


Model Order Reduction of Rarefied Gases Using Neural Networks

Zachary Schellin | Institut für Numerische Fluiddynamik

Outline

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Governing equations

Boltzmann equation with the BGK operator

$$\underbrace{\partial_t f + v\partial_x f}_{\text{transport}} = \underbrace{\frac{1}{\tau}(M_f - f)}_{\text{collisions}} \quad (1)$$

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[1] Florian Bernard, Angelo Iollo, and Sebatian Riffaud. **Reduced-order model for the BGK equation based on POD and optimal transport**. 2018.

Governing equations

Boltzmann equation with the BGK operator

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Equilibrium solution: Maxwellian distribution $\boldsymbol{M_f}$

$$M_f = \frac{\rho(x,t)}{(2\pi RT(x,t))^{\frac{3}{2}}} \exp\left(-\frac{(v-u(x,t))^2}{2RT(x,t)}\right) \tag{2}$$

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Duration to evolve into equilibrium: relaxation time $\boldsymbol{\tau}$

$$\tau^{-1} = \frac{\rho(x,t)T^{1-\nu}(x,t)}{Kn} \tag{3}$$

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$$\tau^{-1} = \frac{\rho(x,t)T^{1-\nu}(x,t)}{Kn} \quad (3)$$

Rarefaction level: Knudsen number $\boldsymbol{Kn}$

$$Kn = \frac{\lambda}{l} \quad (4)$$

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Discretization in space and velocity space in 1D

- **Space and time discretization**:
  $x_j = j\Delta x$ and $j \in \mathbb{Z}$, $v_k = k\Delta v$ and $k \in \mathbb{Z}$, $t^i = i\Delta t$ and $t \in \mathbb{N}$,

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[2] Gabriella Puppo. "Kinetic models of BGK type and their numerical integration". In: (2019). arXiv: 1902.08311 [physics.comp-ph].

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- **Leads to:** set of ODE's in time

$$\partial_t f_{j,k} = -(v_k)_1 D_x f\big|_{j,k}(t) + \frac{1}{\tau}(M_{f\,j,k}(t) - f_{j,k}(t)). \tag{5}$$

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- **KJ first-order differential equations**:
  K gridpoints in space & J number of gridpoints in velocity space

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  $K^3 J^3$ first-order differential equations

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- **KJ first-order differential equations**:
  K gridpoints in space & J number of gridpoints in velocity space
- **3D**:
  $K^3 J^3$ first-order differential equations
- Solution is $\mathbf{f}(\mathbf{x}, \mathbf{v}, \mathbf{t})$ in 1D and $\mathbf{f}(\mathbf{x}, \mathbf{y}, \mathbf{v_x}, \mathbf{v_y}, \mathbf{t})$ in 2D and $\mathbf{f}(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{v_x}, \mathbf{v_y}, \mathbf{v_z}, \mathbf{t})$ in 3D

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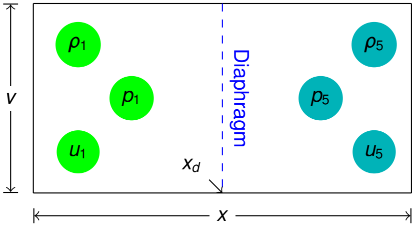
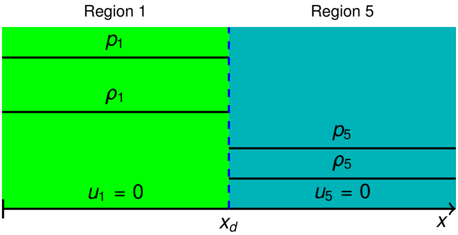


Figure: Problem setup of Sod's shock tube for the BGK model in 1D at $t = 0s$.

- **Idea**:
  - Solve problem analytically (Rankine-Hugoniot jump conditions)
  - Solve problem numerically
  - Compare results expecially **resolution of discontinuities**

Sod's shock tube



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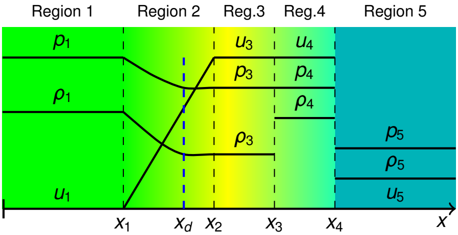

Figure: Problem setup of Sod's shock tube for the BGK model in 1D at $t > 0s$.

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[3] G. A. Sod. "Review. A Survey of Several Finite Difference Methods for Systems of Nonlinear Hyperbolic Conservation Laws". In: **Journal of Computational Physics** 27.1 (Apr. 1978), pp. 1–31. DOI: 10.1016/0021-9991(78)90023-2.

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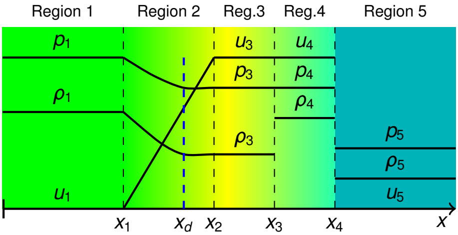

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  - » $\mathbf{x_1}$ head of rarefaction wave
  - » $\mathbf{x_2}$ tail of rarefaction wave

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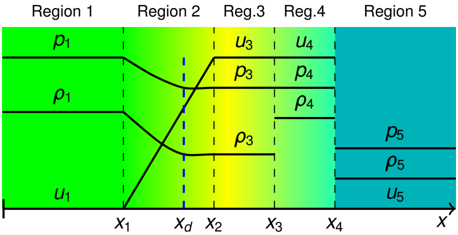

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  - » $\mathbf{x_3}$ contact discontinuity

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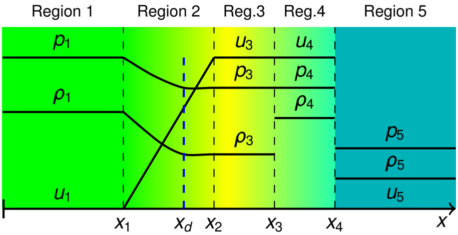

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  - » **x_1** head of rarefaction wave
  - » **x_2** tail of rarefaction wave
  - » **x_3** contact discontinuity
  - » **x_4** position of shockwave

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Two Case Studies

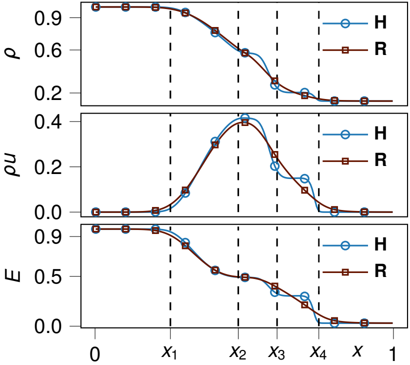
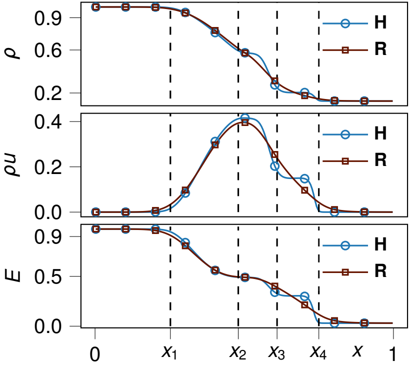


Figure: Moments of **H** and **R** at $t = 0.12s$ and $v = v_0$ in Sod's shock tube.

– Two solutions of the BGK model in Sod's shock tube

Two Case Studies



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- Two solutions of the BGK model in Sod's shock tube
- Two levels of rarefaction
  - **H**, Kn = 0.00001, "Continuum Flow"
  - **R**, Kn = 0.001, "Slip flow"

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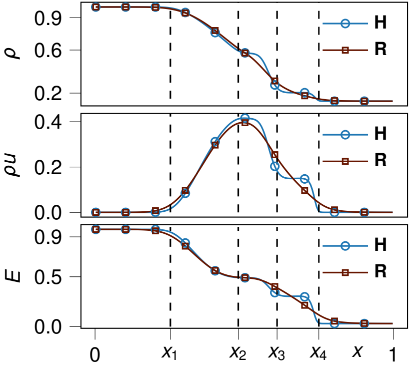

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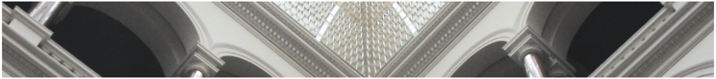
- Pronounced discontinuities

H

- x_1
- x_2
- x_3
- x_4

R

- x_1
- x_2
- x_3
- x_4



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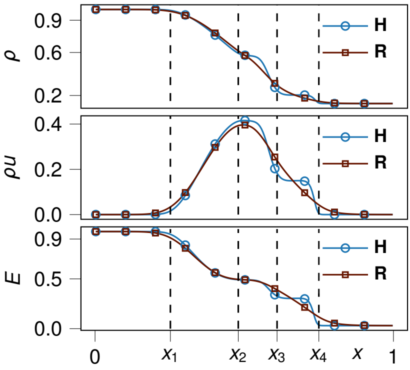

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H	**R**
x_1	x_1
x_2	x_2
x_3	x_3
x_4	x_4

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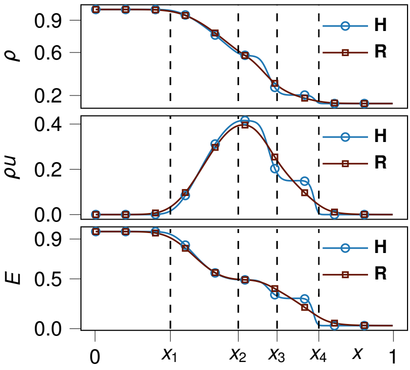

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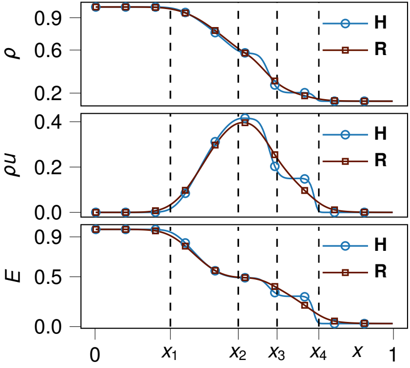
H	**R**
• x_1	• x_1
• x_2	• x_2
• x_3	• x_3
• x_4	• x_4

Two Case Studies



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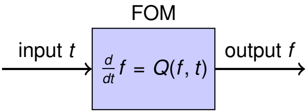
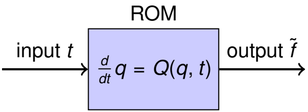
Model Order Reduction

– **Goal**: Reduce computational cost



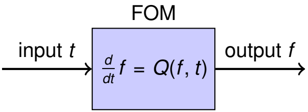
(a) Evolving the FOM in time.



(b) Evolving the ROM in time.

Figure: In the online phase the operator Q is different for the FOM and the ROM.

Model Order Reduction



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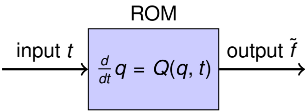
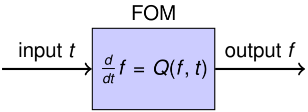


(b) Evolving the ROM in time.

Figure: In the online phase the operator Q is different for the FOM and the ROM.

- **Goal**: Reduce computational cost
  - $f(x, v, t)$ with KJ ODE's in time for 1D

Model Order Reduction



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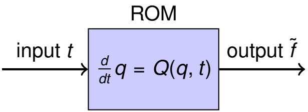

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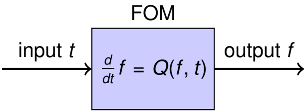

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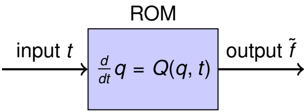

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  - Proper Orthogonal Decomposition **(POD)**
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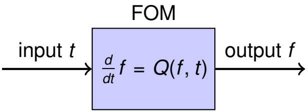
Model Order Reduction



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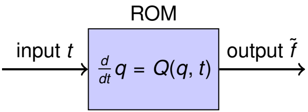

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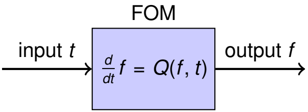
- **Require**: Solution of f (only few timesteps)

Model Order Reduction



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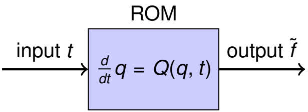

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- **Require**: Reduction algorithm
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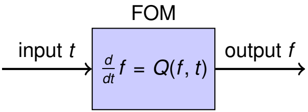
- **Require**: Solution of f (only few timesteps)
- **Reduce**: $POD(f(x, v, t)) = q(x, n, t)$

Model Order Reduction



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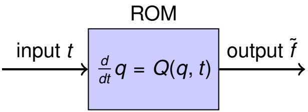

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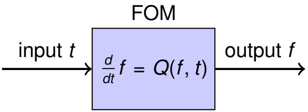
  - P is # n with $P << K$

Model Order Reduction



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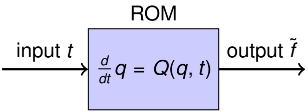

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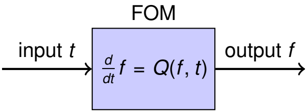
Model Order Reduction



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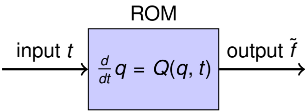

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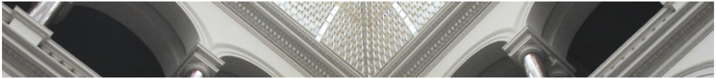
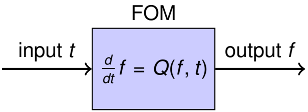
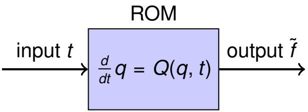
  - $f(x, v, t)$ with KJ ODE's in time for 1D
- **Require**: Reduction algorithm
  - Proper Orthogonal Decomposition **(POD)**
  - Neural Networks **(NN)**
- **Require**: Solution of f (only few timesteps)
- **Reduce**: $POD(f(x, v, t)) = q(x, n, t)$
  - P is # n with $P << K$
  - KJ ODE's vs. PJ ODE's
- **Evolve in time**: $\rightarrow Q(q, t) = \tilde{f}$



Model Order Reduction



(a) Evolving the FOM in time.



(b) Evolving the ROM in time.

Figure: In the online phase the operator Q is different for the FOM and the ROM.

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- **Evaluate mistake**: $f - \tilde{f} < \epsilon$

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Proper Orthogonal Decomposition

– Solution of a PDE is $f(x, v, t)$ can be obtained

Proper Orthogonal Decomposition

- Solution of a PDE is $f(x, v, t)$ can be obtained
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- Solution of a PDE is $f(x, v, t)$ can be obtained
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  - Separation of variables ansatz

Proper Orthogonal Decomposition

- Solution of a PDE is $f(x, v, t)$ can be obtained
  - Discretization into a system of ODE's
  - Separation of variables ansatz
    - » $f(t, v, x) = \sum_{i=1}^{n} \boxed{a_i(t)} \boxed{\Phi_i(x, v)}$ (6)

Proper Orthogonal Decomposition

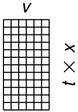
– How to get $\boxed{\Phi_i}$?

4

[4] Steve L. Brunton and J. Nathan Kutz. **Data driven science and engineering. Machine learning, dynamical systems and control**. Cambridge University Press, 2019.

Proper Orthogonal Decomposition

- How to get Φ_i?
  - **Preprocessing**: Separating the spatial and temporal axis of the solution $f(x, v, t)$

    » $X =$ 

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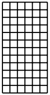
   » $X =$ 

- **Sigular Value Decomposition**: $X = \underbrace{U}_{\text{LSV}} \underbrace{\Sigma}_{\text{SV}} \underbrace{V^*}_{\text{RSV}}$ (6)

- **Truncation**: $\tilde{X} = \underbrace{\tilde{U}}_{\Phi} \tilde{\Sigma} \tilde{V}^*$ (7), $\tilde{U} = \Phi = [\Phi_1, \Phi_2, \dots, \Phi_p]$ (8)

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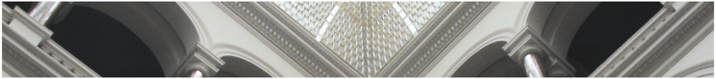

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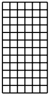
  » $X =$ 

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- **Truncation**: $\tilde{X} = \underbrace{\tilde{U}}_{\Phi}\tilde{\Sigma}\tilde{V}*$ (7), $\tilde{U} = \Phi = [\Phi_1, \Phi_2, \dots, \Phi_p]$ (8)
- **Eckard-Young Theorem**:

$$\underset{\tilde{X}, s.t. rank(\tilde{X})=p}{\operatorname{argmin}} \|X - \tilde{X}\|_F = \tilde{U}\tilde{\Sigma}\tilde{V}^* \qquad (9)$$

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Autoencoders

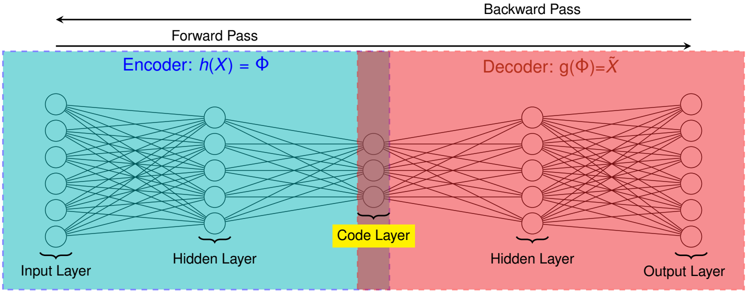
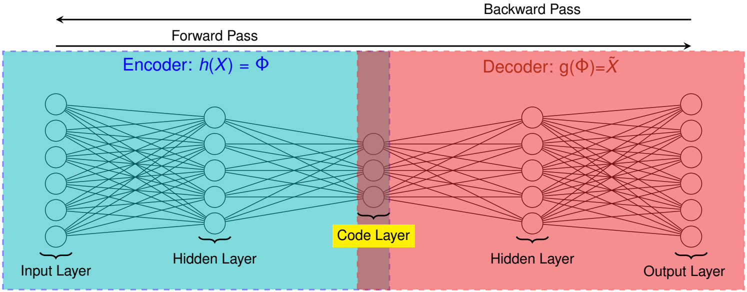


Figure: A fully connected autoencoder.

Autoencoders



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– **Structure**: Encoder & Decoder

Autoencoders

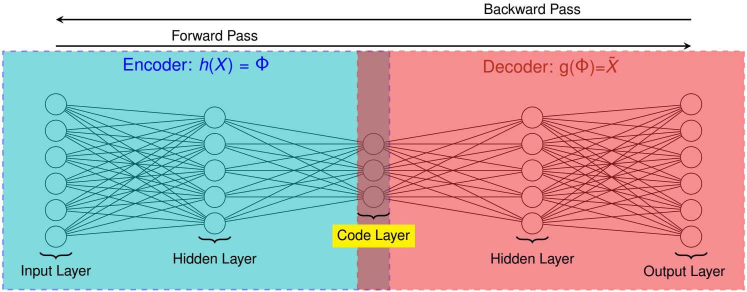
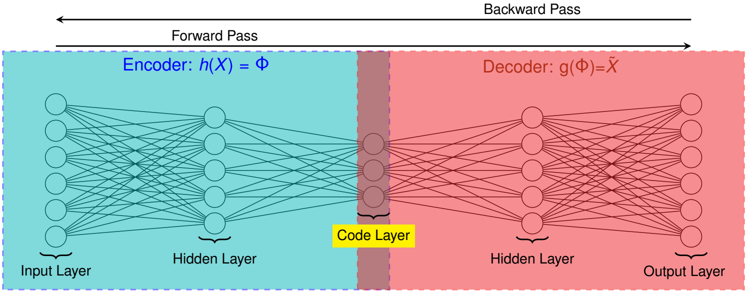


Figure: A fully connected autoencoder.

- **Structure**: Encoder & Decoder
- **Layers**: Input-, Output- **and** Code layer

Autoencoders



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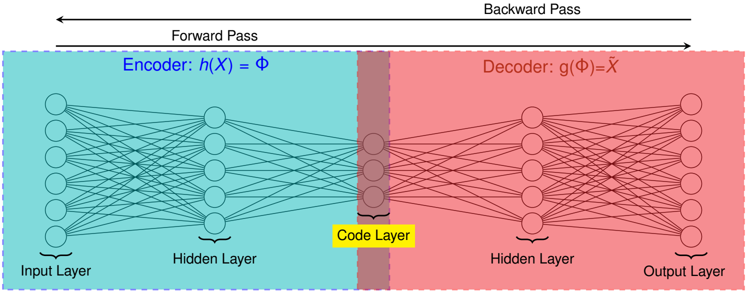
- **Compress** $\rightarrow$ Salient features $\rightarrow$ **Decompress** $\rightarrow$ Reconstruction

Autoencoders



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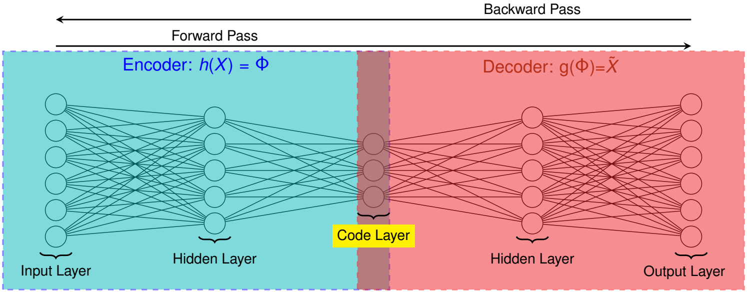

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- **Layers**: Input-, Output- **and** Code layer
- **Compress**$\rightarrow$ Salient features $\rightarrow$ **Decompress** $\rightarrow$ Reconstruction
- **Category**: Self-supervised learning
- **Main hyperparameters**: Number & size of hidden layers esp. size of code layer

Training

$$y \xrightarrow{g} z \xrightarrow{h} \tilde{y}$$

Figure: A very simple network

– Network with three layers

5

[5] Steve L. Brunton and J. Nathan Kutz. **Data driven science and engineering. Machine learning, dynamical systems and control**. Cambridge University Press, 2019.

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$$\tilde{y} = h(z, b) = h((g(y, a)), b) \qquad (10)$$

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– **Optimize**:

- $$a_{i+1} = a_i + \epsilon \frac{\partial E}{\partial a_i} \tag{14}$$
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- **Hyperparameter**: learning rate ϵ

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Concepts

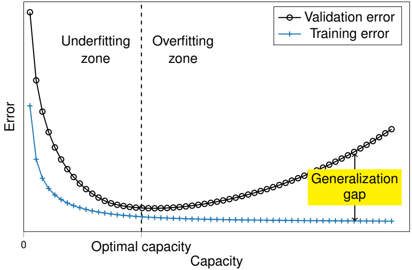

Figure: Influence of capacity

– **Over- and Underfitting**:

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

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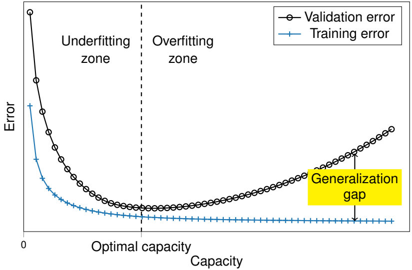

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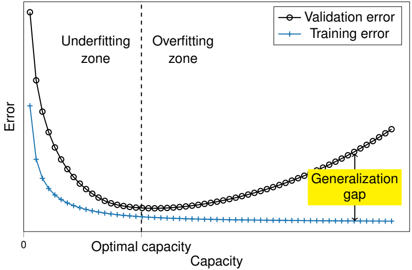

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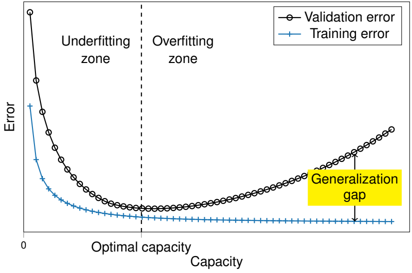

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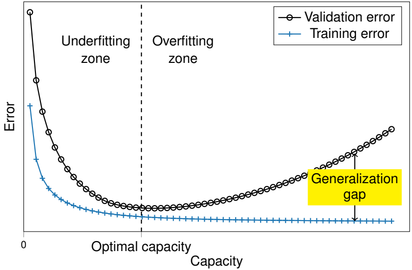

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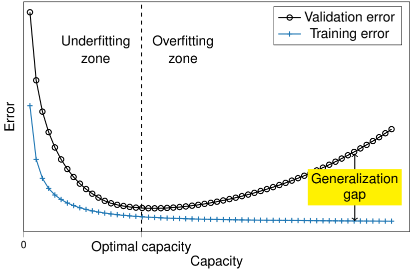

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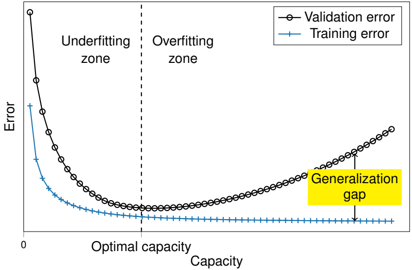

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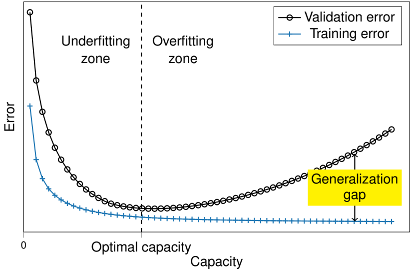

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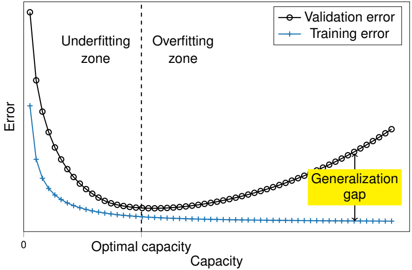

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- **Initialization**

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Number of intrinsic variables

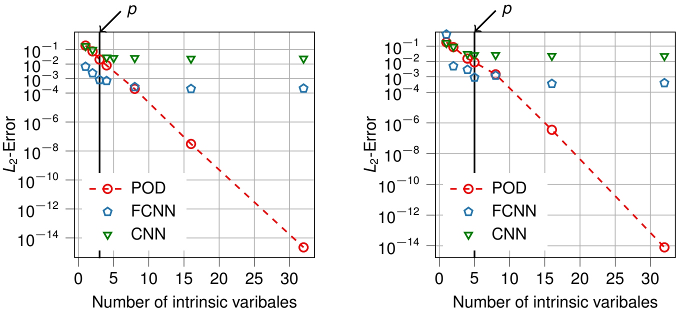
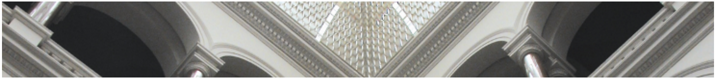


Figure: Variation of p for **H** left and **R** right.

– **Evaluation metric**:

$$L_2\text{-Error} = \frac{||f - \tilde{f}||_2}{||f||_2} \tag{16}$$



Amount of parameters

Table: Amount of parameters used to reconstruct f, the number of intrinsic variables p and the corresponding L_2-Error for POD, the FCNNs, and the CNN.

Algorithm	Parameters		Int. variables p		Ł2-error	
	H	**R**	**H**	**R**	**H**	**R**
POD	15129	25225	3	5	0.0205	0.0087
FCNN	2683	3725	3	5	0.0008	0.0009
CNN	8246	8246	5	5	0.025	0.027

A detailed look at reconstructions

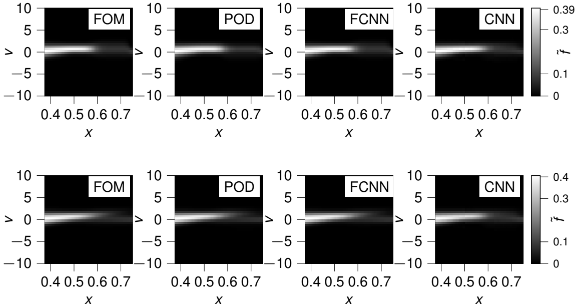


Figure: Comparision of f and $\tilde{f}$ at $t = t_{end}$ and $x \in [0.375, 0.75]$, **H** top and **R** bottom.

A detailed look at reconstructions

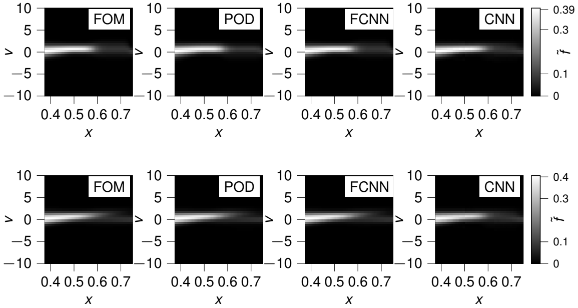


Figure: Comparision of f and $\tilde{f}$ at $t = t_{end}$ and $x \in [0.375, 0.75]$, **H** top and **R** bottom.

- **POD**:
  - **H** - defective after $x = 0.6$: Errors in temperature
  - **R** - almost exact

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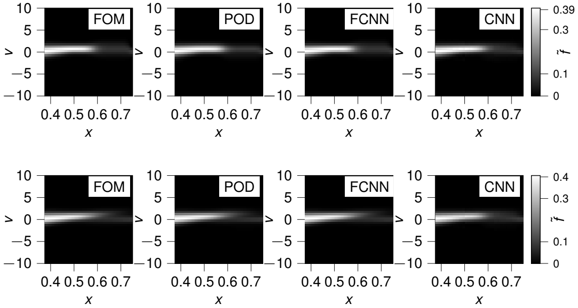

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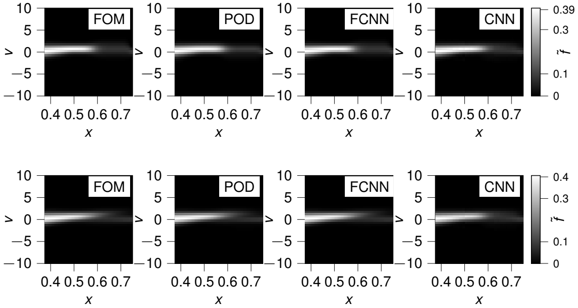
  - **R** - almost exact
- **FCNN**:
  - **H** & **R** - almost exact

A detailed look at reconstructions



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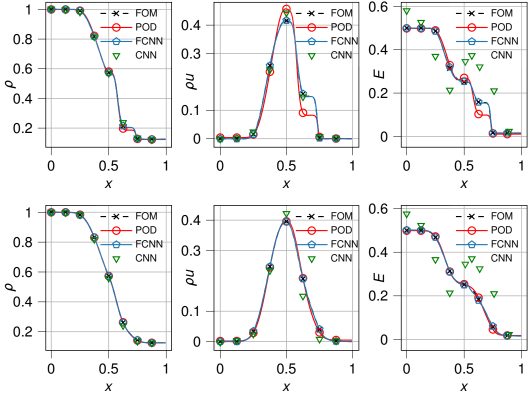
  - **R** - almost exact
- **FCNN**:
  - **H** & **R** - almost exact
- **CNN**:
  - **H** & **R** - average of **H** & **R**

Moments of f and $\tilde{f}$



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Moments of f and $\tilde{f}$

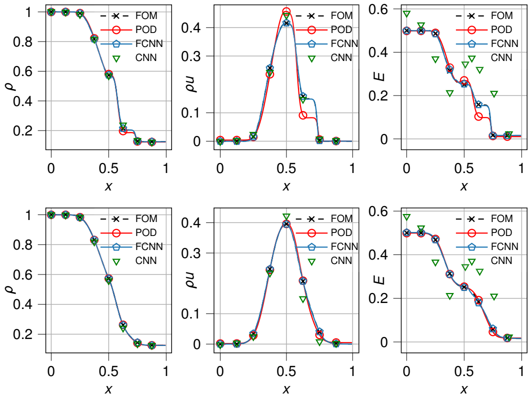

Figure: Moments of f and $\tilde{f}$ at $t = t_{end}$, **H** top and **R** bottom.

– **POD**:
  - **H** - undercuts shockwave in ρ, ρu and E
    ++ - ρu exceeds tail of rarefaction wave
  - **R** - only small deviations at shockwave for ρu and E

Moments of f and $\tilde{f}$

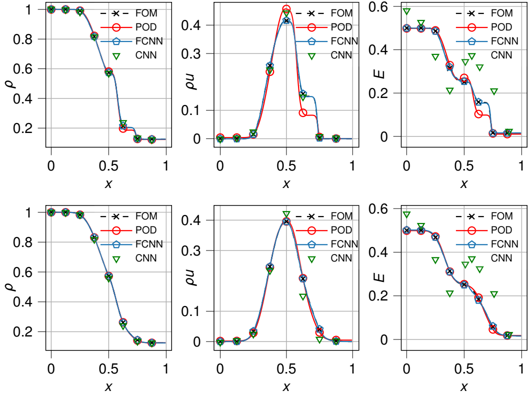

Figure: Moments of f and $\tilde{f}$ at $t = t_{end}$, **H** top and **R** bottom.

- **POD**:
  - **H** - undercuts shockwave in ρ, ρu and E
    ++ - ρu exceeds tail of rarefaction wave
  - **R** - only small deviations at shockwave for ρu and E
- **FCNN**:
  - **R** - severe deviation at transition: tail of rarefaction wave $\rightarrow$ shockfront

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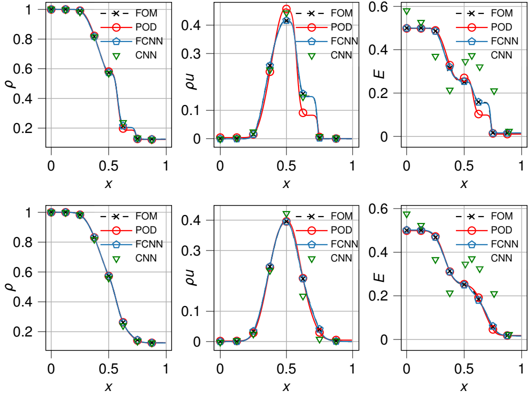

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- **CNN**:
  - **R** is copy of **H**

Physical consistency

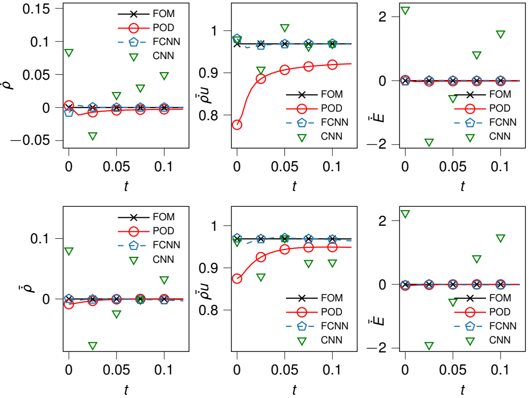


Figure: Conservation properties of f and $\tilde{f}$, **H** top and **R** bottom.

Physical consistency

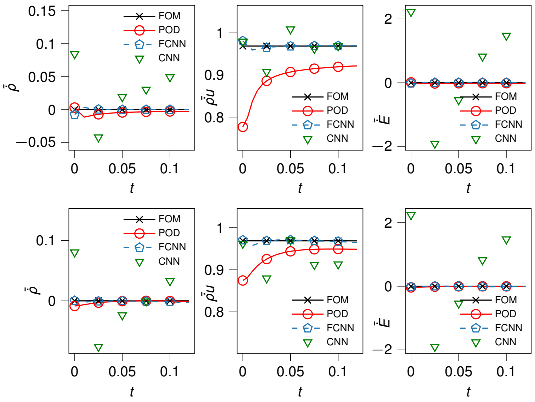
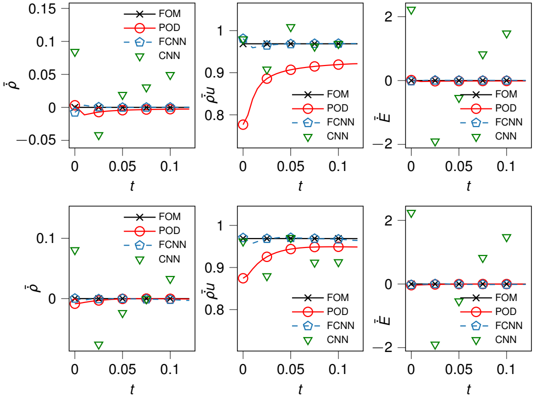


Figure: Conservation properties of f and $\tilde{f}$, **H** top and **R** bottom.

– **POD**:
- **H** & **R** - mass & + mass
- **H** & **R** +++ momentum
- **H** & **R** energy

Physical consistency



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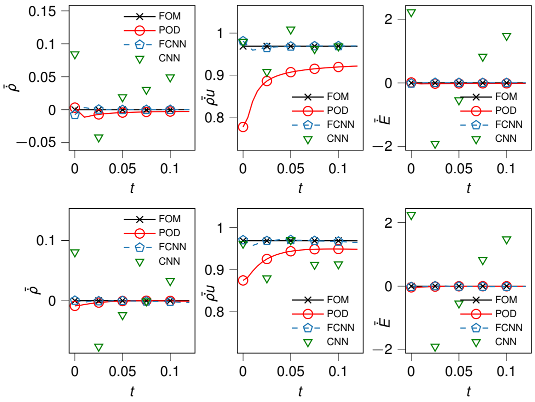

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  - **H** & **R** energy
- **CNN**:
  - No conservation

Interpretabiliy

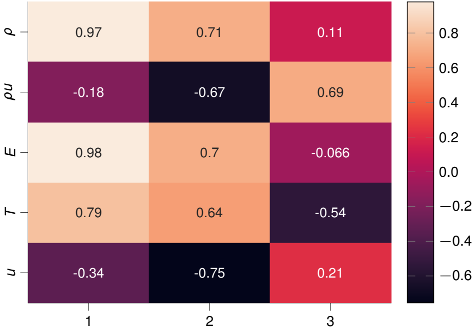

Figure: Pearson correlation between of macroscopic quantities and intrinsic variables for **H**

- **1**:
  - E: 0.98 & ρ: 0.97
- **2**:
  - u: -0.75 & ρ: 0.71
- **3**:
  - ρu: 0.69 & T: -0.54

Interpretabiliy

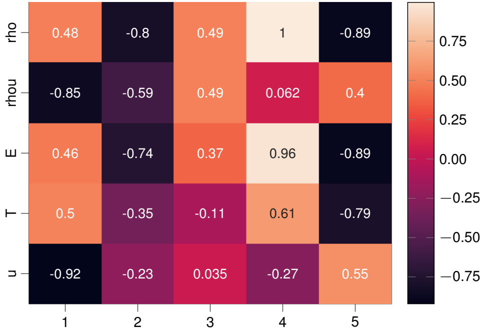

Figure: Pearson correlation between of macroscopic quantities and intrinsic variables for **R**

- **1**:
  - u: -0.92 & ρu: -0.85
- **2**:
  - ρ: -0.8 & E: -0.74
- **3**:
  - ρ: 0.49 & ρu: 0.49
- **4**:
  - ρ: 1 & E: 0.96
- **5**:
  - ρ: -0.89 & T: -0.89

Interpolation

Table: Validation and metric results for the interpolation task with 13, 9, 7 and 5 time steps.

n	Δt^*	Validation error		L_2-error		L_2-error	
		$\mathbf{H}^*$	$\mathbf{R}^*$	$\mathbf{H}^*$	$\mathbf{R}^*$	$\tilde{\mathbf{H}}^*$	$\tilde{\mathbf{R}}^*$
13	0.01s	2.5×10^{-8}	2.9×10^{-7}	0.0018	0.0054	0.0036	0.0058
9	0.015s	2.9×10^{-8}	9.5×10^{-8}	0.0017	0.0038	0.0067	0.0056
7	0.02s	2.5×10^{-8}	1.6×10^{-7}	0.0019	0.0042	0.0101	0.0073
5	0.025s	1.7×10^{-7}	1.6×10^{-7}	0.0039	0.0051	0.0367	0.0138

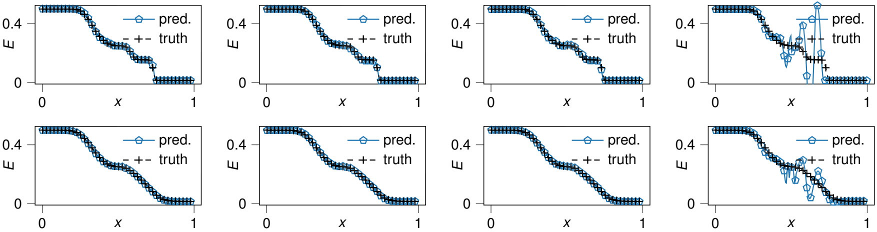

Figure: Energy after interpolation using the FCNN trained on 13,9,7 and 5 time steps, **H** top and **R** bottom.

Table of Contents

– **Outlook**:

- disentangle intrinsic variables
- train a model on various rarefaction levels
- evolve intrinsic variables in time with an LSTM

– **Discussion**:

- When does the training time and finding of hyperparameters pay up?

Thank you for your attention!

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Knudsen number

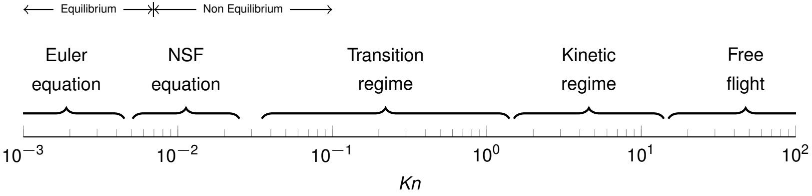

Figure: Partitioning of Kn into levels of rarefaction.

[7]

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[7] Julian Koellermeier et al. "Moment Models for Kinetic Equations". NUMA seminar, KU Leuven. 2020. URL: https://wms.cs.kuleuven.be/groups/NUMA/events.

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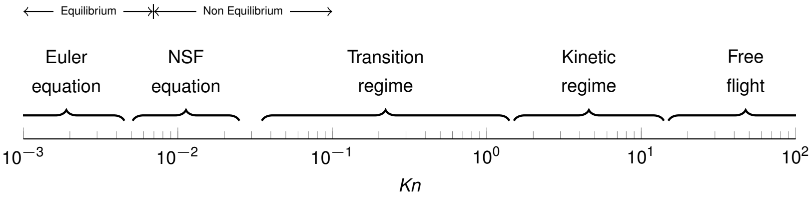

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[7]

– Solution is $\mathbf{f}(\mathbf{x}, \mathbf{v}, \mathbf{t})$ in 1D and $\mathbf{f}(\mathbf{x}, \mathbf{y}, \mathbf{v_x}, \mathbf{v_y}, \mathbf{t})$ in 2D and $\mathbf{f}(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{v_x}, \mathbf{v_y}, \mathbf{v_z}, \mathbf{t})$ in 3D

[7] Julian Koellermeier et al. “Moment Models for Kinetic Equations”. NUMA seminar, KU Leuven. 2020. URL: https://wms.cs.kuleuven.be/groups/NUMA/events.

Moments/ Expected values of f

Question: How do we get the moments of f?

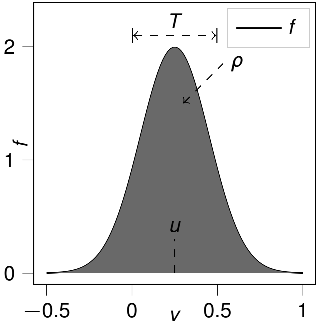

Figure: Illustration of the linkage between f and the moments of f.

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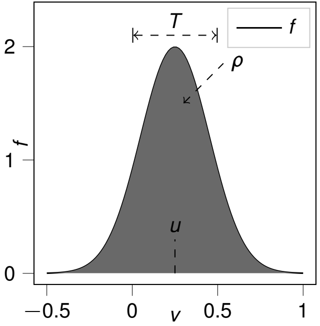

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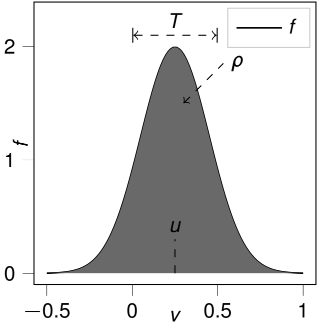
$$\rho(x,t) = \int f \, \mathrm{d}v \,, \tag{17}$$



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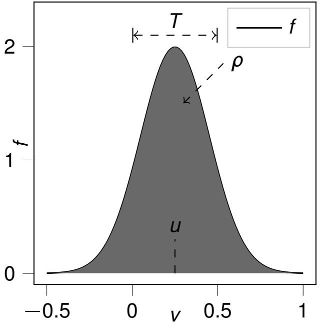

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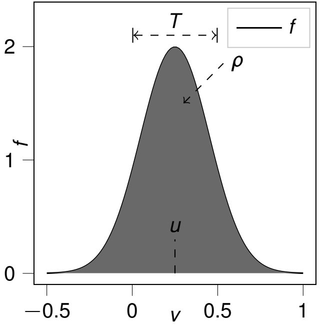
- the third moment/ **Energy** is

$$E(x,t) = \int \frac{1}{2}v^2 f \,\mathrm{d}v\,. \tag{19}$$



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Two Case Studies

- Spatial resolution $J = 200$
- Temporal resolution $I = 25$
- Velocious resolution $K = 40$

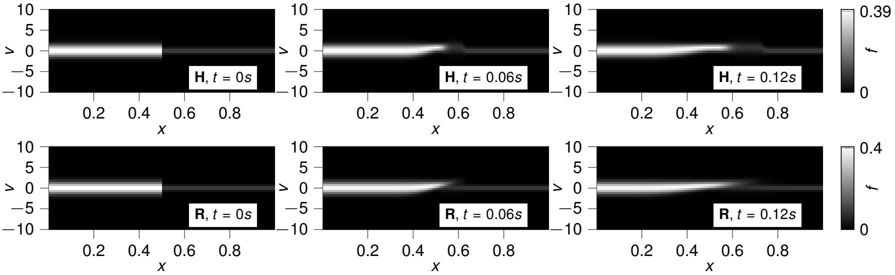


Figure: Solution f top row for **H** and bottom row fro **R** in x and v.

Terminology

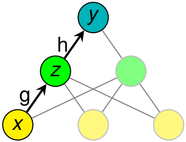
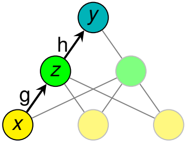


Figure: Example of a simple network.

– Network with three layers

Terminology



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– Network with three layers
  - Input layer
  - Hidden layer
  - Output layer

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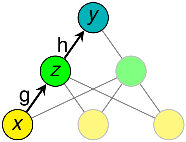

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– **Layer**: Stage of computation

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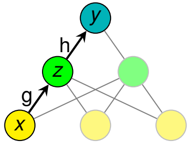

Figure: Example of a simple network.

- **Layer**: Stage of computation
- **Computations**/ Forward pass
  - $g(x) = g(xW + b) = z$
  - $h(z) = h(zW + b) = y$
    - » $h(g(x)) = y$

- Network with three layers
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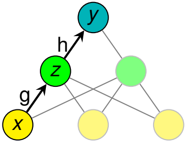

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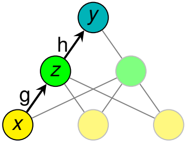
- **Neuron**: Entry in ’Tensor’

Terminology



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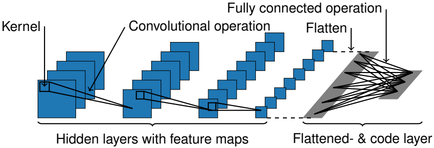
- **Neuron**: Entry in 'Tensor'
- **Trainable parameters**: W, b

Convolutional Autoencoder

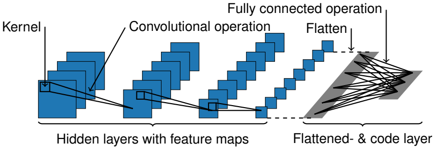


(a) Encoder of a convolutional autoencoder without input layer.

Figure: Fundamental features of conv. networks.

– Designed for 2D/3D input

Convolutional Autoencoder



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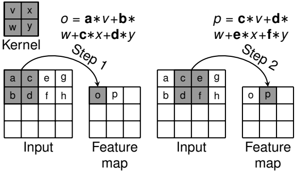

(b) Convolutional operation, 1 strided.

Figure: Fundamental features of conv. networks.

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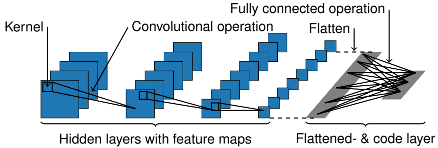
Convolutional Autoencoder



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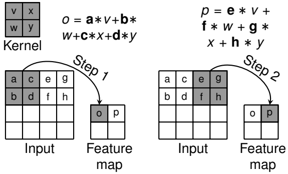

(b) Convolutional operation, 2 strided.

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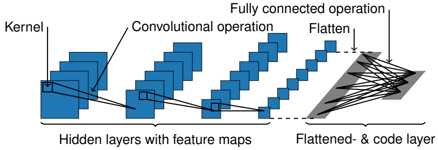
– Designed for 2D/3D input

Convolutional Autoencoder



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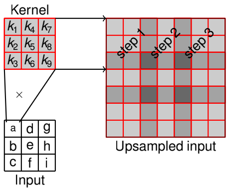

(b) Even deconvolution

Figure: Fundamental features of conv. networks.

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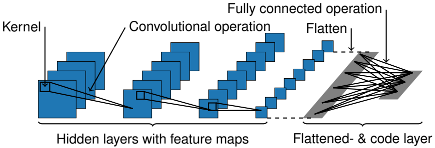
Convolutional Autoencoder



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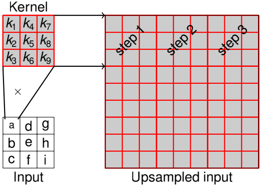

(b) Uneven deconvolution

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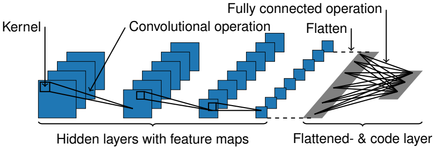

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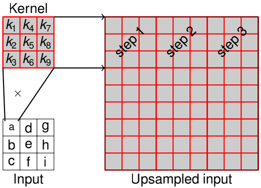

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Figure: Fundamental features of conv. networks.

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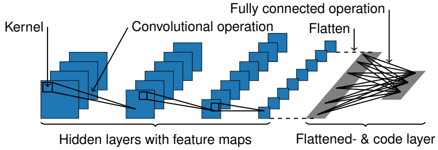
– **Peculiarities**: Sparse connections, parameter sharing

- Promotes generalization

Convolutional Autoencoder



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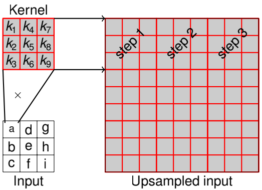

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Figure: Fundamental features of conv. networks.

- Designed for 2D/3D input
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- **Hyperparameters**: Number & size of layers, kernel dimensions, stride increments

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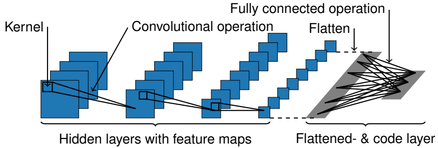

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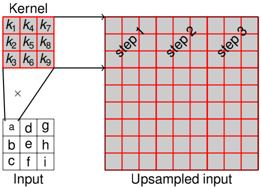

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Figure: Fundamental features of conv. networks.

- Designed for 2D/3D input
- **Peculiarities**: Sparse connections, parameter sharing
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- **Hyperparameters**: Number & size of layers, kernel dimensions, stride increments
  - Non-trivial influence of output dimensions & quality

Time dependece of L_2-Error

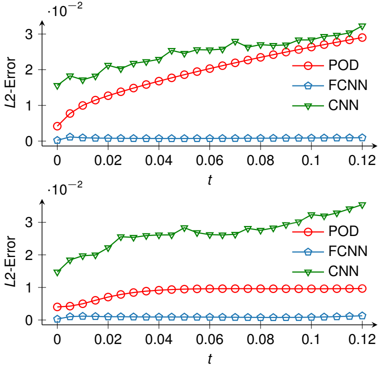

Figure: Comparison of the L_2-Error over time, **H** top and **R** bottom.

- **POD**:
  - **H** - lin. increase of L_2
  - **R** - increase & stagnation of L_2
- **FCNN**:
  - **H** & **R** - no distinct time dependence L_2
  - biggest value at onset
- **CNN**:
  - **H** & **R** - similar evolution