Bachelorarbeit
zur Erlangung des akademischen Grades
Bachelor of Science

Zachary Schellin
376930

October 1, 2020

Contents

1 Introduction

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. (2)[Eckard-Young]. Figure 1 shows the singular

values (left) and the cumulative energy (right) derived from eq. (1):

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

$$\operatorname*{argmin}_{\tilde{X}, s.t. rank(\tilde{X})=r} ||X - \tilde{X}||_F = \tilde{U}\tilde{\Sigma}\tilde{V}^* \tag{2}$$

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 eq. (5), computed from X and $\tilde{X}$.
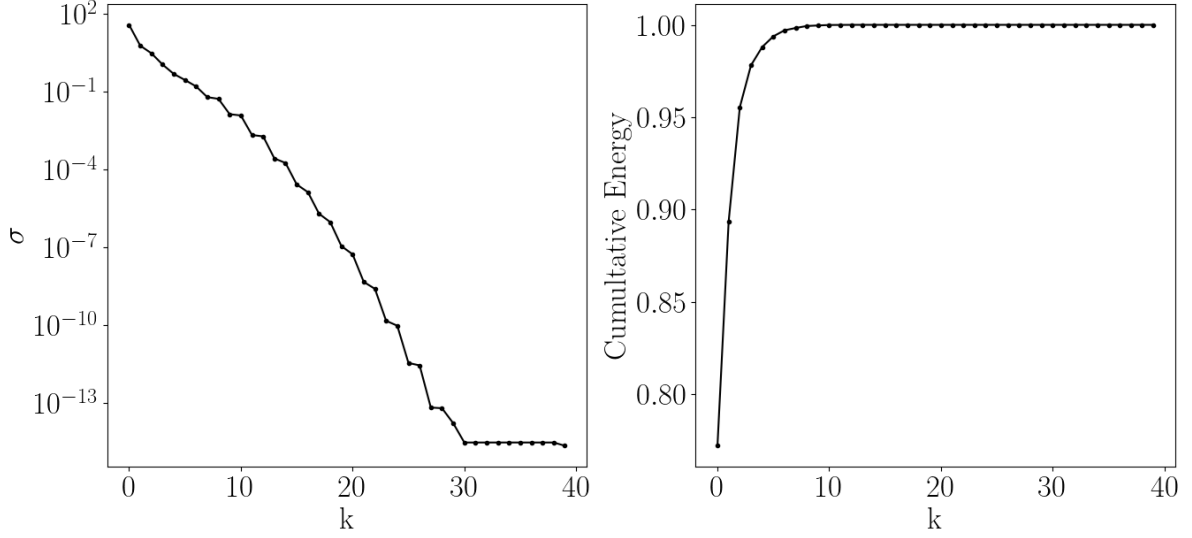

Figure 1: Singular Values (left) and cumultative enrgy (right) over the number of singular values

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 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.

2

4 Results and Latent Manifold Properties

4.1 Evaluation Methods

In oder to evaluate the proposed dimensionality reduction algorithms, two methods are being introduced. The first one constitutes a qualitative analysis using eq. (3) which measures the euclidian distance of every reconstructed sample $\tilde{X}_i$ against it's corresponding original sample X.

$$|X_i - \tilde{X}_i| = \delta_i \qquad \text{with i being the i}^{\text{th}} \text{ sample} \tag{3}$$

$$\sum |\rho_i - \tilde{\rho}_i| = \delta_\rho \qquad \text{with i being the i}^{\text{th}} \text{ sample} \tag{4}$$

As a second quantitative approach a comparison of the density over space in time of the BGK model in eq. (5) is utilized. The sum over all euclidian distances from the original samples ρ_i to their reconstruction $\tilde{\rho}_i$ is evaluated in eq. (4).

$$\int_{\Re^3} f(\mathbf{x}, \xi, t) \begin{pmatrix} 1 \\ \xi \\ \frac{\|\xi\|^2}{2} \end{pmatrix} d\xi = \begin{pmatrix} \rho(\mathbf{x}, t) \\ \rho(\mathbf{x}, t) U(\mathbf{x}, t) \\ E(\mathbf{x}, t) \end{pmatrix} \tag{5}$$

In order to evaluate the performance of the proposed dimensionality reduction algorithms, qualitative and quantitative methods are being introduced. The qualitative analysis comprises a comparision of the sample wise test error following eq. (3) on the microscopic data. The Jacobian of the latent code is strongly linked to this measure, as it measures the contraction of the latent manifold. A quantitative measure is taken on the average test error over all over all samples of the microscopic data as well as on the macroscopic data. Both can lead to different conclusions and will be discussed in Section 4.3.

4.2 Results

A quantitative measure shows, that the linear Autoencoder performs slightly better than the POD on the input data comparing the density of the original data against the reconstruction. In contrast to this measure, the comparison of the original data to the reconstruction yields the opposite conclusion.

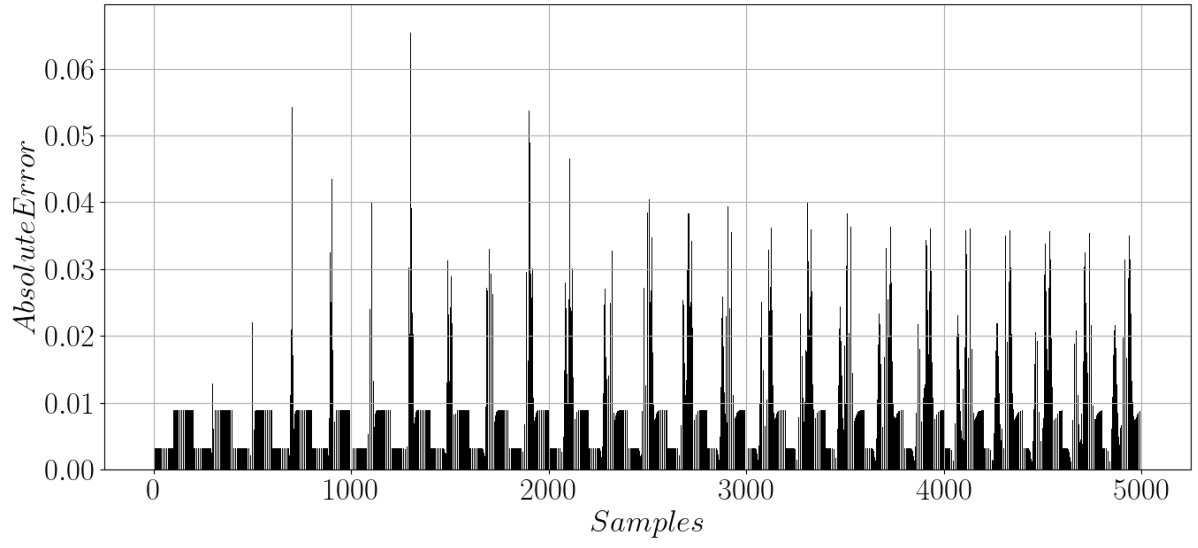| Algorithm	Euclidian distance in Density	Euclidian Distance	Jacobian
POD	0.151	0.0101	
AE	0.101	0.0102	
CAE 1	0.205	0.0106	
CAE 2	0.669	0.001	
CAE 2 + tw	0.385	0.0117	

4.3 Discussion and Outlook

Figure 2: Absolute error for every sample in euklidian distance for the POD
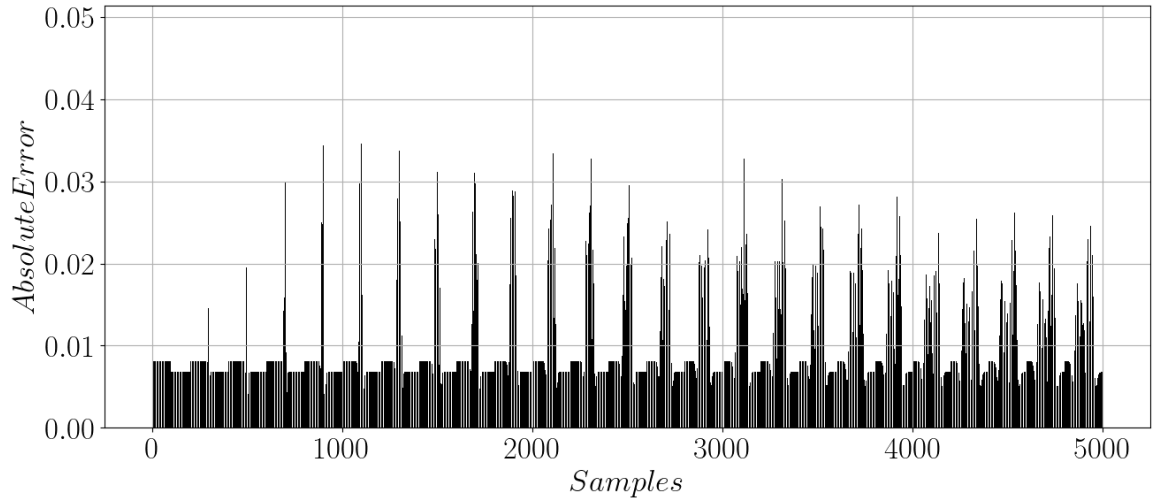

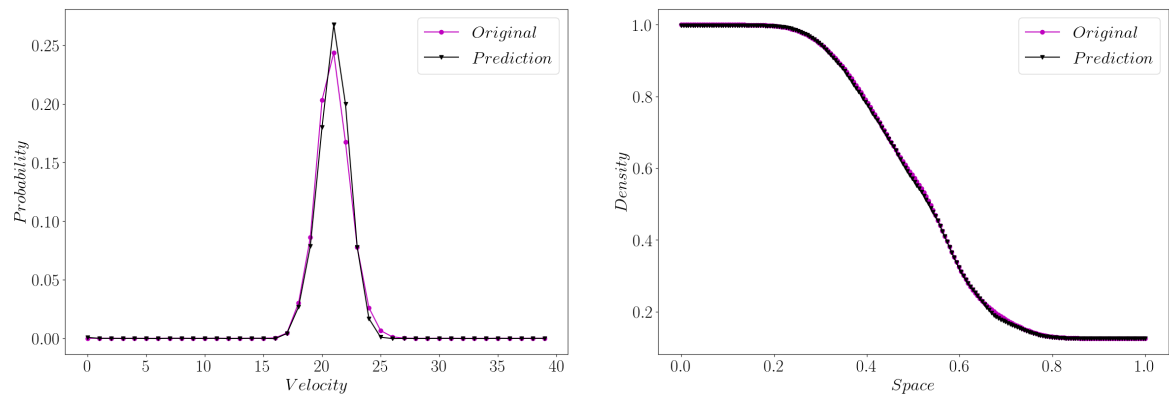Figure 3: Absolute error for every sample in euklidian distance for the linear autoencoder

4

Figure 4: Error of each sample