SiSc Seminar

Reduced Order Modeling for Transport Problems

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Abstract

Snapshot matrices built from solutions to transport problems have large Kolmogorov n-widths, while small n-widths are necessary in order for reduced order modelling techniques to succeed. To overcome this issue, a new algorithm based on solving an optimization problem is proposed in this work, which looks for mappings that represent the whole set of snapshots in terms of a few reference modes and then use the Proper Orthogonal Decomposition method (POD) to find a low-rank representation of the mappings. The algorithm is illustrated on both linear and non-linear problems where it is seen to perform well in case of the former.

Chapter 1

Introduction

Reduced order models (ROMs) can imitate the behaviour of full order models (FOMs) with a reasonable accuracy at a reduced computational cost and are therefore used as their replacement in many applications including real time analysis, optimization problems and optimal control.

Different model order reduction techniques have been developed and applied to various types of partial differential equations (PDEs) in literature. The method in focus in this report is called the reduced basis method. In this, first a sequence of low dimensional spaces (called reduced basis spaces) is found out which are approximations to the actual space of solutions (called the solution manifold) to the parametric PDE and then based on such spaces, an approximate solution is calculated for the parameter of interest. However, the success of the reduced basis method depends on the Kolmogorov n-width of the solution manifolds, which roughly speaking reflects how well the solution manifold can be emulated by a finite dimensional linear space. More precisely, for a manifold $\mathscr{M}$ embedded in some normed linear space X, the Kolmogorov n-width is defined as -

$$w_N(\mathscr{M}, X) = \inf_{E_N} \sup_{f \in \mathscr{M}} \inf_{g \in E_N} \|f - g\|_X \tag{1.1}$$

where the first infimum is taken over all N-dimensional subspaces of X.

Till now, majority of the work on this topic has focused on problems wherein the solution manifold has a small Kolmogorov n-width i.e. it rapidly converges with increasing N. However, there are cases in which this is not the situation and some additional manipulations need to be performed in order for the ROM theory to work. The case of transport problems falls in this category for which the solution manifolds have large n-widths and there are a few works in literature dealing with this issue.

In [1], the solution $u(t)$ is decomposed into a group component $g(t)$ and a shape component $v(t)$ ($u(t) = g(t).v(t)$) by imposing appropriate algebraic constraints on the decomposition such that the shift in the solutions is captured by $g(t)$ while $v(t)$ is as stationary as possible, only capturing the change of shape in $u(t)$. The approach is presented in the frame of Lie group action and the notion of equivariance is introduced with respect to the group action.

The method presented in [2] is similar to the current work in many aspects, particularly in looking for mappings that transform the initial mode u_0 to the subsequent snapshots. The idea there is to find a change of variable/mapping (written as a sum of advection modes) that represents the subsequent snapshots in terms of u_0 and this is achieved by evaluating the Wasserstein distances of the snapshots w.r.t. the reference mode u_0 by solving the Monge-Kantorovich optimal transport problems.

In [3], the authors perform a "preconditioning" of the solution manifold based on a prior expertise of the problem they are dealing with (the case of viscous Burger's equation is considered as an example) so as to transform the manifold to a structure having a small Kolmogorov n-width and finally performing a POD on this preconditioned manifold to recover the reduced basis modes.

The approach presented in [4] is similar to what is being done here in the sense that the former also applies a template fitting strategy. The authors try to fit the solution snapshots in the Krylov space of a matrix (obtained from finite volume discretization) and a few reference modes (mainly the initial mode u_0). A greedy algorithm is introduced that captures the transport structure by building on the template fitting strategy, which is extended to accommodate more complex situations.

In [5], the authors introduce an algorithm called sPOD (shifted POD) which generalizes the common POD by allowing for time dependent shifts of the snapshot matrix i.e. the solution is shifted at every time step to compensate for the transport that took place.

In the current work, an algorithm based on solving an optimization problem is presented which looks for mappings that transforms the reference grid in such a way that the solution manifold can be expressed in terms of a few reference modes. Once these mappings are obtained, a low-rank representation of their space is sought out by applying POD. These steps form the offline stage of the algorithm after which the online stage is performed with the obtained modes and all these have been discussed thoroughly in Chapter 2. In Chapter 3, the proposed algorithm is illustrated on the linear advection and the burger's equations to test its efficacy.

Chapter 2

Methodology

In this chapter, the strategy devised in the current work for applying the reduced basis method to transport problems is described, delineating the steps for performing the offline and online stages of the algorithm.

Let us consider the Cauchy problem of finding $u(\cdot, t; \mu)$ in some physical space $\Omega \subset \mathbb{R}^d, d = 1, 2, 3$ such that

$$\begin{cases} u_t + \mathscr{L}(u; \mu) = 0 & \text{in } [0, T] \times \Omega \\ u(\cdot, t = 0; \mu) = u_0(\cdot; \mu) & \text{in } \Omega \\ u & \text{is periodic} \end{cases} \tag{2.1}$$

where μ varies in some compact parameter space $\mathscr{C}$.

2.1 Model Order Reduction - Offline Stage

At each time step, co-ordinates α_i^n and an application $F_n \in \mathscr{F}_{\mathscr{C}}$ are looked for such that $u(\cdot, t^n; \mu)$ is well approximated by:

$$u^n := \sum_{i=1}^{M} \alpha_i^n \phi_i \circ F_n \tag{2.2}$$

where u^n is the solution to (2.1) at t^n. $F \in \mathscr{F}_{\mathscr{C}}$ here is defined as a map transforming the grid

$$\begin{aligned} F : \Omega &\mapsto \Omega \\ x &\mapsto x + \Gamma(x, t; \mu) \end{aligned} \tag{2.3}$$

The idea behind defining F in this way is to now choose a few of the solution modes u_i (precomputed using high-fidelity solver) as basis modes

ϕ_i and take their composition with the transformed/distorted grid $(x + \Gamma_i)$ to span the entire solution manifold. Γ is added to the reference grid x to get the distorted grid and is referred to as the "grid distortion" function in this report. In most cases, considering only the initial mode u_0 as ϕ_i will serve the purpose here and the problem would also become easier to solve as compared to the case when more number of modes are considered. Having said that, equation (2.3) can now be re-written as:

$$u^n := \sum_{i=1}^{M} \alpha_i^n u_i(x + \Gamma_i^n) \tag{2.4}$$

Γ_i^n for each time step n and for each mode u_i is calculated by solving a minimization problem of the form:

$$(\alpha_i^n, \Gamma_i^n) = \underset{(\alpha_i, \Gamma_i)}{\operatorname{argmin}} \left\| u^n - \sum_i \alpha_i u_i(x + \Gamma_i) \right\| \tag{2.5}$$

for some appropriate norm $\| \cdot \|$ on X.

The following generic algorithm based on coordinate descent method is proposed for solving the minimization problem (2.5) :

Initialize α_i and Γ_i

$$(\alpha_i^{n,0}, \Gamma_i^{n,0}) = (\alpha_i^{ini}, \Gamma_i^{ini}) \tag{2.6}$$

Then assuming that $(\alpha_i^{n,q}, \Gamma_i^{n,q})$ are known for some internal iteration $q \geq 0$

Fit the α_i given $\Gamma_i^{n,q}$

Find $\alpha_i^{n,q+1}$ that minimizes the following quantity (in some sense) :

$$u^n - \sum_i \alpha_i^{n,q+1} u_i(x + \Gamma_i^{n,q}) \tag{2.7}$$

Fit the Γ_i given $\alpha_i^{n,q+1}$

Find $\Gamma_i^{n,q+1}$ that minimizes the following quantity (in some sense) :

$$u^n - \sum_i \alpha_i^{n,q+1} u_i(x + \Gamma_i^{n,q+1}) \tag{2.8}$$

until convergence (for which, say $q = q^*$). Then set:

$$(\alpha_i^n, \Gamma_i^n) = (\alpha_i^{n,q^*+1}, \Gamma_i^{n,q^*+1}) \tag{2.9}$$

Although the α_i^ns have to be calculated for solving the minimization problem, only the functions Γ_i^n are needed for further analysis purpose.

Next a low dimensional representation of the space spanned by functions Γ_i^n in terms of the basis functions $\gamma_{i,j}$ is sought out i.e. Γ_i^n is expressed in the form:

$$\Gamma_i^n = \sum_{j=1}^{N_i} d_{i,j}^n \gamma_{i,j} \tag{2.10}$$

where $d_{i,j}^n$ are the coordinates on the reduced basis which are looked for in the online stage. The basis functions $\gamma_{i,j}$ are obtained by applying the Proper Orthogonal Decomposition (POD) on the functions Γ_i^n.

Finally, using (2.10), equation (2.4) can be re-written and the solution $u(\cdot, t^n; \mu)$ to (2.1) at t^n can be expressed in the reduced basis form as :

$$u^n := \sum_{i=1}^{M} \alpha_i^n u_i(x + \sum_{j=1}^{N_i} d_{i,j}^n \gamma_{i,j}) \tag{2.11}$$

The steps described above form the offline stage of the method which provide the basis functions u_i and $\gamma_{i,j}$, using which a reduced basis representation of the solution manifold is established.

2.2 Model Order Reduction - Online Stage

For simplicity, the explicit Euler scheme is used for the time discretization in the numerical tests which gives the semi-discretized form of (2.1) as-

$$\begin{cases} \dfrac{u^{n+1} - u^n}{dt} + \mathscr{L}(u^n; \mu) = 0 & \text{in } \Omega \\ u(\cdot, t = 0; \mu) \qquad\qquad = u_0(\cdot; \mu) & \text{in } \Omega \\ u & \text{is periodic} \end{cases} \tag{2.12}$$

Here dt denotes the time step and u^n represents the approximate solution to (2.1) at time ndt.

Now in terms of the reduced basis form (2.11) derived in the previous section, the solution $u(\cdot, t^{n+1}; \mu)$ to (2.1) at time t^{n+1} can be represented as:

$$u^{n+1} := \sum_{i=1}^{M} \alpha_i^{n+1} u_i(x + \sum_{j=1}^{N_i} d_{i,j}^{n+1} \gamma_{i,j}) \tag{2.13}$$

So, in order to find u^{n+1}, the coordinates α_i^{n+1} and $d_{i,j}^{n+1}$ need to be determined, which is done by solving a minimization problem of the form:

$$(\alpha_i^{n+1}, d_{i,j}^{n+1}) = \underset{(\alpha_i, d_{i,j})}{\operatorname{argmin}} \left\| \sum_i \alpha_i u_i(x + \sum_j d_{i,j} \gamma_{i,j}) - u^n + dt \mathscr{L}(u^n; \mu) \right\| \tag{2.14}$$

for some appropriate norm $\| \cdot \|$ on X.

The minimization problem (2.14) can be solved in the same way as (2.5) :

Initialize α_i and $d_{i,j}$

$$(\alpha_i^{n+1,0}, d_{i,j}^{n+1,0}) = (\alpha_i^{ini}, d_{i,j}^{ini}) \tag{2.15}$$

Then assuming that $(\alpha_i^{n+1,q}, d_{i,j}^{n+1,q})$ are known for some internal iteration $q \geq 0$

Fit the α_i given $d_{i,j}^{n+1,q}$

Find $\alpha_i^{n+1,q+1}$ that minimizes the following quantity (in some sense) :

$$\sum_i \alpha_i^{n+1,q+1} u_i(x + \sum_j d_{i,j}^{n+1,q} \gamma_{i,j}) - u^n + dt \mathscr{L}(u^n; \mu) \tag{2.16}$$

Fit the $d_{i,j}$ given $\alpha_i^{n+1,q+1}$

Find $d_{i,j}^{n+1,q+1}$ that minimizes the following quantity (in some sense) :

$$\sum_i \alpha_i^{n+1,q+1} u_i(x + \sum_j d_{i,j}^{n+1,q+1} \gamma_{i,j}) - u^n + dt \mathscr{L}(u^n; \mu) \tag{2.17}$$

until convergence (for which, say $q = q^*$). Then set:

$$(\alpha_i^{n+1}, d_{i,j}^{n+1}) = (\alpha_i^{n+1,q^*+1}, d_{i,j}^{n+1,q^*+1}) \tag{2.18}$$

Chapter 3

Numerical Results

In this chapter, the algorithm presented in Chapter 2 is illustrated on the linear advection equation and the Burger's equation and the results obtained from them are discussed.

3.1 Linear Advection Equation

The linear advection equation along with the initial and boundary conditions is given by:

$$\begin{cases} u_t + a u_x = 0 \quad \text{in } [0,T] \times \Omega \\ u \mid_{t=0} = u_0 \\ u \text{ is periodic} \end{cases} \tag{3.1}$$

The parameters of this problem are: $\mu = (u_0, a)$. The parameter domain $\mathscr{C}$ is chosen such that the problem is convection dominated in order to have a solution manifold with a large Kolmogorov n-width. Figure 3.1 shows solution snapshots $\{u(\cdot, t^k; \mu), k \in 1 \ldots K\}$ of (3.1) for some value of parameters.

Now for performing the offline stage, going by the basic expertise on the linear advection equation, only the initial mode u_0 is considered as u_i and in that case, the solution snapshots of (3.1) can be written in the form of (2.4) as:

$$u^n := u_0(x + \Gamma_0^n) \tag{3.2}$$

Here, the coefficient α_0 has been taken equal to 1 since we have only one mode u_0.

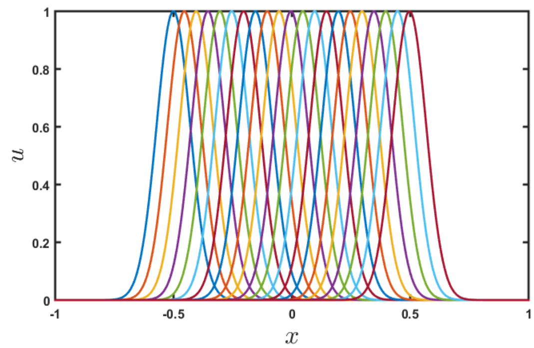

Figure 3.1: Snapshots of the solution to linear advection equation with a sharp Gaussian pulse as $u_0 = \exp[\frac{(-x+0.5)^2}{0.01}]$ and $a = 1$

Following the strategy described in chapter 2 for solving (2.5), a minimization problem of the form (3.3) is solved to obtain the grid distortion functions Γ_0^n which are shown in Figure 3.2 (left).

$$\Gamma_0^n = \underset{\Gamma_0}{\operatorname{argmin}} \|u^n - u_0(x + \Gamma_0)\| \tag{3.3}$$

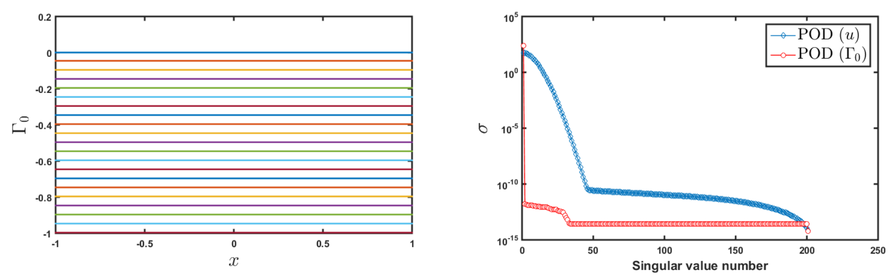

Figure 3.2: Grid distortion functions Γ_0 obtained from the offline phase for the linear advection equation (left). Singular values σ of the POD decomposition of the solution snapshots u (in blue) and of the grid distortion functions Γ_0 (in red) (right).

For the considered example, a very slow decay of the singular values of the POD decomposition of the solution snapshots is observed (cf. Figure 3.2 (right)). This means that many POD modes are required for a good representation of the solution manifold even though it is known that a single mode, namely the transported initial mode is enough for this purpose. However, from the same figure it is seen that the POD singular values of the grid distortion functions Γ_0 have a rapid decay and indeed, only one POD mode (say γ_0) is sufficient enough to represent the space of these functions and hence the entire solution manifold.

After obtaining the mode γ_0 from the offline phase, next the online stage is performed. The solution $u(\cdot, t^{n+1}; \mu)$ to (2.1) at time t^{n+1} can be expressed as:

$$u^{n+1} := u_0(x + d_0^{n+1}\gamma_0) \tag{3.4}$$

The reduced basis coefficients d_0^{n+1} are obtained by solving the minimization problem (3.5) following the strategy presented in chapter 2 for solving (2.14).

$$d_0^{n+1} = \underset{d_0}{\operatorname{argmin}} \|u_0(x + d_0\gamma_0) - u^n + dtau_x^n\| \tag{3.5}$$

Figure 3.3 depicts the solutions obtained using the full order model and the reduced model presented here, which shows a good match between the two indicating that the current method works properly for the case of linear advection equation.

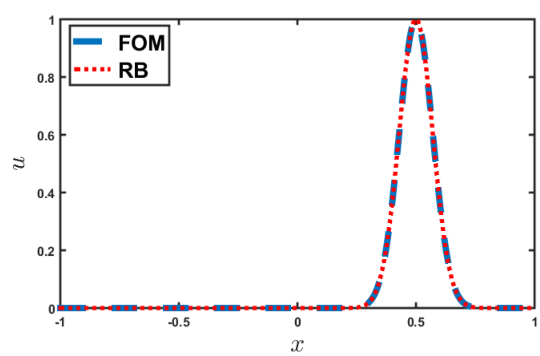

Figure 3.3: Snapshot of the solution to linear advection equation at time $t = 1s$. The FOM solution is given in blue and the reconstructed RB solution in red.

3.2 Burger's Equation with steady shock

The burger's equation along with the initial and boundary conditions is given by:

$$\begin{cases} u_t + uu_x = 0 \quad \text{in } [0,T] \times \Omega \\ u \mid_{t=0} = u_0 \\ u \text{ is periodic} \end{cases} \tag{3.6}$$

The solution snapshots u^n to (3.6) are shown in Figure 3.4. In the reduced form, they are represented in terms of the reference modes u_0 (initial mode) and u_1 (final mode) and the respective grid distortion functions Γ_0 and Γ_1 as :

$$u^n := \alpha_0 u_0(x + \Gamma_0^n) + \alpha_1 u_1(x + \Gamma_1^n) \tag{3.7}$$

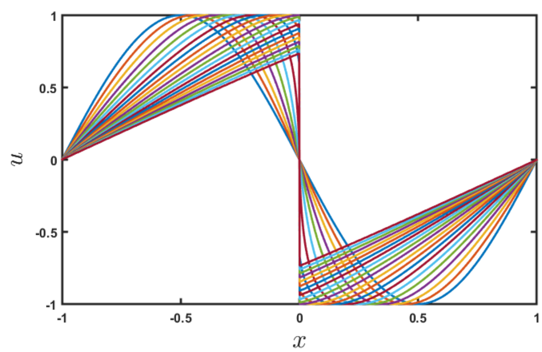

Figure 3.4: Snapshots of the solution to Burger's equation with $u_0 = -\sin(\pi x)$

The functions Γ_0^n and Γ_1^n are obtained by solving a minimization problem as before and are shown in Figure 3.5. In Figure 3.6, the singular values obtained from the POD decompositions of solution modes u^n and of the grid distortion functions Γ_0^n and Γ_1^n are depicted. It is noticed that the decay in the singular values for the solution modes are faster and hence the normal POD would perform better in finding a low rank representation of the solution manifold for the case of Burger's equation as compared to the method presented in this current work.

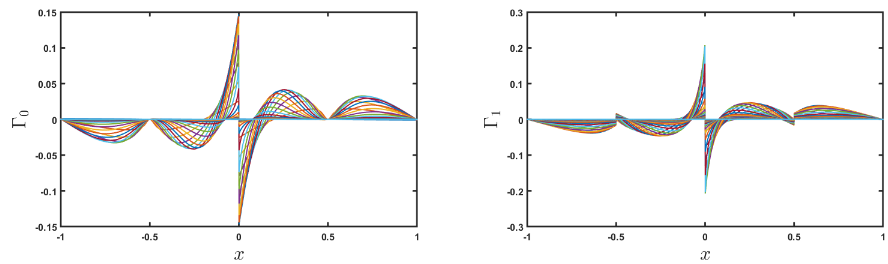

Figure 3.5: Grid distortion functions Γ_0 and Γ_1

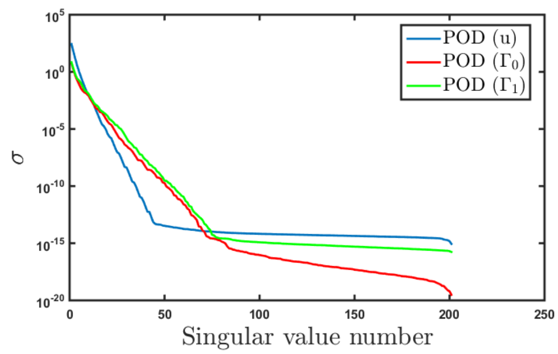

Figure 3.6: Singular values of the POD decomposition of solution snapshots u (in blue) and of the grid distortion functions Γ_0 (in red) and Γ_1 (in green)

The current method can be made to perform better for the case of Burger's equation by considering more number of modes as u_i rather than just the two (u_0 and u_1) as was done here. In that case, a faster decay in the singular values for the grid distortion functions are expected to be observed.

Chapter 4

Conclusion

In this seminar report, an introduction to the theory of reduced order modelling (ROM) for transport problems along with a summary of the related works existing in literature is first given. Next, a novel method for applying ROM to the case of transport problems based on a grid transformation/distortion strategy has been presented, followed by illustrations of the method on the linear advection and the Burger's equations. While the method is seen to perform well in case of the former, it still needs to be improved in order to make it work properly for the latter. As stated previously, one can consider including more number of reference modes u_i (instead of just two) for the representation in the reduced basis form.

However, a definite strategy for selecting the modes u_i based on a greedy procedure needs to be first identified which would be an interesting extension of the current work. While considering the case of Burger's equation with moving shock, it was noticed that the drift in the solution space gets inherited into the space of grid distortion functions, thereby creating an obstacle on the way of finding a low order representation of such functions. To overcome that, one may consider solving the optimization problems encountered in a constrained manner so that the drifts are mainly captured by the reference modes u_i while the distortion functions Γ_i are as stationary as possible, thereby rendering a low rank representation of the latter.

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