Bachelorarbeit
zur Erlangung des akademischen Grades
Bachelor of Science

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Contents

1 Introduction

The Bhatnagar, Gross, Krook equation (BGK) is a kinetic collision model of ionized and neutral gases valid for rarefied as well as other pressure regimes [1]. Generating data of such a flow field is essential for various industry and scientific applications[**REF**]. With the intention to reduce time and cost during the data generating process, experiments were substituted with computational fluid dynamics (CFD) computations. Consequently reduced-order models (ROMs) coupled to aforementioned computations were introduced to further the reduction of time and cost. The thriving field of artificial intelligence operates in model order reduction for data visualization/analysis since the 80's (Quelle?) and has now surfaced in fluid mechanics. This thesis will cover the use of artificial intelligence for model order reduction in fluid mechanics.

1.1 State of the art

State of the art model reduction of dynamical systems is done via proper orthogonal decomposition (POD) which is an algorithm feeding on the idea of singular value decomposition (SVD)[2][3]. POD captures a low-rank representation on a linear manifold. So called POD modes, derived from SVD, describe the principle components of a problem which can be coupled within a Galerkin framework to produce an approximation of lower rank.

$$f(x) \approx \tilde{f}(x) \qquad \text{with} \qquad rk(f(x)) \gg rk(\tilde{f}(x)) \tag{1}$$

Bernard et al. use POD-Galerkin with an additional population of their snapshot database via optimal transport for the proposed BGK equation, bisecting computational run time (cost) in conjunction with an approximation error of 1 % [4]. Artificial intelligence in the form of autoencoders replacing the POD within a Galerkin framework is evaluated against the POD performance by Kookjin et al. for advection-dominated problems[5] resulting in sub 0.1% errors. An additional time inter- and extrapolation is evaluated. Using machine learning/ deep learning for reduced order modeling in CFD is a novel approach although "the idea of autoencoders has been part of the historical landscape of neural networks for decades"[6, p.493]. Autoencoders, or more precisely learning internal representations by the delta rule (backpropagation) and the use of hidden units in a feed forward neural network architecture, premiered by Rumelhart et al. (1986) [7]. Through so called hierarchical training Ballard et al.(1987) introduce a strategy to train auto autoassociative networks (nowadays referred to as autoencoders), in a reasonable time promoting further development despite computational limitations [8]. The so called bottleneck of autoencoders yields a non-smooth and entangled representation thus beeing uninterpretable by practitioners[9] leading to developements in this field. Rifai et al. introduce the contractive autoencoder (CAE) for classification tasks (2011), with the aim to extract robust features which are insensitive to input variations orthogonal to the low-dimensional non-linear manifold by adding a penalty on the frobenius norm of the instrinsic variables with respect to the input, surpassing other classification algorithms [9]. Subsequent development emerges with the manifold tangent classifier (MTC) [10]. A local chart for each datapoint is obtained hence characterizing the manifold which in turn improves classification performance. On that basis a generative process for the CAE is developed. Through movements along the manifold with directions defined by the Jacobian of the bottleneck layer with respect to the input $\vec{x}_m = JJ^T$, sampling is realized [11].

1.2 Objective of this thesis

Due to the non-linearity of transport problems in particular shock fronts, the construction of a robust ROM for those cases poses several challenges. Proper orthogonal decomposition (POD) and it's numerous variants like shifted-POD[?], POD-Galerkin[?], POD+I [?] to name only a few of them, try to solve this problem by......

1.3 Thesis outline

2 The BGK Equation

3 Reduced Order Algorithms

3.1 Data Sampling

3.2 POD

The singular value decomposition of the input X [REF to Section 1] gives the optimal low-rank approximation $\tilde{X}$ of X eq. (3)[Eckard-Young]. Figure 1 shows the singular values (left) and the cumulative energy (right) derived from eq. (2):

$$S_N = \sum_{k=1}^{N} a_k \qquad \text{with a sequence} \qquad \{a_k\}_{k=1}^{n} \tag{2}$$

$$\underset{\tilde{X}, s.t. rank(\tilde{X})=r}{\operatorname{argmin}} \quad ||X - \tilde{X}||_F = \tilde{U}\tilde{\Sigma}\tilde{V}^* \tag{3}$$

The first five singular values give an accurate approximation $\tilde{X}$ of X. As a means to evaluate the low-rank approximation of X we will compare the density derived from **??**, computed from X and $\tilde{X}$.

3.3 Autoencoders

The same matrix as in POD is used as input data for the autoencoder:

$$S = \begin{bmatrix} f(\xi_1, t_1, x_1) & \cdots & f(\xi_n, t_1, x_1) \\ f(\xi_1, t_1, x_2) & \cdots & f(\xi_n, t_1, x_2) \\ f(\xi_1, t_1, x_n) & \cdots & f(\xi_n, t_1, x_n) \\ f(\xi_1, t_2, x_1) & \cdots & f(\xi_n, t_2, x_1) \\ \vdots & \ddots & \vdots \\ f(\xi_1, t_n, x_n) & \cdots & f(\xi_n, t_n, x_n) \end{bmatrix}$$

During training every 1000 epochs a sample against its prediction was printed in order to link the value of the L1-Loss to a prediction. Using this method a first verification of

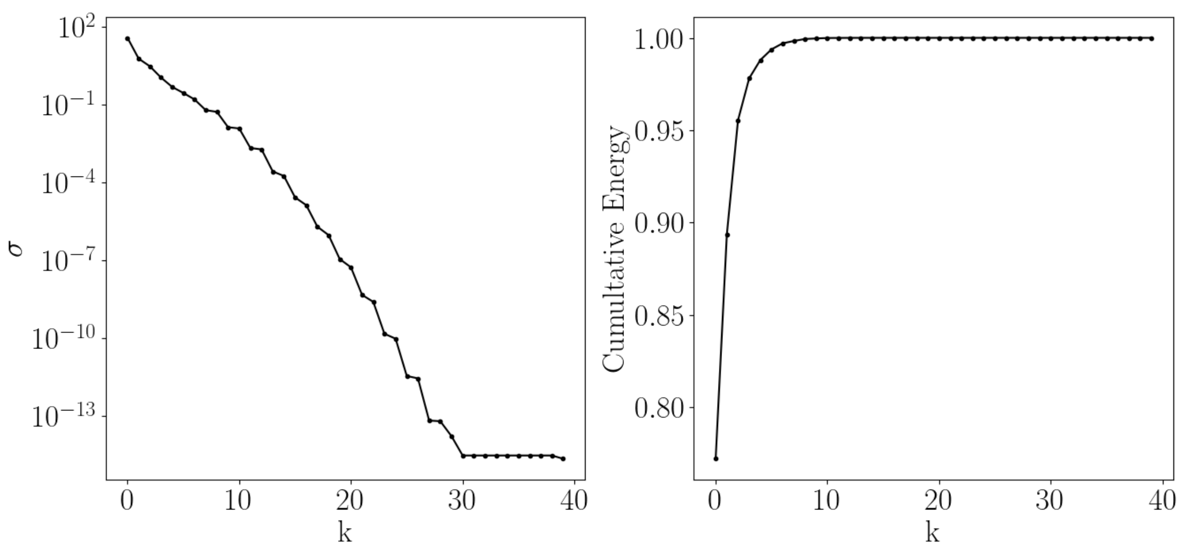

Figure 1: Singular Values (left) and cumultative enrgy (right) over the number of singular values

the model was achieved. Continuing the search for any possible shortage of the models performance, that this method could not cover, eg. samples lying between every 1000 sample, that the model was not able to reconstruct correctly, a second verification process is conducted.

4 Results and Latent Manifold Properties

4.1 Evaluation Methods

4.2 Results

The search for a reduced model of the BGK equation yields a first reduction and analysis of the provided data with a low Knudsen number of $Kn = 0.00001$. For this flow field the Navier Stokes equations are still valid. Analysing the batch size for the architecture 1.0 the test errors in table 1 can be produced. For the evaluation of the prediction the

Architecture	1.0
Batch Size	L2-Error
64	0.008
32	0.0049
16	0.0038
8	0.0037
4	0.0026
2	0.0021

Table 1: L2-Error over Batch-Size

Autoencoder produces normalized conservative quantities are analysed. The conservative quantities are the total energy E, the density ρ and the impulse ρu. Normalization is done over the temporal mean as seen in eq. (4a) to eq. (4c).

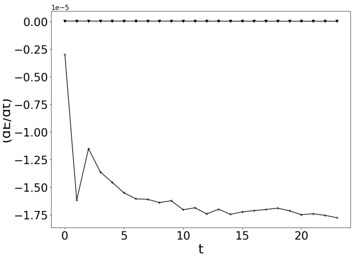

Figure 2: Normalized total change in Energy $\hat{E}$ over time

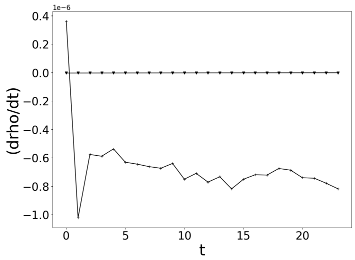

Figure 3: ormalized total change in Energy $\hat{\rho}$ over time

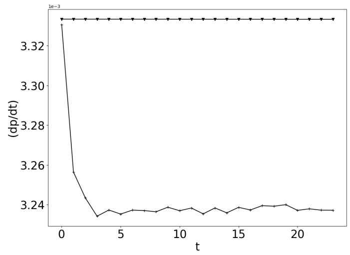

Figure 4: ormalized total change in Energy $\hat{p}$ over time

$$\frac{\frac{d}{dt}\int E\,dx}{\bar{E}} = 0 \qquad \text{with} \quad \bar{E} = \frac{\iint E\,dtdx}{\Delta t} \tag{4a}$$

$$\frac{\frac{d}{dt}\int \rho\,dx}{\bar{\rho}} = 0 \qquad \text{with} \quad \bar{\rho} = \frac{\iint \rho\,dtdx}{\Delta t} \tag{4b}$$

$$\frac{\frac{d}{dt}\int \rho u\,dx}{\bar{\rho u}} = 0 \qquad \text{with} \quad \bar{\rho u} = \frac{\iint \rho u\,dtdx}{\Delta t} \tag{4c}$$

4.3 Discussion and Outlook

References

[1] Bhatnagar, Gross, and Krook. A model for collision processes in gases. 1954.

[2] Thomas Franz. *Reduced-order modeling of steady transonic flows via manifold learning.* 2016.

[3] Steve L. Brunton and J. Nathan Kutz. *Data driven science and engineering.* 2019.

[4] Florian Bernard, Angelo Iollo, and Sebatian Riffaud. Reduced-order model for the bgk equation based on pod and optimal transport. 2018.

[5] Kookjin Lee and Kevin T. Carlberg. Model reduction of dynamical systems on nonlinear manifolds using deep convolutional autoencoders. 2019.

[6] Ian J. Goodfellow, Yoshua Bengio, and Aaron Courville. *Deep Learning.* MIT Press, Cambridge, MA, USA, 2016. `http://www.deeplearningbook.org`.

[7] D.E. Rumelhart, G.E. Hinton, and R.J. Williams. Learning internal representations by error propagation. 1986.

[8] Dana H. Ballard. Modular learning in neural networks. 1987.

[9] Salah Rifai, Pascal Vincent, Xavier Muller, Xavier Glorot, and Yoshua Bengio. Contractive auto-encoders: Explicit invariance during feature extraction. 2011.

[10] Salah Rifai, Yann N Dauphin, Pascal Vincent, Yoshua Bengio, and Xavier Muller. *The Manifold Tangent Classifier*. Curran Associates, Inc., 2011.

[11] Salah Rifai, Yoshua Bengio, Yann Dauphin, and Pascal Vincent. A generative process for sampling contractive auto-encoders, 2012.