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Data-driven reduced order modeling for flows with moving geometries using shifted POD

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1. INTRODUCTION

For transport-dominated problems, the data-driven model reduction using *Proper Orthogonal Decomposition* (POD) suffers from a very low convergence rate, which renders the method impractical for this important class of problems. In Reiss et al. [2018], the *shifted Proper Orthogonal Decomposition* (sPOD) was introduced to speed up the convergence, when decomposing fields of transport dominated systems with the help of the POD. The method builds on the idea that traveling waves or moving localized structures can be perfectly described by their wave profile and a time-dependent transformation, usually a shift operation. Therefore, the shifted POD decomposes transport fields by shifting the data field in a so-called co-moving frame, in which the wave is stationary and can be described by few spatial basis functions determined by the POD. Multiple gradient based optimization algorithms for the sPOD exist already in the literature [Black et al., 2021, Reiss, 2021, Schulze et al., 2019]. However, those formulations of the sPOD have disadvantages, both in practice and theory, which we address in this contribution.

2. ALGORITHMIC APPROACH

The sPOD seeks to decompose traveling wave-fields $Q_{ij} = q(x_i, t_j)$, $Q \in \mathbb{R}^{M,N}$, $M > N$ by solving the optimization problem:

$$\min_{\{Q^k\}_k} \sum_{k=1}^F \|Q^k - [Q^k]_{r_k}\|^2 \quad \text{s.t.} \quad Q = \sum_{k=1}^F \mathcal{T}^k(Q^k) \quad (1)$$

with pre-determined shift-transforms $\mathcal{T}^{\pm k}(Q)_{ij} = q(x_i \mp \Delta_k(t)_i, t_j)$ parametrizing the translation of the wave. Here, F denotes the number of co-moving frames and $\|A\|^2 = \langle A, A \rangle$ with $\langle A, B \rangle = \text{tr}(A^H B)$. The resulting *co-moving frames* $Q^k \in \mathbb{R}^{M,N}$ are therefore of low rank and can be decomposed efficiently using a truncated singular value decomposition (SVD), denoted by $[Q^k]_{r_k}$. However, the co-moving ranks $r_k > 0$ have to be chosen a priori. For complicated systems, this choice is often critical for the quality of the decomposition and the additional freedom

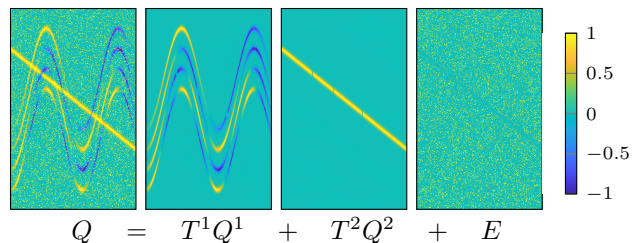


Fig. 1. Given the transport-dominated data-matrix Q with 12.5% noise, our algorithm decomposes it in co-moving frames Q^1, Q^2 and noise E .

of co-moving ranks leads to the question whether the decomposition into co-moving frames is globally optimal.

For this reason, we investigate the shifted POD, formulated as a convex optimization problem, based on minimizing the one-norm $\|Q^k\|_* = \sum_i \sigma_i(Q^k)$ over the set of all singular values $\{\sigma_i(Q^k)\}_{k,i}$ in the shifted frames.

Problem 1. For given shifts $\{\Delta_k\}$, $\lambda > 0$ and $Q \in \mathbb{R}^{M,N}$, $M > N$ with $Q_{ij} = q(x_i, t_j)$ find $\{Q^k \in \mathbb{R}^{M,N}\}$

$$\min_{Q^k} \sum_k \|Q^k\|_* \quad \text{s.t.} \quad Q = \sum_{k=1}^F \mathcal{T}^k(Q^k) \quad (2)$$

where $\mathcal{T}^k(Q)_{ij} = q(x_i - \Delta(t)_i, t_j)$.

As stated in Reiss [2021], this optimization problem is convex, but difficult to solve with a gradient based algorithm. Therefore, in this work we use an alternative formulation based on an augmented Lagrangian with multiplier Y following Bertsekas [2014]:

$$\mathcal{L}(\{Q^k\}_k, Y) = \sum_{k=1}^F \|Q^k\|_* + \frac{\mu}{2} \|Q - \sum_{k=1}^F \mathcal{T}^k(Q^k)\|^2 \quad (3)$$

$$+ \langle Y, Q - \sum_{k=1}^F \mathcal{T}^k(Q^k) \rangle \quad (4)$$

With the new formulation we can employ the *alternating direction method* (ADM, see for review Boyd et al. [2011]), which allows a rapid minimization of the one-norm with help of the singular value thresholding operator:

$$\text{svt}(A, \tau) = US_\tau(\Sigma)V^* \quad (5)$$

$$= \underset{\tilde{A}}{\text{argmin}} \tau \|\tilde{A}\|_* + \frac{1}{2} \|\tilde{A} - A\|^2 \quad (6)$$

$$\mathcal{S}_\tau(x) = \text{sign}(x) \max(|x| - \tau, 0), \quad (7)$$

which technically boils down to a singular value decomposition of the matrix $A = U\Sigma V^*$ with a soft thresholding operator \mathcal{S}_τ (threshold $\tau > 0$) applied to the singular values. For the data displayed in fig. 1 the algorithm converges to the exact numerical ranks after approximately 25 iterations as shown in fig. 2. To further improve the

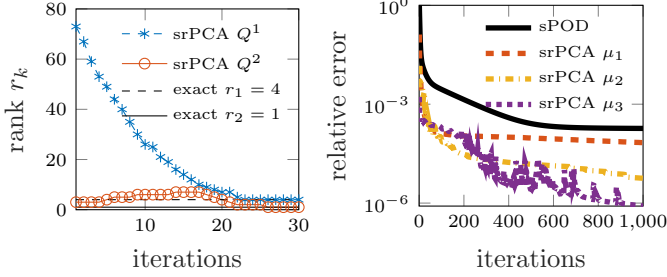


Fig. 2. Convergence of the decomposition for the data shown in figure 1 without the noise. On the left, the numerical ranks of Q^1 and Q^2 at each iteration and on the right the overall error of the data for different stiffness coefficients $(\mu_1, \mu_2, \mu_3) = (0.1, 1, 10)\mu_0$.

decomposition we can make the algorithm robust against outliers or noisy input data, by adding an additional sparsity constraint, as done by Lin et al. [2010, 2011]. We therefore decompose $Q = \tilde{Q} + E$ in a low rank part $\tilde{Q} = \sum_k \mathcal{T}^k(Q^k)$ and the noise is captured in $E \in \mathbb{R}^{M,N}$. The Lagrange function becomes:

$$\mathcal{L}_E(\{Q^k\}_k, E, Y) = \frac{\mu}{2} \|Q - \sum_{k=1}^F \mathcal{T}^k(Q^k) - E\|^2 \quad (8)$$

$$+ \lambda \|E\|_1 + \sum_{k=1}^F \|Q^k\|_* + \langle Y, Q - \sum_{k=1}^F \mathcal{T}^k(Q^k) - E \rangle. \quad (9)$$

The resulting algorithm 1 is therefore more robust against interpolation noise of the shift-operators, corrupted measurements or numerical artifacts. It can be interpreted as a shifted version of the *robust Principle Component Analysis* (srPCA). Its performance scales with the complexity of the singular value decomposition, which can be further accelerated by randomized- or wavelet-techniques (see Halko et al. [2011], Krah et al. [2020]).

3. RESULTS - 2D VORTEX SHEDDING OF A MOVING CYLINDER AT $Re = 200$

To illustrate the applicability of the decomposition to large data sets, we computed a 2D vortex shedding of two cylinders using the *artificial compressibility method* (ACM) to simulate incompressible Navier Stokes equations on a highly resolved adaptive grid [Engels et al., 2021]. In the simulation domain of size $L \times L$, a stationary cylinder is placed at $(x_1, y_1) = (0.125, 0.5)L$, followed by a moving cylinder $(x_2, y_2) = (0.5L, 0.5L + \Delta(t))$, simulated over one period $T = 1/f$. The mean flow going from left to right is tuned such that the *Reynolds number* $Re = 200$ in reference to the first cylinder is achieved. The shift of the second

Algorithm 1 ADM for shifted rPCA

Require: $Q \in \mathbb{R}^{m \times n}$, $\{\mathcal{T}^k\}_k$, $\mu, \lambda > 0$

- 1: init $Q^k = 0 \forall k, \tilde{Q} = E = Y = 0$
- 2: **while** not converged **do**
- 3: **for** frame $p = 1, \dots, N$ **do**
- 4: $\tilde{Q}^p = \mathcal{T}^{-p}(Q - \sum_{k=1, k \neq p}^F \mathcal{T}^k(Q^k) - E + \frac{1}{\mu}Y)$
- 5: apply singular value thresholding
- 6: $Q^p \leftarrow \text{svt}(\tilde{Q}^p, \mu^{-1})$
- 7: **end for**
- 8: **for** frame $p = 1, \dots, N$ **do**
- 9: Update $Q^p = \tilde{Q}^p$
- 10: **end for**
- 11: update noise matrix:
- 12: $E = \mathcal{S}_{\lambda\mu^{-1}}(Q - \sum_k \mathcal{T}^k(Q^k) + \frac{1}{\mu}Y)$
- 13: update multiplier: $Y \leftarrow Y + \mu(Q - \sum_k \mathcal{T}^k(Q^k) - E)$
- 14: **end while**
- 15: **return** $\{Q^k\}$

cylinder $\Delta(t) = 0.25L \sin(2\pi ft)$ is compensated by our algorithm and the data are decomposed in two co-moving frames, which are illustrated in fig. 3. A clear separation

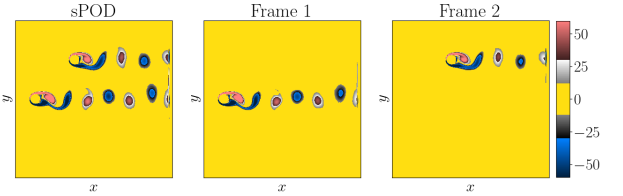


Fig. 3. sPOD: Results of the algorithm for the vorticity field at $t = T/4$.

of the two cylinder shedding is achieved, with an overall relative error of about 1%, when stopping the algorithm at $(r_1, r_2) = (37, 35)$. Comparing this result to the POD with $r = r_1 + r_2$ shown in fig. 4 (relative error 2%), we see typical staircase effects of the POD located at the discontinuities at the fluid-solid interfaces. In the conference talk we will

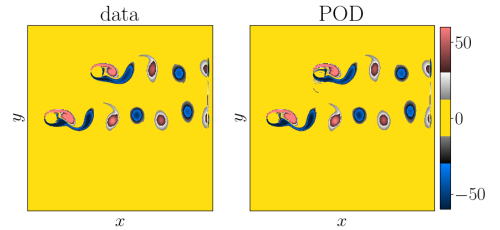


Fig. 4. Vorticity field (left) and its decomposition with the POD (right) at $t = T/4$.

further address the ability to predict and optimize flows using the low rank structure computed by our algorithm.

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