Nonlinear ROM for gradient-flow dynamics

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Abstract

Reduced Order Models (ROMs) are simplified representations of large systems designed to reduce the computational cost while retaining the essential features. Their key challenges are the identification of such important features and the accurate quantification of the error committed in the reduced representation. This work develops ROMs in metric spaces, highlighting the novelties of this perspective and addressing the advantages it brings to tackle the above-mentioned points.

Metric ROMs [3] are built to accurately capture what is known about the geometric structure of the problem. By identifying significant topological features of the potentially nonlinear data manifold at disposal, this approach provides geometry-aware models, addressing some relevant limitations of traditional ROM techniques [6, 4]. Indeed, taking into consideration such geometric information about the data that is used to build the reduced model leads to a significant enhancement of its reliability, possibly allowing a-priori error estimation and interpretability of its hyperparameters.

This work proposes the construction of nonlinear ROMs within the Wasserstein metric space $\mathcal{P}_2(\Omega; \mathcal{W}_2)$ for gradient flow-based dynamics. Such a setting is particularly well-suited for handling both advective and diffusive behaviors, whose coexistence is notoriously problematic for the identification of accurate ROMs. Indeed, considering $\rho_0 \in \mathcal{P}_2(\Omega)$ a probability density with finite second-order moment and $v_t \in L_2(\rho_t; \Omega)$, $\forall t \in [0, T]$, a smooth bounded vector field tangent to the boundary $\partial\Omega$, i.e. $\rho_t v_t \cdot \nu\big|_{\partial\Omega} = 0$, the gradient flow dynamics is expressed with $\rho_t \in \mathcal{P}_2(\Omega)$ solving the continuity equation

$$\partial_t \rho_t + \nabla \cdot (\rho_t v_t) = 0$$

in the distributional sense. It is known [1] that v_t can be seen as the gradient of the L_2-first variation of a functional $\mathcal{F} : \mathcal{P}_2(\Omega) \to \mathbb{R}$, so that $v_t = -\nabla \frac{\delta \mathcal{F}}{\delta \rho}[\rho_t]$. Therefore, the parametric diffusion-advection-reaction PDE with Neumann boundary conditions, parameters $p \in \mathbb{P}$ and potential $V : \Omega \times \mathbb{P} \to \mathbb{R}$ given by

$$\begin{cases} \partial_t \rho_t(x;p) = \Delta \rho_t(x;p) + \nabla \rho_t(x;p) \cdot \nabla V(x;p) + \rho_t(x;p) \Delta V(x;p) & x \in \Omega \\ \frac{\partial \rho_t(x;p)}{\partial \nu}\Big|_{\partial\Omega} = 0 \end{cases}$$

can be represented as a gradient flow [7], choosing the functional

$$\mathcal{F}[\rho] = \int_\Omega \rho(x;p) \log(\rho(x;p)) + V(x;p)\rho(x;p) dx.$$

In particular, we aim to build a dynamical low-rank approximation [5] of $\rho_t(x;p)$ including the geometrical constraints of the problem, providing some estimates on the accuracy of the approximation in the parameter space. Commonly, nonlinear ROMs are built by applying linear reduction on a transformed manifold that is the result of a nonlinear transformation of the original snapshots [8, 2], following the pipeline shown in Figure 1. In this way, the original data manifold $\mathcal{M}$ is transformed

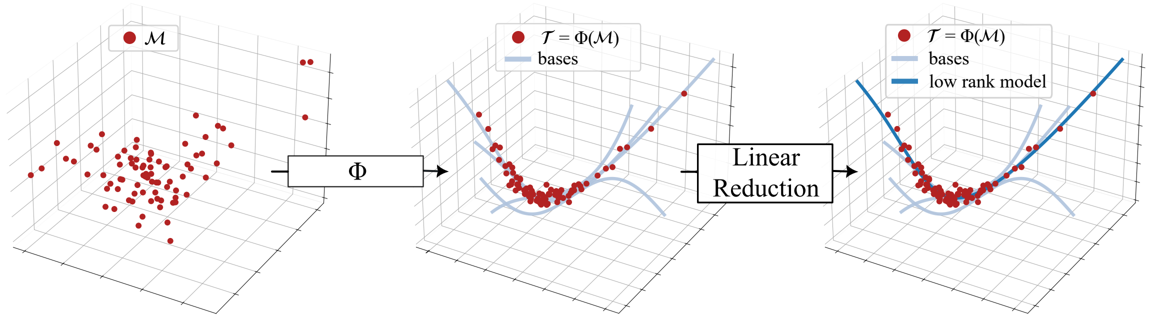

Figure 1: Nonlinear reduction pipeline: a nonlinear map Φ transforms the original data manifold $\mathcal{M}$ into the new manifold $\mathcal{T}$, which has an accurate low rank representation.

through a nonlinear map Φ into the manifold $\mathcal{T}$, which in general has a better Kolmogorov decay, being more suitable for linear reduction. We propose a nonlinear ROM for advection-diffusion problems in which linear reduction is performed on an appropriately chosen data manifold given the geometric assumptions derived from its gradient flow structure. We demonstrate that this improves the generalization capabilities in the entire parameter space $\mathbb{P}$ of the reduced model, and apply the method to different scenarios.

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