Abstract

Fluid flow in the transonic regime finds relevance in aerospace engineering, particularly in the design of commercial air transportation vehicles. Computational fluid dynamics models of transonic flow for aerospace applications are computationally expensive to solve due to high degrees of freedom as well as the coupled nature of the conservation laws. While this poses a bottleneck for the use of such models in aerospace design, computational costs can be significantly minimized by constructing special, structure-preserving surrogate models called reduced order models. However, such models are known to incur huge off-line costs which can sometimes outweigh their potential benefits. Furthermore, their prediction accuracy is known to be poor under transonic flow conditions. In this work, we propose a machine learning method to construct reduced order models via deep neural networks. Application to the inviscid transonic flow past the RAE2822 airfoil under varying freestream Mach numbers and angles of attack show that the proposed approach adapts to parameter variation very well. Notably, the proposed framework precludes knowledge of numerical operators utilized in the data generation phase. Furthermore, the proposed approach incurs significantly lower offline costs compared to existing approaches while still producing comparable accuracy.

1 Introduction

Projection based model order reduction is a structure-preserving technique to develop computationally cheap but accurate surrogate models of systems of partial differential equations (PDEs) and have seen widespread interest in the recent years due to the promise they have shown in efficient compression of spatio-temporal dynamics for a variety of systems [1][2][3][4]. As such, this field finds extensive application in control [5], multi-fidelity optimization [6] and uncertainty quantification [7][8] among others. We direct the interested reader to [9] for an excellent review on the recent advances and opportunities in ROMs. Such reduced order models (ROMs) are derived via reducing the dimensionality
of the full order model (FOM) which are the PDEs in their discrete or semi-discrete form. The dimensionality reduction is mainly achieved via a projection step where the FOM is projected onto a suitably chosen test basis set. The proper orthogonal decomposition (POD) \[10\] is a suitable choice to extract such bases, specifically for PDEs governing fluid flow due to its physical interpretability. Such models are referred to as POD-ROM in this work. Furthermore, the state space dimension of the PDE is directly reduced via POD by expressing the FOM state as a linear expansion of the POD modes.

To illustrate the mechanics of a POD-ROM, consider a state variable \( u \in \mathbb{R}^n \) which is the numerical solution of a PDE on a computational mesh of size \( n \). Then the POD-ROM approximates \( u \) as the linear expansion on a finite number of \( k \) orthonormal basis vectors \( \phi_i \in \mathbb{R}^n \). That is,

\[
    u \approx \sum_{i=1}^{k} \tilde{u}_i \phi_i, \tag{1}
\]

where, \( \tilde{u}_i \in \mathbb{R} \) is the \( i \)th component of \( \tilde{u} \in \mathbb{R}^k \), which are the coefficients of the basis expansion, also known as the reduced state and the \( \{ \phi_i \}, \phi_i \in \mathbb{R}^n \) are also called as POD modes. It can be shown that \[10, 11\] the POD modes in the above equation are the same as the left singular vectors of the snapshot matrix (obtained by stacking \( m \) snapshots of \( u \)), \( \mathbf{U} = [u_1, \ldots, u_m] \), extracted by performing a singular value decomposition (SVD) on \( \mathbf{U} \). That is,

\[
    \mathbf{U} = \Phi \mathbf{D} \Psi^\top \tag{2}
\]

where, \( \Phi \in \mathbb{R}^{n \times m} \) and \( \Phi_k \) represents the first \( k \) columns of \( \Phi \) after truncating the last \( m - k \) columns based on the relative magnitudes of the cumulative sum of their singular values. The \( L_2 \) error in approximation of the state variables due to the POD basis expansion is then given as

\[
    \sum_{j=1}^{m} \|u_j - (\Phi_k \Phi_k^\top)u_j\|_2^2 = \sum_{i=k+1}^{m} d_i^2 \tag{3}
\]

where \( d_i \) is the singular value corresponding to the \( i \)th column of \( \Phi \) and is also the \( i \)th diagonal element of \( \mathbf{D} \).

In the case of dynamical systems, the reduced state \( \tilde{u} \) is assumed to be a function of time with the POD basis set fixed in the time domain. In this work however, we consider static-parametric systems, in which case, the \( \tilde{u} \) is assumed to be a function of the parameters while the POD basis set is globally fixed across the parameter domain. Therefore, the POD-ROM reduces the unknowns \( u \) of the FOM to the \( \tilde{u} \) in the ROM, which is significantly cheaper to solve. A fundamental challenge arises when the FOM is available as a simulation code (black-box). In such a situation, the full-order system matrices are not available for the projection step. To overcome this, \[12\] showed that the system matrices can be constructed via a linearization assumption based on Koopman theory \[13\] following which projection-based model reduction proceeds in the traditional fashion. One of the primary limitations observed with the aforementioned approach is that in the transonic regime when the flow encounters sharp gradients due to shocks, the prediction accuracy suffers unless a densely populated training dataset is used. Moreover, such a limitation is typical of any projection-based framework and the typical workaround is to isolate the regions of the shock via domain decomposition and solve the FOM in this region (see \[14\] and \[15\]); although such approaches are intrusive and do not apply to simulation codes which is the scope of our work. The second limitation is that such an approach incurs a significant offline cost towards the construction of the reduced operators which is exacerbated with more snapshots. While the offline cost is inevitable in any projection-based approach, additional price must be paid when the FOM is available as a simulation code, particularly for parametric systems (for further details also see \[16\]).

In this work, we hypothesize that with an approach that circumvents the projection-based solution altogether, the heavy offline costs associated with projection-based ROMs can be significantly reduced. Furthermore, by leveraging state of the art machine learning models that can learn highly nonlinear embeddings from data, a potentially cheap-but-accurate surrogate model can be constructed for complex fluid flow in the transonic regime. In this regard, this work focuses on specifically the use of deep neural networks (DNNs) to approximate \( u \) in the parameter space for static-parametric POD-ROMs. Furthermore, we compare the DNN-based approach to the projection-based approach in \[12\] as a means to evaluate the effectiveness of our approach.

The rest of the article is organized as follows. The problem setup is discussed in section\[2\] the proposed DNN-based approach and the results are presented in section\[3\]. The paper concludes with a summary of the key findings and some directions for future work.
Table 1: Ambient flight conditions

| $P_\infty$ | 28,745 Pa |
| $\rho_\infty$ | 0.44 kg/m$^3$ |
| $a_\infty$ | 301.86 m/s |

## 2 Problem setup

### 2.1 Compressible Euler equations

The Euler equation governing the two-dimensional, compressible, inviscid flow past an airfoil is the chosen FOM on which we perform model reduction. The equation in conservation form is given in Eq. (4) below,

$$\nabla_x F + \nabla_y G = 0$$

where

$$F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho w \\ \rho u H \end{bmatrix}, \quad G = \begin{bmatrix} \rho v \\ \rho w \\ \rho v^2 + p \\ \rho v H \end{bmatrix}$$

$$H = E + \frac{p}{\rho}$$

$$\rho E = \frac{1}{2} \rho (u^2 + v^2) + \frac{p}{\gamma - 1}.$$ 

$\rho$, $u$, $v$, $p$ are the primitive variables namely the density, velocity components and pressure respectively, $H$ is the enthalpy, $E$ is the internal energy and $\gamma$ is the ratio of specific heats. Furthermore, $\nabla_x$ and $\nabla_y$ are the $x$ and $y$ components of the gradient operator $\nabla$ respectively. The farfield ($\infty$) boundary conditions are specified with a flow direction, the Mach number ($Ma$), static pressure ($p$) and static temperature ($T$). The free-stream boundary values on the boundary face of the computational domain are computed based on extrapolation of Riemann invariants under the assumption of irrotational, quasi-1D flow in the boundary-normal direction. The airfoil surface is modeled as an adiabatic, slip wall where all the primitive and thermodynamic variables are extrapolated from the interior domain via reconstruction gradients. The numerical solution to the nonlinear system is obtained with a coupled implicit finite volume based solver with 2nd order spatial discretization. The gradients are computed with the Hybrid-Gauss-Least-Squares method and the Venkatakrishnan limiter [17]. All the FOM snapshots are obtained via the commercial black-box CFD solver Star-CCM+.

### 2.2 The RAE2822 airfoil

The RAE2822 is a commonly used canonical test case for aerospace engineering problems under transonic flight conditions which is also used in this work. A spherical domain of 100 airfoil chord length radius is used to model the fluid domain which is meshed with 27857 polyhedral mesh elements with near-field refinement to capture the shock (see Figure 1). The ambient flight conditions are summarized in Table 1. In this work, our quantity of interest is the normalized pressure, also known as the coefficient of pressure ($C_p$) which is defined as

$$C_p = \frac{p - p_\infty}{\frac{1}{2} \rho_\infty (Ma_\infty \times a_\infty)^2}$$

which follows from the fact that this is a two-dimensional simulation and the chord length is set to unity.

The free-stream Mach number ($Ma$) and the flow incidence angle or angle of attack $\alpha$ are the chosen parameters. Therefore, a database of solution snapshots ($C_p$ distributions) are generated by solving a predetermined set of combinations of ($Ma$, $\alpha$) within a specified range which we set as $0.8 \leq Ma \leq 0.9$ and $0 \leq \alpha \leq 2$. A total of $m = 90$ such points are generated via a space-filling design of experiments namely the Latin Hypercube design [18].

## 3 Machine learning enabled model order reduction

In the recent past, there have been several studies into the integration of machine learning techniques within the projection-based ROM methodology. These have generally focused on improving the capture of transient dynamics
within the reduced space spanned by the POD bases [19, 20, 21] or on determining projections where advective dynamics may be captured more confidently [22, 23, 24] among others. In this article, we introduce a machine learning framework to predict the coefficients (the reduced state) of the POD modes obtained from our simulation database where all snapshots generated for the purpose of reduced-basis identification are at steady state. We remind the reader that the POD modes were obtained using the training dataset (corresponding to 80 simulations only). We outline a learning task which seeks to learn a map between inputs given by our control parameters θ and Ma and our outputs given by the coefficients of these POD modes. Therefore our training data set consists of coefficients obtained by projecting the training snapshots at steady-state for a variety of control parameters onto their global POD modes. For capturing approximately 97% of the total variance in the pressure fields, we retain 16 POD modes for the pressure snapshots. The eigenvalue-variance decay plot is shown on the left in Figure 2. To train this map, we utilize a fully-connected feed-forward neural network composed of six hidden layers and 50 neurons in each layer. Our training is performed using the Adam optimizer ([25]) with a learning rate of 0.001 and our batch size is 40 samples. The progress to convergence for the framework on the training data is shown on the right in Figure 2.

A first validation of the proposed framework is performed through the use of 5-fold cross-validation which provides a more trustworthy estimate of the test accuracy of the proposed model. Our average coefficient of determination for this cross-validation was around 0.94. This indicated that the proposed framework was performing in the expected manner and not due to a fortuitous selection of training snapshots. We further validate the training of our framework through quantitative assessments on the testing dataset as shown through the comparison of POD coefficient values. Predictions for four of these coefficients are shown in Figure 3. The proposed framework is seen to perform quite accurately. We also perform statistical assessments on the predicted snapshots obtained by reconstructing the field using the predicted POD coefficients. These are shown in Figure 4, which demonstrate that the distribution of the true field is recovered accurately. A scatter plot is also shown which shows that the vast majority of predicted values of the absolute pressure lie close to their true values. We remind the reader that all these assessments are performed for snapshots that the learning framework has not seen previously.

Finally, we assess C_p profiles for the testing dataset using the snapshots predicted by the proposed framework. These are shown, for all the testing dataset, in Figure 5. The plots compare the predictions of the proposed DNN-based approach against that of [12] as well as the FOM solution. The proposed approach clearly adapts well to parametric variation as demonstrated by how well it captures the location and strength of the shock. Particularly at the flight conditions in Figures 5h and 5j, it marginally outperforms the projection-based approach. Finally, the proposed approach incurs only a small fraction of the offline cost involved in the projection-based approach as mentioned before. This shows great promise with the scalability of the proposed approach when the inputs are high dimensional.
4 Conclusion

Projection-based POD-ROMs are known to be limited in accuracy when the FOM contains parameter-dependent discontinuities or sharp gradients. This has been a particularly limiting factor in their successful application towards transonic wing/airfoil design in aerospace engineering. This work proposes a machine learning-based approach based on deep neural networks to firstly circumvent the expensive projection step and secondly learn the nonlinear parameter dependence of the shock. Upon application of the proposed approach on the flow past the RAE2822 airfoil under inviscid transonic flight conditions, it is observed that the proposed approach performs on par with the projection-based approach while marginally outperforming it in a select few cases. Future directions in this work includes evaluation of the proposed approach with high dimensional inputs and eventual incorporation into aerodynamic optimization workflows.

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Figure 3: The prediction ability of the trained framework for the testing dataset. The panels show the ability to predict different POD coefficients of this dataset unseen during training.
Figure 4: The prediction ability of the trained framework for one snapshot of the testing dataset. The left panel shows the distribution of the true and predicted values of the absolute pressure while the right panel shows the scatter between true and predicted values.

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Figure 5: Comparison of the proposed DNN-based method predictions against other approaches

(a) $Ma = 0.887$, $\alpha = 0.944$
(b) $Ma = 0.816$, $\alpha = 1.011$
(c) $Ma = 0.866$, $\alpha = 1.146$
(d) $Ma = 0.823$, $\alpha = 0.899$
(e) $Ma = 0.853$, $\alpha = 1.798$
(f) $Ma = 0.839$, $\alpha = 0.854$
(g) $Ma = 0.829$, $\alpha = 1.708$
(h) $Ma = 0.862$, $\alpha = 1.483$
(i) $Ma = 0.817$, $\alpha = 0.270$
(j) $Ma = 0.884$, $\alpha = 1.348$
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