf{C}(j\omega\mathbf{E} - \mathbf{A})^{-1}\mathbf{B} = \mathbf{C}\boldsymbol{\Phi}(j\omega)\mathbf{B}, \tag{3}$$

where $\boldsymbol{\Phi}(s) := (s\mathbf{E} - \mathbf{A})^{-1}$, $\forall s \in \mathbb{C}$. Furthermore, one can write the second transfer function as

$$\mathbf{H}_2(j\omega) = \mathbf{C}\boldsymbol{\Phi}(2j\omega)\mathbf{Q}\Big[\boldsymbol{\Phi}(j\omega)\mathbf{B} \otimes \boldsymbol{\Phi}(j\omega)\mathbf{B}\Big]. \tag{4}$$

In general, the n^{th} transfer function can be recursively written in terms of the first $n-1$ functions $\mathbf{G}_\ell$ as

$$\mathbf{H}_n(j\omega) = \mathbf{C}\boldsymbol{\Phi}(nj\omega)\mathbf{Q}\Big[\sum_{\ell=1}^{n-1} \mathbf{G}_\ell(j\omega) \otimes \mathbf{G}_{n-\ell}(j\omega)\Big], \ \forall n \geqslant 1.$$

3. THE LOEWNER FRAMEWORK

Given the following scalar data partitioned into

$$\begin{aligned} &\text{right data} : (\lambda_i; \mathbf{w}_i), \ i = 1, \cdots, k, \quad \text{and,} \\ &\text{left data} : (\mu_h; \mathbf{v}_h), \ h = 1, \cdots, k, \end{aligned} \tag{5}$$

find the function $\mathbf{H}(s)$, such that the following interpolation conditions are (approximately) fulfilled:

$$\mathbf{H}(\lambda_i) = \mathbf{w}_i, \quad \mathbf{H}(\mu_h) = \mathbf{v}_h. \tag{6}$$

The Loewner matrix $\mathbb{L} \in \mathbb{C}^{k\times k}$ and the shifted Loewner matrix $\mathbb{L}_s \in \mathbb{C}^{k\times k}$ are defined as follows

$$\mathbb{L}_{(i,h)} = \frac{\mathbf{v}_i - \mathbf{w}_h}{\mu_i - \lambda_h}, \ \mathbb{L}_{s(i,h)} = \frac{\mu_i\mathbf{v}_i - \lambda_h\mathbf{w}_h}{\mu_i - \lambda_h} \tag{7}$$

while the data vectors $\mathbb{V}, \mathbb{W}^T \in \mathbb{R}^k$ are introduced as

$$\mathbb{V}_{(i)} = \mathbf{v}_i, \quad \mathbb{W}_{(h)} = \mathbf{w}_h. \tag{8}$$

The Loewner model is composed of

$$\mathbf{E} = -\mathbb{L}, \quad \mathbf{A} = -\mathbb{L}_s, \quad \mathbf{B} = \mathbb{V}, \quad \mathbf{C} = \mathbb{W}.$$

In practical applications, the pencil $(\mathbb{L}_s, \mathbb{L})$ is often singular. In these cases, perform a rank revealing singular value decomposition (SVD) of the Loewner matrix $\mathbb{L}$

$$\mathbb{L} = \mathbf{X}\mathbf{S}\mathbf{Y}^* \approx \mathbf{X}_r\mathbf{S}_r\mathbf{Y}_r^*, \quad \text{with } \mathbf{X}_r, \mathbf{Y}_r \in \mathbb{C}^{k\times r}, \ \mathbf{S}_r \in \mathbb{C}^{r\times r}.$$

The system matrices corresponding to a projected Loewner model of dimension r can be computed as follows

$$\hat{\mathbf{E}} = -\mathbf{X}_r^*\mathbb{L}\mathbf{Y}_r, \quad \hat{\mathbf{A}} = -\mathbf{X}_r^*\mathbb{L}_s\mathbf{Y}_r, \quad \hat{\mathbf{B}} = \mathbf{X}_r^*\mathbb{V}, \quad \hat{\mathbf{C}} = \mathbb{W}\mathbf{Y}_r.$$

4. THE PROPOSED METHOD FOR ESTIMATING A QUADRATIC MODEL FROM DATA

In this contribution, the proposed procedure represents a natural extension of the method introduced in Karachalios et al. [2019] from the case of bilinear systems to the case of quadratic systems.

Using the classical Loewner framework introduced in Section 3, we first fit a linear model that matches samples of the first (linear) transfer function. Then, from samples of the second transfer function (that includes the nonlinear behavior), we are able to fit appropriate quadratic terms. The data required for this procedure can be estimated from direct numerical simulations in the time domain.

One can use the classical Loewner framework approach to directly construct a reliable reduced-order linear model $(\hat{\mathbf{A}}, \hat{\mathbf{B}}, \hat{\mathbf{C}})$ of order r from samples of the first transfer function $\mathbf{H}_1(j\omega)$ in (3).

The next step is to fit an appropriate matrix $\mathbf{Q} \in \mathbb{C}^{r\times r^2}$ that supplements the linear model into a quadratic model. In this direction, it is assumed that information about the second transfer function $\mathbf{H}_2(j\omega)$ in (4) is known at $2k$ points $\{j\omega_1, \ldots, j\omega_{2k}\}$. Introduce the following vectors $\mathbf{r}_\ell \in \mathbb{C}^r$ and $\mathbf{o}_\ell \in \mathbb{C}^{1\times r}$ for $\ell \in \{1, 2, \ldots, 2k\}$:

$$\begin{aligned} \mathbf{r}_\ell &= (j\omega_\ell\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} = \boldsymbol{\Phi}(j\omega_\ell)\mathbf{B}, \\ \mathbf{o}_\ell &= \mathbf{C}(2j\omega_\ell\mathbf{I} - \mathbf{A})^{-1} = \mathbf{C}\boldsymbol{\Phi}(2j\omega_\ell). \end{aligned} \tag{9}$$

One can write the second transfer function evaluated at $j\omega_\ell$, $\ell \in \{1, 2, \ldots, 2k\}$, in terms of the vectors $\mathbf{r}, \mathbf{o}^* \in \mathbb{C}^r$ in (9), as follows

$$\begin{aligned} \mathbf{H}_2(j\omega_\ell) &= \mathbf{C}\boldsymbol{\Phi}(2j\omega_\ell)\mathbf{Q}\Big[\boldsymbol{\Phi}(j\omega_\ell)\mathbf{B} \otimes \boldsymbol{\Phi}(j\omega_\ell)\mathbf{B}\Big] \\ &= \mathbf{o}_\ell\mathbf{Q}[\mathbf{r}_\ell \otimes \mathbf{r}_\ell]. \end{aligned} \tag{10}$$

Denote with $\mathbf{v_Q} \in \mathbb{C}^{r^3}$ the vectorization of $\mathbf{Q} \in \mathbb{C}^{r\times r^2}$, i.e.

$$\mathbf{v_Q} = [\mathbf{Q}(:,1) \ ; \ \mathbf{Q}(:,2) \ \cdots \ \mathbf{Q}(:,r^2)]. \tag{11}$$

From (10), we can write that $(\mathbf{r}_\ell^T \otimes \mathbf{r}_\ell^T \otimes \mathbf{o}_\ell)\mathbf{v_Q} = \mathbf{H}_2(j\omega_\ell)$, $\forall 1 \leq \ell \leq 2k$. By collecting this $2k$ equalities into a matrix format, we put together the following linear equation:

$$\mathbf{T}\mathbf{v_Q} = \mathbf{Z}, \tag{12}$$

where $\mathbf{T} \in \mathbb{C}^{2k\times r^3}$, $\mathbf{Z} \in \mathbb{C}^{2k}$ are matrices such that

$$\begin{cases} \mathbf{T}(\ell,:) = \mathbf{r}_\ell^T \otimes \mathbf{r}_\ell^T \otimes \mathbf{o}_\ell, \\ \mathbf{Z}(\ell) = \mathbf{H}_2(j\omega_\ell). \end{cases} \tag{13}$$

Finally, one can write the solution of (12) by means of the Moore-Penrose pseudo-inverse matrix $\mathbf{T}^\dagger \in \mathbb{C}^{r^3\times 2k}$.

More exactly, write the solution vector as

$$\mathbf{v_Q} = \mathbf{T}^\dagger\mathbf{Z}.$$

Afterwards, one can directly put together the recovered matrix $\mathbf{Q} \in \mathbb{C}^{r\times r^2}$ based on the formula from (11).

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5. TEST CASES

In 1963, Edward Lorenz proposed a simple model to represent the unpredictable behavior of weather (see Lorenz [1963]). He used fluid convection theory to model the motion of a two-dimensional cell of fluid cooled from above and warmed from below. Thus, the simplified model was proposed

$$\begin{aligned} \dot{x}_1 &= -\sigma x_1 + \sigma x_2, \\ \dot{x}_2 &= \rho x_1 - x_2 - x_1 x_3, \\ \dot{x}_3 &= -\beta x_3 + x_1 x_2. \end{aligned} \tag{14}$$

The following quantities enter the equations in (14):

(1) x_1 represents the convective fluid motion;
(2) x_2 denotes the horizontal temperature variation;
(3) x_3 denotes the vertical temperature variation.
(4) σ and ρ are related to the Prandtl and, respectively the Rayleigh number.
(5) β is a geometric factor.

Note that the Lorenz system in (14) can be rewritten in the format introduced in (1). Let $\mathbf{x} = [x_1\ x_2\ x_3]^T \in \mathbb{R}^3$ be the new augmented system variable. Then, write

$$\dot{\mathbf{x}} = \underbrace{\begin{bmatrix} -\sigma & \sigma & 0 \\ \rho & -1 & 0 \\ 0 & 0 & -\beta \end{bmatrix}}_{\mathbf{A}} \mathbf{x} + \underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{\mathbf{Q}} (\mathbf{x} \otimes \mathbf{x}).$$

We will consider the controlled case for which an external control input also enters the equations, i.e. only in the first equation and without any scale.

The observed output is given by the average of variables x_2 and x_3, i.e., the vertical temperature variation.

In this way, we define the appropriate scaling vectors $\mathbf{B} = [1\ \ 0\ 0]^T$ and $\mathbf{C} = \frac{1}{2}[0\ \ 1\ \ 1]$ that appear in the definition of the transfer functions.

The first and second transfer functions defined in (3), and in (4), respectively, can be explicitly computed as

$$\begin{aligned} \mathbf{H}_1(s) &= \frac{\rho}{2(s^2 + s + \sigma s + \sigma - \sigma\rho)}, \\ \mathbf{H}_2(s, s) &= \frac{\rho(s+1)}{2(\beta + 2s)(s^2 + s + \sigma s + \sigma - \sigma\rho)^2}. \end{aligned} \tag{15}$$

Another numerical example treated in this contribution is the coupled van der Pol oscillator from Kawano and Scherpen [2017].

The dynamics are characterized by the following six differential equations with linear and nonlinear (cubic) terms:

$$\begin{aligned} \dot{x}_1 &= x_2, \\ \dot{x}_2 &= -x_1 - \mu(x_1^2 - 1)x_2 + a(x_3 - x_1) + b(x_4 - x_2), \\ \dot{x}_3 &= x_4, \\ \dot{x}_4 &= -x_3 - \mu(x_3^2 - 1)x_4 + a(x_1 - x_3) + b(x_2 - x_4), \\ &\quad + a(x_5 - x_3) + b(x_6 - x_4) + u, \\ \dot{x}_5 &= x_6, \\ \dot{x}_6 &= -x_5 - \mu(x_5^2 - 1)x_6 + a(x_3 - x_5) + b(x_4 - x_6). \end{aligned} \tag{16}$$

The output is chosen to be $y = x_3$. Note that by introducing three additional surrogate states, e.g. $x_7 = x_1^2, x_8 = x_2^2$ and $x_9 = x_3^2$, one can rewrite the cubic nonlinear system in (16) of order $n = 6$ as an order $n_q = 9$ quadratic system.

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