Data-Driven Reduced-Order Models for Physics-Based Machine Learning

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Numerical Linear Algebra

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Problem Statement

Consider the 1-D diffusion PDE:

$$-\frac{\partial}{\partial x}\left(k(x)\frac{\partial u}{\partial x}\right) + \frac{\partial u}{\partial x} = 0 \tag{1}$$

for $x \in [0, 1]$ with initial conditions $u(t = 0) = \delta(x - x_0)$ and boundary conditions $u(0) = u(1) = 0$.
In the Laplace domain:

$$-\frac{\partial}{\partial x}\left(k\frac{\partial \hat{u}}{\partial x}\right) + \lambda \hat{u} = \delta(x - x_0) \tag{2}$$

with discretization:

$$Au + \lambda u = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \lambda u_i = e_1 \tag{3}$$

Solve this equation for arbitrary λ by creating a reduced-order model fit to some solutions.

Framework

1. Suppose known data are $d(\lambda) = \hat{u}(\lambda, \tilde{x})$, where $\tilde{x} \in x$ is a known point and $\hat{u}$ is solved directly for $\lambda = \lambda_1, ..., \lambda_k$.
2. Let $\vec{d} = [d(\lambda_1), ..., d(\lambda_k)]^*$.
3. Define a matrix from a rational Krylov subspace: $V_k = [v_1, v_2, ..., v_k] = \left[(A + \lambda_1)^{-1} e_1, ..., (A + \lambda_k)^{-1} e_1\right] \in \mathbb{R}^{(n-1)\times k}$.
4. Then $v_j^* A v_i + \lambda v_j^* v_i = d(\lambda_j)$ and $v_i^* A v_j + \lambda v_i^* v_j = d(\lambda_i)$.

This gives us matrices $S \in \mathbb{R}^{k\times k}$ and $M \in \mathbb{R}^{k\times k}$, where:

$$S_{ij} + \lambda M_{ij} = d(\lambda_j) \tag{4}$$
$$S_{ij} + \lambda M_{ij} = d(\lambda_i) \tag{5}$$
$$S_{ii} = \left(\lambda d(\lambda)\right)'|_{\lambda=\lambda_i} \tag{6}$$
$$M_{ii} = -d'(\lambda_i) \tag{7}$$

Solve $Sw + \hat{\lambda} Mw = \vec{d}$ for w so that the approximated solution for arbitrary $\hat{\lambda}$ is:

$$u(\hat{\lambda}, \tilde{x}) = V_k w_k = \vec{d}^* w \tag{8}$$

Figure

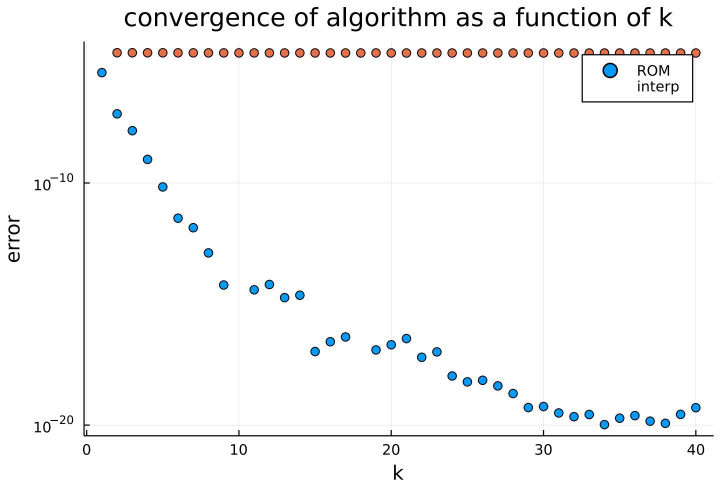

Figure: Algorithm L_2 accuracy as a function of k. ROM model is in blue and linear interpolation is in orange. $k > 50$ causes numerical instability.