Noisy Data Driven Reduced Order Models

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Outline

Introduction

Model Problems
- Time-Dependent Advection Diffusion Models
- Laplace Transform

Loewner Framework ROM

Loewner Method with Noisy Data

Resources

Problem

Given

$\mathbf{A}, \mathbf{E} \in \mathbb{R}^{n\times n}$, $\mathbf{B} \in \mathbb{R}^{n\times m}$, $\mathbf{C} \in \mathbb{R}^{k\times n}$, and $\mathbf{D} \in \mathbb{R}^{k\times m}$

consider a system with m inputs and k outputs of the type:

$$\begin{aligned}\mathbf{E}\frac{d}{dt}\mathbf{y}(t) &= \mathbf{A}\mathbf{y}(t) + \mathbf{B}\mathbf{u}(t)\\ \mathbf{z}(t) &= \mathbf{C}\mathbf{y}(t) + \mathbf{D}\mathbf{u}(t)\end{aligned}$$

with n large (> 1000). !!Expensive to solve!!

Goal - Create a reduced order model

$\widehat{\mathbf{A}}, \widehat{\mathbf{E}} \in \mathbb{R}^{r\times r}$, $\widehat{\mathbf{B}} \in \mathbb{R}^{r\times m}$, $\widehat{\mathbf{C}} \in \mathbb{R}^{k\times r}$, and $\widehat{\mathbf{D}} \in \mathbb{R}^{k\times m}$

with r small (< 20) that approximates the original model

Reduced Order Model Techniques

Our research focuses on:

- Interpolatory techniques
  - Projection Based
  - Loewner Method

Each technique will require working in frequency space.

To operate in frequency space, we must apply the Laplace Transform to the time-dependent system.

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SISO Notation

Proposed system is single input ($\mathbf{u}(t) \in \mathbb{R}$) and single output ($\mathbf{z}(t) \in \mathbb{R}$)

Change of notation:

$\mathbf{A}, \mathbf{E} \in \mathbb{R}^{n \times n}$, $\mathbf{b}, \mathbf{c} \in \mathbb{R}^n$, and $\mathbf{d} \in \mathbb{R}$

$$\begin{aligned} \mathbf{E}\frac{d}{dt}\mathbf{y}(t) &= \mathbf{A}\mathbf{y}(t) + \mathbf{b}\mathbf{u}(t) \\ \mathbf{z}(t) &= \mathbf{c}^T\mathbf{y}(t) + \mathbf{d}\mathbf{u}(t) \end{aligned}$$

1D Time-Dependent Advection Diffusion Equation

Partial differential equation (PDE):

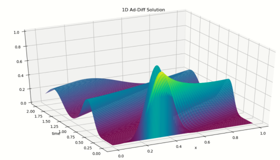
$$
\begin{aligned}
\frac{\partial}{\partial t}y(x,t) - \alpha\frac{\partial^2}{\partial x^2}y(x,t) + \beta\frac{\partial}{\partial x}y(x,t) &= 0 && x \in (0,1), t \in (0,T),\\
y(0,t) &= u(t), && t \in (0,T),\\
y_x(1,t) &= 0, && t \in (0,T),\\
y(x,0) &= y_0(x), && x \in (0,1),
\end{aligned}
$$

with $\alpha > 0$ and $\beta > 0$. We use

$$\alpha = 0.01, \beta = 1, T = 0.5.$$

Output:

$$z(t) = \int_0^1 y(x,t)dx$$



PDE solution

1D Advection Diffusion Discretization

Upwind finite difference discretization in space leads to

$$\frac{d}{dt}\mathbf{y}(t) = \mathbf{A}\mathbf{y}(t) + \mathbf{b}\mathbf{u}(t), \quad t \in (0,T), \qquad \mathbf{y}(0) = \mathbf{y}_0,$$

where $\mathbf{A} = \alpha\mathbf{A}^{diff} + \beta\mathbf{A}^{conv}$

$$\mathbf{A}^{diff} = \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 2 & -2 \end{bmatrix} \mathbf{A}^{conv} = \begin{bmatrix} -1 & & & & \\ 1 & -1 & & & \\ & \ddots & \ddots & & \\ & & 1 & -1 & \\ & & & 1 & -1 \end{bmatrix}$$

$$\mathbf{y}_0 = \Big(y_0(x_0,t), \dots, y_0(x_{n_x-1},t)\Big)^T \in \mathbb{R}^{n_x}$$

$$\mathbf{b} = \Big(\frac{\alpha}{h^2} + \frac{\beta}{h}, 0, \dots, 0\Big)^T \in \mathbb{R}^{n_x}$$

1D Advection Diffusion Discretization (cont.)

Composite Trapezoidal Rule:

$$\int_0^1 y(x,t)dx \approx \frac{h}{2}y(x_0,t) + hy(x_1,t) + \ldots + hy(x_{n_x-1},t) + \frac{h}{2}y(x_n,t)$$
$$= \frac{h}{2}u(t) + hy(x_1,t) + \ldots + hy(x_{n_x-1},t) + \frac{h}{2}y(x_n,t)$$

Leads to:

$$\int_0^1 y(x,t)dx \approx \frac{h}{2}u(t) + hy_1(t) + \ldots + hy_{n_x-1}(t) + \frac{h}{2}y_{n_x}(t)$$
$$= \mathbf{c}^T\mathbf{y}(t) + \mathbf{d}\mathbf{u}(t)$$

with

$$\mathbf{c} = \left(h, h, \ldots, h, \frac{h}{2}\right)^T \in \mathbb{R}^{n_x}$$
$$\mathbf{d} = \frac{h}{2}$$

Laplace Transform

Transforms a function of time to function of a frequency

Let $q(t)$ be function of time where $t \in \mathbb{R}$

Denote $\mathcal{L}(q)$ as $q(s)$ where $s \in \mathbb{C}$ is frequency

Laplace Transform

Apply the Laplace Transform to the system:

$$\begin{aligned} \mathbf{E}\frac{d}{dt}\mathbf{y}(t) &= \mathbf{A}\mathbf{y}(t) + \mathbf{b}\mathbf{u}(t) \\ \mathbf{z}(t) &= \mathbf{c}^T\mathbf{y}(t) + \mathbf{d}\mathbf{u}(t) \end{aligned}$$

which turns into:

$$\begin{aligned} s\mathbf{E}\mathbf{y}(s) - \mathbf{y}(0) &= \mathbf{A}\mathbf{y}(s) + \mathbf{b}\mathbf{u}(s) \\ \mathbf{z}(s) &= \mathbf{c}^T\mathbf{y}(s) + \mathbf{d}\mathbf{u}(s) \end{aligned}$$

Laplace Transform

Assume $\mathbf{y}(0) = 0$

Rearrange and solve:

$$\mathbf{y}(s) = \left(\left(s\mathbf{E} - \mathbf{A}\right)^{-1}\mathbf{b}\right)\mathbf{u}(s)$$

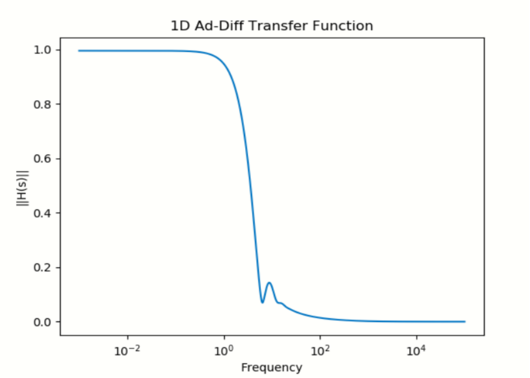
Substitute to get:

$$\mathbf{z}(s) = \left(\mathbf{c}^T\left(s\mathbf{E} - \mathbf{A}\right)^{-1}\mathbf{b} + \mathbf{d}\right)\mathbf{u}(s)$$

Which gives the following transfer function $\mathbf{H}(s)$:

$$\mathbf{H}(s) = \mathbf{c}^T\left(s\mathbf{E} - \mathbf{A}\right)^{-1}\mathbf{b} + \mathbf{d}, \quad s \in \mathbb{C}$$

1D Advection Diffusion Transfer Function



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Loewner Method Motivation

The projection based ROM works very well, as proven by the error plot. What do we need the Loewner Method for?

Reasons:

- To use the projection method, need $\mathbf{A}$,$\mathbf{b}$,$\mathbf{c}$,$\mathbf{d}$, and $\mathbf{E}$
- In some applications, matrices not given
- Can be used with only transfer function data
- Retains interpolation property, mimics projection method

Downsides:

- Loewner matrices might become singular if too many sample frequencies are used
- Which frequencies to sample data from?
- Needs $\mathbf{d}$ in FOM

Loewner Data Setup

First, lets assume that in the FOM $\mathbf{d} = 0$

Left frequencies:

$$\mathbf{\Sigma} = \{\sigma_1, \ldots, \sigma_r\} \subset \mathbb{I}$$

Right frequencies:

$$\mathbf{\Theta} = \{\theta_1, \ldots, \theta_r\} \subset \mathbb{I}$$

with

$$\mathbf{\Sigma} \cap \mathbf{\Theta} = \emptyset$$

Loewner Matrices and ROM

Construct the Loewner Matrix:

$$\mathbb{L}_{ij} = \frac{\mathbf{H}(\sigma_i) - \mathbf{H}(\theta_j)}{\sigma_i - \theta_j}$$

Construct the Shifted Loewner Matrix:

$$\mathbb{M}_{ij} = \frac{\sigma_i \mathbf{H}(\sigma_i) - \theta_j \mathbf{H}(\theta_j)}{\sigma_i - \theta_j}$$

Loewner Matrices and ROM

Construct the Loewner ROM:

$$\begin{aligned}
\widehat{\mathbf{A}} &= -\mathbb{M} \\
\widehat{\mathbf{b}} &= [\mathbf{H}(\sigma_1), \ldots, \mathbf{H}(\sigma_r)]^T \\
\widehat{\mathbf{c}}^T &= [\mathbf{H}(\theta_1), \ldots, \mathbf{H}(\theta_r)] \\
\widehat{\mathbf{E}} &= -\mathbb{L} \\
\widehat{\mathbf{d}} &= 0
\end{aligned}$$

$$\widehat{\mathbf{H}}(s) = \widehat{\mathbf{c}}^T \left(s\widehat{\mathbf{E}} - \widehat{\mathbf{A}}\right)^{-1} \widehat{\mathbf{b}} + \widehat{\mathbf{d}}$$

Loewner Interpolation Theorem

Theorem

Assume $\mathbb{M} - s\mathbb{L}$ *is invertible for all* $s \in \Sigma \cup \Theta$.

Then, the previously described ROM transfer function interpolates at the left and right training frequencies:

$\mathbf{H}(s) = \widehat{\mathbf{H}}(s)$ *for all* $s \in \Sigma \cup \Theta$

Loewner Interpolation Property Proof

Simplify the constructed Loewner ROM

$$\widehat{\mathbf{H}}(s) = \widehat{\mathbf{c}}^T \left(s\widehat{\mathbf{E}} - \widehat{\mathbf{A}}\right)^{-1} \widehat{\mathbf{b}}$$
$$\widehat{\mathbf{H}}(s) = \left[\mathbf{H}(\theta_1), \ldots, \mathbf{H}(\theta_r)\right] (\mathbb{M} - s\mathbb{L})^{-1} \left[\mathbf{H}(\sigma_1), \ldots, \mathbf{H}(\sigma_r)\right]^T$$

Consider the matrix $\mathbb{M} - s\mathbb{L}$ where $s \in \mathbb{C}$.

$$(\mathbb{M} - s\mathbb{L})_{i,j} = \frac{s - \theta_j}{\sigma_i - \theta_j}\mathbf{H}(\theta_j) + \frac{\sigma_i - s}{\sigma_i - \theta_j}\mathbf{H}(\sigma_i)$$

Two interpolatory cases for s:

1. $s = \theta_k$ for some k
2. $s = \sigma_k$ for some k

Loewner Interpolation Property Proof

Consider case where $s = \theta_k$.

Recall:

$$(\mathbb{M} - s\mathbb{L})_{i,j} = \frac{s - \theta_j}{\sigma_i - \theta_j}\mathbf{H}(\theta_j) + \frac{\sigma_i - s}{\sigma_i - \theta_j}\mathbf{H}(\sigma_i)$$

$$(\mathbb{M} - \theta_k\mathbb{L})e_k = \left[\mathbf{H}(\sigma_1), \ldots, \mathbf{H}(\sigma_r)\right]^T \implies$$
$$e_k = (\mathbb{M} - \theta_k\mathbb{L})^{-1}\left[\mathbf{H}(\sigma_1), \ldots, \mathbf{H}(\sigma_r)\right]^T$$

$$\left[\mathbf{H}(\theta_1), \ldots, \mathbf{H}(\theta_r)\right] e_k = \mathbf{H}(\theta_k)$$
$$\left[\mathbf{H}(\theta_1), \ldots, \mathbf{H}(\theta_r)\right](\mathbb{M} - \theta_k\mathbb{L})^{-1}\left[\mathbf{H}(\sigma_1), \ldots, \mathbf{H}(\sigma_r)\right]^T = \widehat{\mathbf{H}}(\theta_k)$$

Therefore, $\mathbf{H}(\theta_k) = \widehat{\mathbf{H}}(\theta_k)$

Loewner Interpolation Property Proof

Consider case where $s = \sigma_k$.

Recall:

$$(\mathbb{M} - s\mathbb{L})_{i,j} = \frac{s - \theta_j}{\sigma_i - \theta_j}\mathbf{H}(\theta_j) + \frac{\sigma_i - s}{\sigma_i - \theta_j}\mathbf{H}(\sigma_i)$$

$$e_k^T(\mathbb{M} - \sigma_k\mathbb{L}) = [\mathbf{H}(\theta_1), \ldots, \mathbf{H}(\theta_r)] \implies$$
$$e_k^T = [\mathbf{H}(\theta_1), \ldots, \mathbf{H}(\theta_r)]\,(\mathbb{M} - \sigma_k\mathbb{L})^{-1}$$

$$e_k^T\,[\mathbf{H}(\sigma_1), \ldots, \mathbf{H}(\sigma_r)]^T = \mathbf{H}(\sigma_k)$$
$$[\mathbf{H}(\theta_1), \ldots, \mathbf{H}(\theta_r)]\,(\mathbb{M} - \sigma_k\mathbb{L})^{-1}\,[\mathbf{H}(\sigma_1), \ldots, \mathbf{H}(\sigma_r)]^T = \widehat{\mathbf{H}}(\sigma_k)$$

Therefore, $\mathbf{H}(\sigma_k) = \widehat{\mathbf{H}}(\sigma_k)$

Dealing with Singular Loewner Matrices

Necessary that Loewner matrices are nonsingular

- More frequencies leads to singular Loewner matrices
- ROM transfer function will be undefined

Use SVD to extract independent columns of matrices:

$$\mathbf{U_1 \Sigma_1 V_1^*} = [\mathbb{L}\ \mathbb{M}]$$
$$\mathbf{U_2 \Sigma_2 V_2^*} = [\mathbb{L}\ \mathbb{M}]^T$$

Given a tolerance for the normalized singular values, let $k_1, k_2 =$ number of normalized singular values $>$ the tolerance. Set k $=$ max(k_v, k_w).

Let $\mathbf{U} = \mathbf{U_{1k}}$ and $\mathbf{V} = \mathbf{V_{2k}}$.

Dealing with Singular Loewner Matrices

Construct the new Loewner ROM as:

$$\begin{aligned}
\widehat{\mathbf{A}} &= -\mathbf{U}^*\mathbb{M}\mathbf{V} \\
\widehat{\mathbf{b}} &= \mathbf{U}^*\left[\mathbf{H}(\sigma_1), \ldots, \mathbf{H}(\sigma_r)\right]^T \\
\widehat{\mathbf{c}}^T &= \left[\mathbf{H}(\theta_1), \ldots, \mathbf{H}(\theta_r)\right]\mathbf{V} \\
\widehat{\mathbf{E}} &= -\mathbf{U}^*\mathbb{L}\mathbf{V} \\
\widehat{\mathbf{d}} &= 0
\end{aligned}$$

$$\widehat{\mathbf{H}}(s) = \widehat{\mathbf{c}}^T\left(s\widehat{\mathbf{E}} - \widehat{\mathbf{A}}\right)^{-1}\widehat{\mathbf{b}} + \widehat{\mathbf{d}}$$

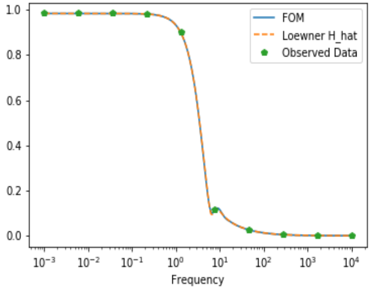
Interpolatory properties of the new Loewner ROM are beyond the scope of this presentation

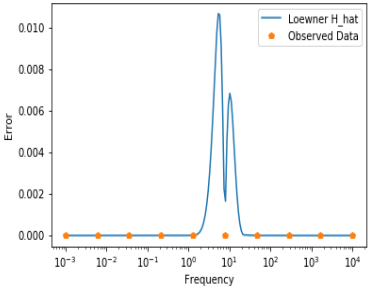
Lowner Framework Implementation

1. Choose disjoint imaginary left and right frequencies $\{\sigma_1, \ldots, \sigma_r\}$ and $\{\theta_1, \ldots, \theta_r\}$, respectively
2. Compute $\mathbb{L}$ and $\mathbb{M}$
   - $\mathbb{L}_{ij} = \frac{\mathbf{H}(\sigma_i) - \mathbf{H}(\theta_j)}{\sigma_i - \theta_j}$
   - $\mathbb{M}_{ij} = \frac{\sigma_i \mathbf{H}(\sigma_i) - \theta_j \mathbf{H}(\theta_j)}{\sigma_i - \theta_j}$
3. Compute $\mathbf{U}$ and $\mathbf{V}$ from the SVD of the Loewner pencils
4. Use the Loewner matrices, $\mathbf{U}$, $\mathbf{V}$, and the left and right transfer function data to compute the ROM

Actual H(s) vs Loewner H(s)

Using 5 left and 5 right frequencies:





Converting Loewner to Real

Since the right and left frequencies are complex, the ouput of the transfer function at these frequencies will be complex as well. This leads to complex Loewner matrices.

The original problem is in the time domain.

- Need real matrices $\widehat{\mathbf{A}}$, $\widehat{\mathbf{b}}$, $\widehat{\mathbf{c}}$, $\widehat{\mathbf{d}}$, and $\widehat{\mathbf{E}}$

Compute real $\mathbb{L}$ and $\mathbb{M}$

- Problem:
  - How do we retain the info in $\mathbb{L}$, $\mathbb{M}$?

Utilize the fact that $\overline{\mathbf{H}(\mathbf{s})} = \mathbf{H}(\overline{\mathbf{s}})$.

Converting Loewner to Real

First include the complex conjugate data in the setup.

Left frequencies:

$$\mathbf{\Sigma} = \{\sigma_1, \ldots, \sigma_{2r}\} \subset \mathbb{I}$$

where $\sigma_{2i} = \overline{\sigma}_{2i-1}$

Right frequencies:

$$\mathbf{\Theta} = \{\theta_1, \ldots, \theta_{2r}\} \subset \mathbb{I}$$

where $\theta_{2i} = \overline{\theta}_{2i-1}$

Converting Loewner to Real

Let $\mathbf{J} \in \mathbb{C}^{n \times n}$ be a block diagonal matrix with $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -i \\ 1 & i \end{bmatrix}$ repeated on the diagonal.

Use the following real Loewner matrices to compute $\mathbf{U}_R$ and $\mathbf{V}_R$:

$$\mathbb{L}_R = \mathbf{J}^* \mathbb{L} \mathbf{J}$$
$$\mathbb{M}_R = \mathbf{J}^* \mathbb{M} \mathbf{J}$$

Converting Loewner to Real

Construct the real Loewner ROM as:

$$\begin{aligned}
\widehat{\mathbf{A}} &= -\mathbf{U}_R^T \mathbb{M}_R \mathbf{V}_R \\
\widehat{\mathbf{b}} &= \mathbf{U}^T \mathbf{J}^* \left[\mathbf{H}(\sigma_1), \ldots, \mathbf{H}(\sigma_r)\right]^T \\
\widehat{\mathbf{c}}^T &= \left[\mathbf{H}(\theta_1), \ldots, \mathbf{H}(\theta_r)\right] \mathbf{J}\mathbf{V} \\
\widehat{\mathbf{E}} &= -\mathbf{U}_R^T \mathbb{L}_R \mathbf{V}_R \\
\widehat{\mathbf{d}} &= 0
\end{aligned}$$

$$\widehat{\mathbf{H}}(s) = \widehat{\mathbf{c}}^T \left(s\widehat{\mathbf{E}} - \widehat{\mathbf{A}}\right)^{-1} \widehat{\mathbf{b}} + \widehat{\mathbf{d}}$$

How does this work?

Consider computing $\mathbb{L}_R$ in the case where $\Sigma = \{\sigma, \overline{\sigma}\}$ and $\Theta = \{\theta, \overline{\theta}\}$:

$$\mathbb{L}_R = \frac{1}{2}\begin{bmatrix}1 & 1\\ i & -i\end{bmatrix}\begin{bmatrix}\frac{\mathbf{H}(\sigma)-\mathbf{H}(\theta)}{\sigma-\theta} & \frac{\overline{\mathbf{H}(\sigma)}-\mathbf{H}(\theta)}{\overline{\sigma}-\theta}\\ \frac{\mathbf{H}(\sigma)-\overline{\mathbf{H}(\theta)}}{\sigma-\overline{\theta}} & \frac{\overline{\mathbf{H}(\sigma)}-\overline{\mathbf{H}(\theta)}}{\overline{\sigma}-\overline{\theta}}\end{bmatrix}\begin{bmatrix}1 & -i\\ 1 & i\end{bmatrix}$$

$$\mathbb{L}_R = \begin{bmatrix} re(\frac{\mathbf{H}(\sigma)-\mathbf{H}(\theta)}{\sigma-\theta}) & im(\frac{\mathbf{H}(\sigma)-\mathbf{H}(\theta)}{\sigma-\theta})\\ -im(\frac{\mathbf{H}(\sigma)-\mathbf{H}(\theta)}{\sigma-\theta}) & re(\frac{\mathbf{H}(\sigma)-\mathbf{H}(\theta)}{\sigma-\theta})\end{bmatrix}$$

The matrix $\mathbb{L}_R$ is real but encapsulates the same information as the complex number $\frac{\mathbf{H}(\sigma)-\mathbf{H}(\theta)}{\sigma-\theta}$.

Same holds for $\mathbb{M}_R$.

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Output Function Performance

Singular Value Comparison

Eigenvalue Comparison

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[1] A.C. Antoulas, C. Beattie, S. Gugercin, *Interpolatory Methods for Model Reduction*, pg. 33-85, June 14, 2019

[2] M. Heinkenschloss, a big thanks for mentoring this project!