

A Gentle Introduction to Model Order Reduction via Proper Orthogonal Decomposition

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Outline

- 1 The Model Reduction Problem
- 2 Solution Strategy
- 3 Example: Heat Equation

Large Dynamical Systems

Many computational science, engineering, and mathematics applications eventually reduce to the problem of solving a (very) large system of ordinary differential equations:

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(t, \mathbf{x}(t)), \quad \mathbf{x}(0) = \mathbf{x}_0, \quad (*)$$

where

$$\mathbf{x} : \mathbb{R} \rightarrow \mathbb{R}^n, \quad \mathbf{f} : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n, \quad \mathbf{x}_0 \in \mathbb{R}^n.$$

We call $(*)$ the *full-order model (FOM)*.

Some assumptions:

- We know \mathbf{f} and that it is “nice”
- The dimension n is large ($n \sim 10^8$)
- We can solve $(*)$, but it is computationally expensive to do so

Small Dynamical Systems

The goal of model order reduction (MOR) is to construct a low-dimensional system

$$\frac{d}{dt}\hat{\mathbf{x}}(t) = \hat{\mathbf{f}}(t, \hat{\mathbf{x}}(t)), \quad \hat{\mathbf{x}}(0) = \hat{\mathbf{x}}_0, \quad (**)$$

where

$$\hat{\mathbf{x}} : \mathbb{R} \rightarrow \mathbb{R}^r, \quad \hat{\mathbf{f}} : \mathbb{R} \times \mathbb{R}^r \rightarrow \mathbb{R}^r, \quad \hat{\mathbf{x}}_0 \in \mathbb{R}^r,$$

with $r \ll n$ and $\hat{\mathbf{x}}$ related to \mathbf{x} somehow.

We call $(**)$ the *reduced-order model* (ROM).

The goal is typically $r < 50$ or so.

Strategy: Projection to a Linear Subspace

Idea: approximate $\mathbf{x} \in \mathbb{R}^n$ as a linear combination of r vectors.

That is, find $V \in \mathbb{R}^{n \times r}$ such that

$$\mathbf{x}(t) \approx V \hat{\mathbf{x}}(t),$$

meaning $\text{Range}(V) \approx \{\mathbf{x}(t) \mid t \geq 0\}$.

But how?

Strategy: Collect Snapshot Data

To approximate the solution set $\{\mathbf{x}(t) \mid t \geq 0\}$, simulate the FOM (*) and record the solution $\mathbf{x}(t)$ at times $0 = t_0 < t_1 < \dots < t_{k-1}$. Stack the results column-wise to get the *snapshot matrix*,

$$X = \left[\begin{array}{c|c|c|c} \mathbf{x}(t_0) & \mathbf{x}(t_1) & \dots & \mathbf{x}(t_{k-1}) \end{array} \right] \in \mathbb{R}^{n \times k}.$$

Now the column space (range) of X is an approximation to $\{\mathbf{x}(t) \mid t \geq 0\}$.

But we want $V \in \mathbb{R}^{n \times r}$ (probably $r < k < n$)...

Strategy:

Use the SVD!

Strategy: Use the SVD!

Theorem

Let $A \in \mathbb{R}^{n \times k}$ have the singular value decomposition

$$A = \Phi \Sigma \Psi^T.$$

Then the first r columns of Φ are the best rank- r approximation of the column space of A . In other words, $\{\phi_j\}_{j=1}^r$ solves the minimization problem

$$\operatorname{argmin}_{\tilde{\phi}_1, \dots, \tilde{\phi}_r \in \mathbb{R}^n} \sum_{j=1}^k \left\| \mathbf{x}_j - \sum_{i=1}^r \langle \mathbf{x}_j, \tilde{\phi}_i \rangle_{\mathbb{R}^n} \tilde{\phi}_i \right\|_{\mathbb{R}^n}^2$$

such that

$$\langle \tilde{\phi}_i, \tilde{\phi}_j \rangle_{\mathbb{R}^n} = \delta_{ij} \quad \text{for } 1 \leq i, j \leq r.$$

Strategy: Use POD to Define the Linear Subspace

Define

$$V_r := \Phi_{:,r}(X) \in \mathbb{R}^{n \times r},$$

the *POD basis of rank r* corresponding to the snapshot matrix X .

Since Φ has orthonormal columns, so does V_r . In particular,

- $V_r^T V_r = I \in \mathbb{R}^{r \times r}$
- $V_r V_r^T$ is the orthogonal projector onto

$$\text{Range}(V_r) \approx \text{Range}(X) \approx \{\mathbf{x}(t) \mid t \geq 0\}$$

Strategy: Substitute the Approximation

Since V_r is orthonormal,

$$\mathbf{x}(t) \approx V_r \hat{\mathbf{x}}(t) \quad \implies \quad V_r^T \mathbf{x}(t) \approx \cancel{V_r^T V_r} \hat{\mathbf{x}}(t) = \hat{\mathbf{x}}(t).$$

Substituting this into the FOM (*),

$$\frac{d}{dt} \mathbf{x}(t) = \mathbf{f}(t, \mathbf{x}(t)), \quad \mathbf{x}(0) = \mathbf{x}_0,$$

we obtain

$$\begin{aligned} \frac{d}{dt} V_r \hat{\mathbf{x}}(t) &= \mathbf{f}(t, V_r \hat{\mathbf{x}}(t)), & V_r \hat{\mathbf{x}}(0) &= \mathbf{x}_0, \\ \cancel{V_r^T V_r} \frac{d}{dt} \hat{\mathbf{x}}(t) &= V_r^T \mathbf{f}(t, V_r \hat{\mathbf{x}}(t)), & \cancel{V_r^T V_r} \hat{\mathbf{x}}(0) &= V_r^T \mathbf{x}_0, \end{aligned}$$

$$\boxed{\frac{d}{dt} \hat{\mathbf{x}}(t) = V_r^T \mathbf{f}(t, V_r \hat{\mathbf{x}}(t))},$$

$$\boxed{\hat{\mathbf{x}}(0) = V_r^T \mathbf{x}_0 =: \hat{\mathbf{x}}_0}.$$

Strategy: Precompute When Possible

Suppose the FOM operator \mathbf{f} is of the form

$$\mathbf{f}(t, \mathbf{x}(t)) = A\mathbf{x}(t) + \mathbf{c},$$

where

$$A \in \mathbb{R}^{n \times n}, \quad \mathbf{c} \in \mathbb{R}^n.$$

Then the corresponding ROM is

$$\begin{aligned} \frac{d}{dt} \hat{\mathbf{x}}(t) &= V_r^\top \mathbf{f}(t, V_r \hat{\mathbf{x}}(t)) = V_r^\top A V_r \hat{\mathbf{x}}(t) + V_r^\top \mathbf{c} \\ &= \hat{A} \hat{\mathbf{x}}(t) + \hat{\mathbf{c}}, \end{aligned}$$

where

$$\hat{A} := V_r^\top A V_r \in \mathbb{R}^{r \times r}, \quad \hat{\mathbf{c}} := V_r^\top \mathbf{c} \in \mathbb{R}^r.$$

Summary

Offline Phase (construct the ROM)

- 1 Simulate the n -dimensional FOM to collect snapshots, stacked column-wise into the matrix X .
- 2 Compute the rank- r POD basis matrix V_r corresponding to X (the first r left singular vectors).
- 3 Construct \hat{A} , \hat{c} from A , c , and V_r . This defines an r -dimensional ROM.

Online Phase (simulate the ROM)

Given an initial value \mathbf{x}_0 ,

- 1 Project the initial value as $\hat{\mathbf{x}}_0 = V_r^T \mathbf{x}_0$.
- 2 Solve the ROM with initial value $\hat{\mathbf{x}}_0$, obtaining $\hat{\mathbf{x}}(t)$
- 3 Reconstruct the solution in the initial space as $\mathbf{x}_{\text{ROM}}(t) = V_r \hat{\mathbf{x}}(t)$.

Example: Heat Equation

Consider the following one-dimensional parabolic PDE.

$$\begin{aligned}x_t(t, \omega) &= \frac{1}{\pi^2} x_{\omega\omega}(t, \omega), & (t, \omega) &\in (0, T] \times \Omega, \\x_\omega(t, 0) &= x_\omega(t, 1) = 0, & t &> 0, \\x(0, \omega) &= \cos(\pi\omega) + \varepsilon \cos(4\pi\omega) + 2, & \omega &\in \Omega.\end{aligned}$$

Discretizing with a simple finite difference scheme yields a linear ODE,

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

We can reduce this system!

<https://tinyurl.com/v5mjcn6>