Sampling low-dimensional Markovian dynamics for pre-asymptotically recovering reduced models from data with operator inference

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Setting

Consider the model reduction problem of reducing a large discrete dynamical system (the *full-order model* or FOM)

$$\mathbf{x}_{j+1} = \mathbf{f}(\mathbf{x}_j, \mathbf{u}_j)$$

to a smaller system (the *reduced-order model* or ROM)

$$\hat{\mathbf{x}}_{j+1} = \hat{\mathbf{f}}(\hat{\mathbf{x}}_j, \mathbf{u}_j)$$

where

$$\mathbf{u}_j \in \mathbb{R}^m \qquad \mathbf{x}_j \in \mathbb{R}^n, \qquad \mathbf{f} : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n,$$
$$\hat{\mathbf{x}}_j \in \mathbb{R}^r, \qquad \hat{\mathbf{f}} : \mathbb{R}^r \times \mathbb{R}^m \to \mathbb{R}^r.$$

with $r \ll n$ and $\hat{\mathbf{x}}_j$ related to $\mathbf{x}_j$. Usually $\mathbf{x}_j \approx V\hat{\mathbf{x}}_j$ where $V \in \mathbb{R}^{n \times r}$ is a POD basis matrix derived from FOM snapshot data.

Problem

Given a basis $V \in \mathbb{R}^{n \times r}$, the standard *intrusive* approach is to define

$$\tilde{\mathbf{f}}(\tilde{\mathbf{x}}, \mathbf{u}) := V^\mathsf{T} \mathbf{f}(V\tilde{\mathbf{x}}, \mathbf{u}), \qquad \tilde{\mathbf{x}}_0 := V^\mathsf{T} \mathbf{x}_0.$$

For example,

$$\mathbf{f}(\mathbf{x}, \mathbf{u}) = A\mathbf{x} + B\mathbf{u}, \qquad A \in \mathbb{R}^{n \times n}, \quad B \in \mathbb{R}^{n \times m},$$

$$\implies \quad \tilde{\mathbf{f}}(\tilde{\mathbf{x}}, \mathbf{u}) = \underbrace{V^\mathsf{T} A V}_{\tilde{A}} \tilde{\mathbf{x}} + \underbrace{V^\mathsf{T} B}_{\tilde{B}} \mathbf{u}, \qquad \tilde{A} \in \mathbb{R}^{r \times r}, \quad \tilde{B} \in \mathbb{R}^{r \times m},$$

The computational advantage is that $\tilde{A} = V^\mathsf{T} A V$ and $\tilde{B} = V^\mathsf{T} B$ can be precomputed. **But what if the operators A or B are unknown, or they are hard to access or construct explicitly?**

Approach: Operator Inference

Instead of computing $\tilde{A} \in \mathbb{R}^{r \times r}$ and $\tilde{B} \in \mathbb{R}^{r \times m}$ intrusively, assume that the ROM operator $\hat{\mathbf{f}}$ has the form

$$\hat{\mathbf{f}}(\hat{\mathbf{x}}) = \hat{A}\hat{\mathbf{x}} + \hat{B}\mathbf{u},$$

then solve a least-squares problem to get the best $\hat{A} \in \mathbb{R}^{r \times r}$ and $\hat{B} \in \mathbb{R}^{r \times m}$ according to the snapshot data [PW16]:

$$\underset{\hat{A},\hat{B}}{\arg\min} \sum_{j=0}^{k-1} \left\| \hat{A}\hat{\mathbf{x}}_j + \hat{B}\mathbf{u}_j - \hat{\mathbf{x}}_{j+1} \right\|_2^2.$$

This is a relatively small ordinary linear least squares problem that decouples nicely, and is computationally inexpensive to solve. The problem can be generalized to more complicated forms of $\mathbf{f}$, for example,

$$\underset{\substack{\hat{\mathbf{c}},\hat{A},\\ \hat{H},\hat{B}}}{\arg\min} \sum_{j=0}^{k-1} \left\| \hat{\mathbf{c}} + \hat{A}\hat{\mathbf{x}}_j + \hat{H}(\mathbf{x}_j \otimes \mathbf{x}_j) + \hat{B}\mathbf{u}_j - \hat{\mathbf{x}}_{j+1} \right\|_2^2.$$

Algorithm 1 Operator inference for reducing discrete systems

procedure $\textsc{OpInf}(\mathbf{f},\ \mathbf{x}_0,\ \{\mathbf{u}_j\}_{j=0}^{k},\ r)$

  for $j = 0, 1, \ldots, k-1$ **do**

    $\mathbf{x}_{j+1} \leftarrow \mathbf{f}(\mathbf{x}_j, \mathbf{u}_j)$ ▷ Generate state snapshots.

  end for

  $V \leftarrow \mathrm{POD\_basis}\left(\mathrm{data} = \{\mathbf{x}_j\}_{j=0}^{k},\ \mathrm{rank} = r\right)$

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  for $j = 0, 1, \ldots, k$ **do**:

    $\hat{\mathbf{x}}_j \leftarrow V^{\mathsf{T}}\mathbf{x}_j$ ▷ Project the trajectory.

  end for

  $\hat{A}, \hat{B} \leftarrow \arg\min \sum_{j=0}^{k-1} \left\| \hat{A}\hat{\mathbf{x}}_j + \hat{B}\mathbf{u}_j - \hat{\mathbf{x}}_{j+1} \right\|_2^2$ ▷ Infer operators.

  return $\hat{A},\ \hat{B}$

end procedure

Another Problem: Non-Markovian Dynamics

The intrusive operators $\tilde{A}$ and $\tilde{B}$ often inherit desirable properties from A and B (e.g., $\lambda_{\max}(A) < 0$ often implies $\lambda_{\max}(\tilde{A}) < 0$). However, the inferred operators $\hat{A}$ and $\hat{B}$ are **not** guaranteed to inherit such properties [Peh19] since $\tilde{A} \neq \hat{A}$ in general.

New Approach: Data "Re-projection"

After generating state snapshots $\{\mathbf{x}_j\}_{j=0}^{k} \subset \mathbb{R}^n$ and computing the basis $V \in \mathbb{R}^{n\times r}$, compute the projected snapshot data that would be produced by the corresponding intrusive model. Using this re-projected data with operator inference yields the intrusive model, that is, $\hat{A} = \tilde{A}$ and $\hat{B} = \tilde{B}$.

Algorithm 2 Operator inference with re-projected trajectories

procedure $\textsc{OpInfRP}(\mathbf{f},\ \mathbf{x}_0,\ \{\mathbf{u}_j\}_{j=0}^{k},\ r)$

  for $j = 0, 1, \ldots, k-1$ **do**

    $\mathbf{x}_{j+1} \leftarrow \mathbf{f}(\mathbf{x}_j, \mathbf{u}_j)$ ▷ Generate state snapshots.

  end for

  $V \leftarrow \text{POD\_basis}\left(\text{data} = \{\mathbf{x}_j\}_{j=0}^{k},\ \text{rank} = r\right)$

  $\hat{\mathbf{x}}_0 \leftarrow V^{\mathsf{T}}\mathbf{x}_0$

  for $j = 0, 1, \ldots, k-1$ **do**:

    $\hat{\mathbf{x}}_{j+1} \leftarrow V^{\mathsf{T}}\mathbf{f}(V\hat{\mathbf{x}}_j, \mathbf{u}_j)$ ▷ Re-project the trajectory.

  end for ▷ (was $\hat{\mathbf{x}}_j = V^{\mathsf{T}}\mathbf{x}_j$ before.)

  $\hat{A}, \hat{B} \leftarrow \arg\min \sum_{j=0}^{k-1} \left\| \hat{A}\hat{\mathbf{x}}_j + \hat{B}\mathbf{u}_j - \hat{\mathbf{x}}_{j+1} \right\|_2^2$ ▷ Infer operators.

  return $\hat{A},\ \hat{B}$

end procedure

Results

Theorem (Re-projection)

Re-projection generates the trajectories obtained with the intrusive reduced model with initial condition $\tilde{\mathbf{x}}_0 = V^\mathsf{T}\mathbf{x}_0$.

Corollary (Operator inference)

For a polynomial system of degree ℓ, *if* $k \geq m + \sum_{i=1}^{\ell} \binom{n}{i}$ *and the data matrix* $\hat{X}$ *is full rank, then the operator inference least squares problem with re-projected trajectories has a unique solution: the operators of the intrusive model.*

Complexity of Algorithm 2: if $\mathbf{f} \in \mathcal{O}(F(n))$,

$$\underbrace{\mathcal{O}(kF(n))}_{\text{snapshot generation}} + \underbrace{\mathcal{O}(kn^2)}_{\text{basis computation}} + \underbrace{\mathcal{O}(\mathbf{k}(F(n)+nr))}_{\text{re-projection sampling}} + \underbrace{\mathcal{O}(kr^3)}_{\text{operator inference}}$$

Methodology

For a few different PDE-driven problems,

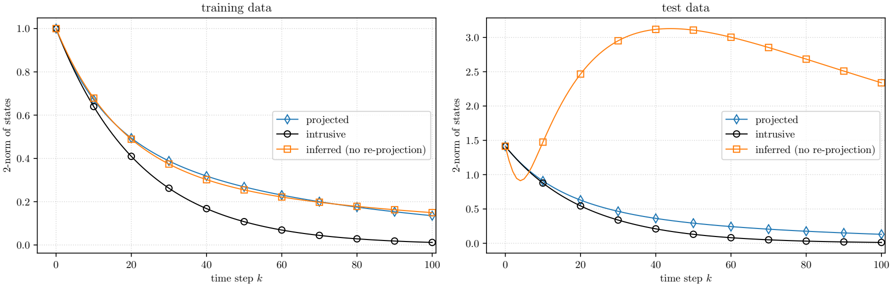
- Construct the FOM.
- Simulate the FOM to generate data and compute a basis.
- Compute the intrusive ROM operators ($\tilde{A}$).
- Use operator inference to compute the ROM operators.
- Re-project the trajectories, then use operator inference to compute the ROM operators ($\hat{A}$).
- Compare intrusive and inferred operators (check $\tilde{A} = \hat{A}$).

We examine

- A motivational toy problem
- A simple homogeneous heat equation
- The viscous Burgers' equation with inputs for boundary conditions

Results: Toy Problem

Let $\mathbf{f}(\mathbf{x}) = A\mathbf{x}$ where $\lambda(A) \subset [.9, .99]$.



Results: Heat Equation

Consider the one-dimensional heat equation

$$\begin{aligned} \frac{\partial x}{\partial t} - \mu \frac{\partial^2 x}{\partial \omega^2} &= 0 && \forall (\omega, t) \in (0, L) \times (0, T] \\ x(0,t) = x(L,t) &= 0 && \forall t \in [0, T], \\ x(\omega, 0) &= g(\omega) && \forall \omega \in [0, L]. \end{aligned}$$

Discretized with simple finite differences, we obtain an ODE of the form

$$\frac{d\mathbf{x}}{dt} = A\mathbf{x}(t).$$

Two experiments:

- <u>Discrete</u>: Implicit Euler takes the form $\mathbf{x}_{j+1} = (I - \delta t A)^{-1}\mathbf{x}_j$. We successfully learned $V^\mathsf{T}(I - \delta t A)^{-1}V$ with re-projection.
- <u>Continuous</u>: with re-projection, $\hat{A} \to V^\mathsf{T} A V$ as $\delta t \to 0$ in the scheme used to compute the snapshots.

Results: Burgers' Equation

Consider the viscous Burgers' equation,

$$\begin{aligned} \frac{\partial x}{\partial t} + x\frac{\partial x}{\partial \omega} - \mu \frac{\partial^2 x}{\partial \omega^2} &= 0 && \forall (\omega, t) \in (-1, 1) \times (0, T] \\ x(-1, t) = u(t), \quad x(1, t) &= -u(t) && \forall t \in [0, T], \\ x(\omega, 0) &= 0 && \forall \omega \in [0, L]. \end{aligned}$$

Discretized in space with finite differences and in time with Explicit Euler, this becomes a discrete system of the form

$$\mathbf{x}_{j+1} = A\mathbf{x}_j + H(\mathbf{x}_j \otimes \mathbf{x}_j) + Bu_j.$$

We confirmed that we can compute the intrusive model,

$$\tilde{\mathbf{x}}_{j+1} = V^\mathsf{T} A V \tilde{\mathbf{x}}_j + V^\mathsf{T} H (V \otimes V)(\tilde{\mathbf{x}}_j \otimes \tilde{\mathbf{x}}_j) + V^\mathsf{T} B u_j,$$

via operator inference with re-projection.

References

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Computer Methods in Applied Mechanics and Engineering, 306:196–215, 2016.

Appendix

Why Re-projection Works (by example)

Consider the FOM $\mathbf{x}_{j+1} = \mathbf{f}(\mathbf{x}_j) := A\mathbf{x}_j$. Given a basis matrix V, the intrusive reduced model is $\tilde{\mathbf{x}}_{j+1} = \tilde{A}\tilde{\mathbf{x}}_j$ where $\tilde{A} = V^\mathsf{T} A V$. In operator inference, we set $\hat{\mathbf{x}}_j := V^\mathsf{T}\mathbf{x}_j$, then minimize

$$\sum_{j=0}^{k-1} \left\| \hat{A}\hat{\mathbf{x}}_j - \hat{\mathbf{x}}_{j+1} \right\|_2^2 = \sum_{j=0}^{k-1} \left\| \hat{A} V^\mathsf{T} \mathbf{x}_j - V^\mathsf{T} A \mathbf{x}_j \right\|_2^2,$$

which gives an answer $\hat{A} \approx V^\mathsf{T} A V = \tilde{A}$ since $\mathbf{x}_j \approx V\hat{\mathbf{x}}_j$. On the other hand, re-projection sets $\hat{\mathbf{x}}_{j+1} = V^\mathsf{T}\mathbf{f}(V\mathbf{x}_j) = V^\mathsf{T} A V \mathbf{x}_j = \tilde{A}\mathbf{x}_j$, so the sum to minimize becomes

$$\sum_{j=0}^{k-1} \left\| \hat{A}\hat{\mathbf{x}}_j - \tilde{A}\hat{\mathbf{x}}_j \right\|_2^2 = \sum_{j=0}^{k-1} \left\| (\hat{A} - \tilde{A})\hat{\mathbf{x}}_j \right\|_2^2,$$

so of course $\hat{A} = \tilde{A}$ as long as the system is overdetermined and well-conditioned.

Extension 1: Continuous Systems (ODEs)

The model reduction is most often posed in the continuous setting, i.e., the full-order model is a differential equation:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t)).$$

The goal of re-projection is to learn the intrusive reduced model,

$$\frac{d\tilde{\mathbf{x}}}{dt} = \tilde{\mathbf{f}}(t, \tilde{\mathbf{x}}(t), \mathbf{u}(t)) := V^{\mathsf{T}}\mathbf{f}(t, V\hat{\mathbf{x}}(t), \mathbf{u}(t)),$$

from data with operator inference.

In this setting, operator inference requires velocity snapshots $\{\dot{\hat{\mathbf{x}}}_j\}_{j=1}^{k}$ that correspond to the state snapshots (these replace $\hat{\mathbf{x}}_{j+1}$ in the least squares problem). Vanilla operator inference sets $\dot{\hat{\mathbf{x}}}_j = V^{\mathsf{T}}\mathbf{f}(\mathbf{x}_j)$, while re-projection sets $\dot{\hat{\mathbf{x}}}_j = V^{\mathsf{T}}\mathbf{f}(V\hat{\mathbf{x}}_j) = V^{\mathsf{T}}\mathbf{f}(VV^{\mathsf{T}}\mathbf{x}_j)$. Only the velocity snapshots are modified; the states remain unchanged. However, the intrusive operator is only recovered in the limit as $\delta t \to 0$ in the scheme that generates the snapshots.

Algorithm 3 Operator inference with re-projected trajectories (continuous)

procedure $\textsc{OpInfRP2}(\mathbf{f},\ \{t_j\}_{j=0}^{k-1},\ \mathbf{x}_0,\ \mathbf{u},\ r)$

  for $j = 0, 1, \ldots, k-1$ **do**

    $\mathbf{x}_j \leftarrow$ solve $\frac{d\mathbf{x}}{dt}(t_j) = \mathbf{f}(t_j, \mathbf{x}(t_j), \mathbf{u}(t_j)), \quad \mathbf{x}(0) = \mathbf{x}_0.$

  end for

  $V \leftarrow \mathrm{POD\_basis}\left(\mathrm{data} = \{\mathbf{x}_j\}_{j=0}^{k-1},\ \mathrm{rank} = r\right)$

  $\hat{\mathbf{x}}_0 \leftarrow V^{\mathsf{T}}\mathbf{x}_0$

  for $j = 0, 1, \ldots, k-1$ **do**:

    $\dot{\hat{\mathbf{x}}}_j \leftarrow V^{\mathsf{T}}\mathbf{f}(V\hat{\mathbf{x}}_j, \mathbf{u}_j)$ ▷ "Re-project" the velocity.

  end for

  $\hat{A}, \hat{B} \leftarrow \arg\min \sum_{j=0}^{k-1} \left\| \hat{A}\hat{\mathbf{x}}_j + \hat{B}\mathbf{u}_j - \dot{\hat{\mathbf{x}}}_j \right\|_2^2$ ▷ Infer operators.

  return $\hat{A},\ \hat{B}$

end procedure

Extension 2: Parametric Systems

Consider the (discrete) full-order model

$$\mathbf{x}_{j+1} = \mathbf{f}(\mathbf{x}_j, \mathbf{u}_j; \boldsymbol{\mu}),$$

where $\boldsymbol{\mu} \in \mathbb{R}^p$ is a parameter. One way to deal with $\boldsymbol{\mu}$ is via interpolation:

1. Select parameter samples $\{\boldsymbol{\mu}_i\}_{i=1}^s \subset \mathbb{R}^p$ to train on.
2. Solve the FOM for each $\boldsymbol{\mu}_i$.
3. Compute a (global) POD basis from the resulting snapshots.
4. Use re-projected operator inference to compute a ROM for each $\boldsymbol{\mu}_i$, using only the data corresponding to that $\boldsymbol{\mu}_i$.
5. For a new parameter $\bar{\boldsymbol{\mu}}$, interpolate between the ROM operators for each $\boldsymbol{\mu}_i$ to get a ROM corresponding to $\bar{\boldsymbol{\mu}}$.

This methodology can be used in the continuous setting as well, but it only works well if the parameter dimension p is small—otherwise, the interpolation becomes unwieldy.