Universität

Model order reduction using nonlinear transformations of space-time domains

Reisensburg Workshop

Hendrik Kleikamp (University of Münster); based on work with Mario Ohlberger and Stephan Rave January 20–22, 2025

living.knowledge



Slowly decaying Kolmogorov N-widths Burgers' equation as a simple example

Example: Moving discontinuities with different speeds in a parametrized Burgers' equation





Slowly decaying Kolmogorov N-widths Burgers' equation as a simple example

Example: Moving discontinuities with different speeds in a parametrized Burgers' equation



Transport-dominated problems suffer from a slow Kolmogorov N-width decay!



Slowly decaying Kolmogorov N-widths Burgers' equation as a simple example

Example: Moving discontinuities with different speeds in a parametrized Burgers' equation



Transport-dominated problems suffer from a slow Kolmogorov N-width decay!
Approximation by linear subspaces not suitable!





Approach: Perform nonlinear transformation of solution snapshots



- Approach: Perform nonlinear transformation of solution snapshots
- Use ideas from (medical) image registration and landmark matching



- Approach: Perform nonlinear transformation of solution snapshots
- Use ideas from (medical) image registration and landmark matching
- Consider space-time snapshots to directly incorporate interacting shocks



- Approach: Perform nonlinear transformation of solution snapshots
- Use ideas from (medical) image registration and landmark matching
- Consider space-time snapshots to directly incorporate interacting shocks
- Assumption: Reference snapshot can be transformed into all other solution snapshots



- Approach: Perform nonlinear transformation of solution snapshots
- Use ideas from (medical) image registration and landmark matching
- Consider space-time snapshots to directly incorporate interacting shocks
- Assumption: Reference snapshot can be transformed into all other solution snapshots
- Align discontinuities by transformations of the underlying space-time domain



- Approach: Perform nonlinear transformation of solution snapshots
- Use ideas from (medical) image registration and landmark matching
- Consider space-time snapshots to directly incorporate interacting shocks
- Assumption: Reference snapshot can be transformed into all other solution snapshots
- Align discontinuities by transformations of the underlying space-time domain

Main question: How to represent transformations in a reduced manner?



Consider a small set of landmarks q_i instead of full "images"









Consider a small set of landmarks q_i instead of full "images"





Consider a small set of landmarks q_i instead of full "images"





- Consider a small set of landmarks q_i instead of full "images"
- Given associated initial momenta pi(0), transform the landmarks according to a geodesic equation





- Consider a small set of landmarks q_i instead of full "images"
- Given associated initial momenta p_i(0), transform the landmarks according to a geodesic equation
- ► Represent vector fields via a kernel k as $v_t(x) = \sum_{i=1}^{n} k(x, q_i(t)) p_i(t)$ position





- Consider a small set of landmarks q_i instead of full "images"
- Given associated initial momenta p_i(0), transform the landmarks according to a geodesic equation
- ► Represent vector fields via a kernel k as $v_t(x) = \sum_{i=1}^{n} k(x, q_i(t)) p_i(t)$ position





- Consider a small set of landmarks qi instead of full "images"
- Given associated initial momenta pi(0), transform the landmarks according to a geodesic equation
- ► Represent vector fields via a kernel k as $\nu_t(x) = \sum_{i=1}^n k(x, q_i(t)) p_i(t)$ position
- Approximate initial momenta as a function of the parameter





- Consider a small set of landmarks q_i instead of full "images"
- Given associated initial momenta pi(0), transform the landmarks according to a geodesic equation
- ► Represent vector fields via a kernel k as $\nu_t(x) = \sum_{i=1}^n k(x, q_i(t)) p_i(t)$ position
- Approximate initial momenta as a function of the parameter
- Offline/online phase: Similar procedure as for the vector fields (but without additional reduction of initial momenta)



Numerical results for Burgers' equation Landmark matching





Matching errors **Relative error** 10^{-1} 10^{-2} 0.5 1.5Parameter μ Offline phase Average (5.3%) Average (5.43%) Online phase

Model order reduction using nonlinear transformations of space-time domains

hendrik.kleikamp@uni-muenster.de 4

Open problems





Intrusive online computations? Residual minimization?

Error estimates (a priori and a posteriori)?

Efficient online evaluations of the solution?

Snapshot reduction and online selection of solution "topology"?

Additional slides

Labeled landmark matching I



 \blacktriangleright The trajectories of the template landmarks x_i are given as solutions to the ODE

$$\frac{dq_i}{dt}(t) = v_t(q_i(t)), \qquad q_i(0) = x_i$$

for $i=1,\ldots,n$, where $q_i\colon [0,1]\to \mathbb{R}^r$ denotes the evolution of the i-th landmark and $\nu_t\colon \mathbb{R}^r\to \mathbb{R}^r$ denotes the vector field at time $t\in[0,1]$.

> The time-dependent vector field admits a representation similar to kernel approximants, namely

$$\nu_t(x) = \sum_{i=1}^n k(x, q_i(t)) p_i(t),$$

where k: $\mathbb{R}^r \times \mathbb{R}^r \to \mathbb{R}^{r \times r}$ is a symmetric matrix-valued kernel and $p_i : [0, 1] \to \mathbb{R}^r$ are momenta associated to the landmarks for i = 1, ..., n.



Labeled landmark matching II

The momenta and landmarks evolve in an energy minimizing way by means of a Hamiltonian function defined as

$$H(q(t), p(t)) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} p_i(t)^{\top} k(q_i(t), q_j(t)) p_j(t) = \frac{1}{2} \| v_t \|_V^2,$$

where $q(t) = (q_1(t), \ldots, q_n(t))$ is the set of landmarks and $p(t) = (p_1(t), \ldots, p_n(t))$ denotes the set of momenta. Here, the space V corresponds to the reproducing kernel Hilbert space.

The evolution of the landmarks and momenta is now in such a way that the Hamiltonian is constant over time, which leads to the system

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial H}{\partial p}(q,p), \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial q}(q,p).$$

The initial momenta are chosen such that they minimize the energy

$$E_{\{\mathbf{x}_i\} \to \{\mathbf{y}_j\}}(p(0)) = H(q(0), p(0)) + \frac{1}{\sigma^2} \sum_{i=1}^n \| q_i(1) - y_i \|_2^2.$$

Unlabeled landmark matching



• Given sets of template landmarks $x_1, \ldots, x_n \in \mathbb{R}^r$ and target landmarks $y_1, \ldots, y_m \in \mathbb{R}^r$, we define the associated signed measures v_{template} and v_{target} as

$$\nu_{\text{template}} \coloneqq \sum_{i=1}^n \delta_{x_i} \qquad \text{and} \qquad \nu_{\text{target}} \coloneqq \sum_{j=1}^m \delta_{y_j}.$$

• Given another kernel $k_{\text{dist}} \colon \mathbb{R}^r \times \mathbb{R}^r \to \mathbb{R}$ we measure the norm of a linear combination $\nu = \sum_{i=1}^n \delta_{x_i}$ as

$$\left\| \boldsymbol{\nu} \right\|^2 = \sum_{i=1}^n \sum_{j=1}^n k_{\mathsf{dist}}(\boldsymbol{x}_i, \boldsymbol{x}_j).$$

• We consider as mismatch term g in the energy the squared norm of the difference,

$$g(q(1)) = \sum_{i=1}^{n_{\text{diff}}} \sum_{j=1}^{n_{\text{diff}}} c_i c_j k_{\text{dist}}(z_i, z_j), \qquad \text{where } \sum_{i=1}^{n_{\text{diff}}} c_i \delta_{z_i} = \sum_{i=1}^n \delta_{q_i(1)} - \sum_{j=1}^m \delta_{y_j}.$$

Landmark matching Efficient point-wise evaluation of the transformation

 \blacktriangleright In order to compute the evolution of a given point $x \in \mathbb{R}^r$ as

$$\frac{\mathrm{d}q}{\mathrm{d}t}(t) = v_t(q(t)), \qquad q(0) = x$$

only the time evolutions of landmarks and momenta are required according to

$$\nu_t(q(t)) = \sum_{i=1}^n k(q(t), q_i(t)) p_i(t).$$

The time evolution of single points can therefore be computed efficiently by solving the corresponding ODE.

• Computational costs for labeled landmark matching when considering $n \in \mathbb{N}$ landmarks, $n_{\text{eval}} \in \mathbb{N}$ points of interest and $n_t \in \mathbb{N}$ time steps:

$$\mathbb{O}\left(n_t n(n+n_{\mathsf{eval}})\right).$$

A similar complexity involving the total number n + m of template and target landmarks is obtained in the case of unlabeled landmarks.

