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8 Generative Artificial Intelligence

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Deep Learning in Computational Mechanics – an introductory course, Herrmann et al. 2025

website

book

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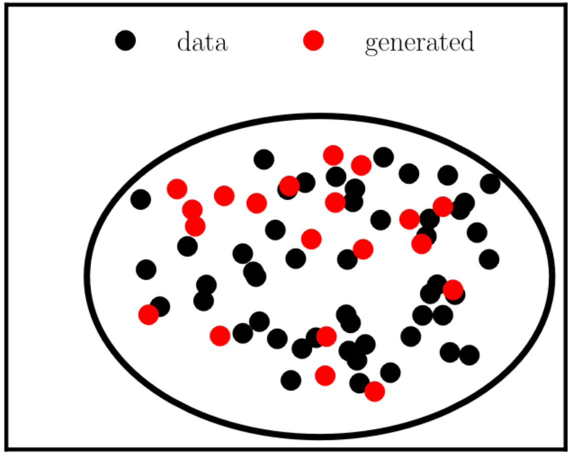
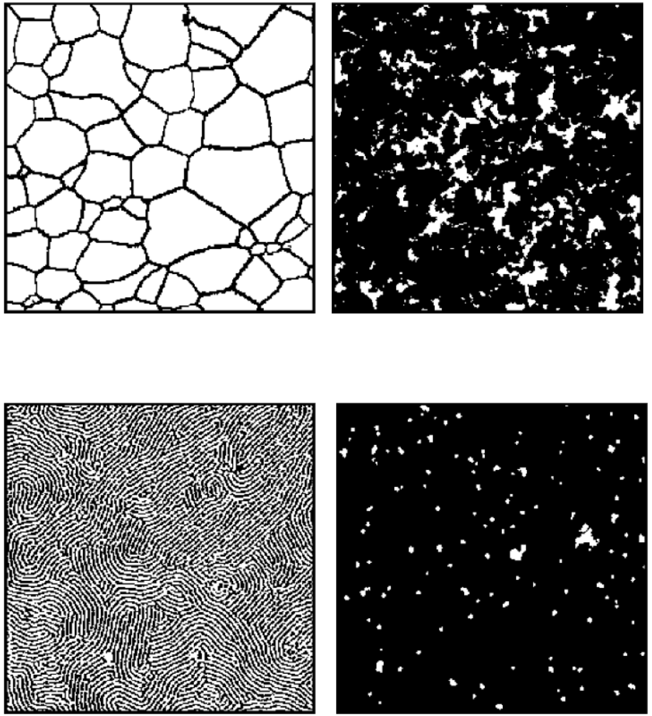
Contents

8 Generative Artificial Intelligence

Generative modeling

- Generate new data points that resemble a given dataset (without simply reproducing given data points)
- Example: Generate new rim designs given a set of rims



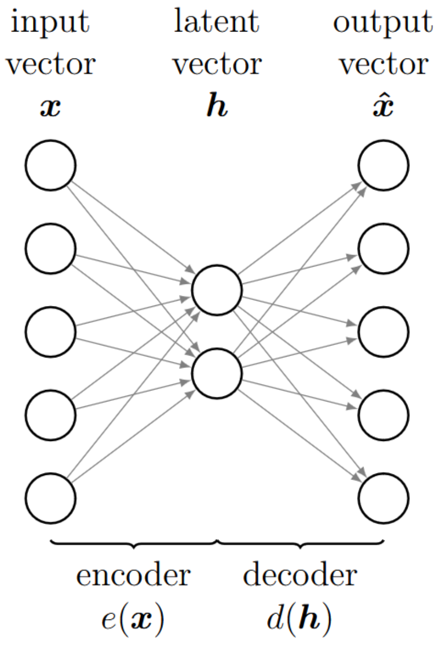


- Variational autoencoders, generative adversarial networks, diffusion models, flow-based models, transformer models

8.1 Autoencoders

Autoencoders learn a compression (and the corresponding decompression)

- **Encoder** e projects data from high-dimensional input x to low-dimensional latent space h
- **Decoder** d reconstructs x from the latent space h, i.e., $\hat{x} = d(e(x))$

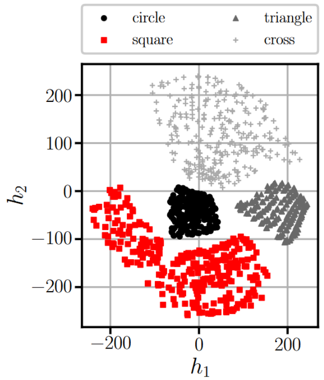


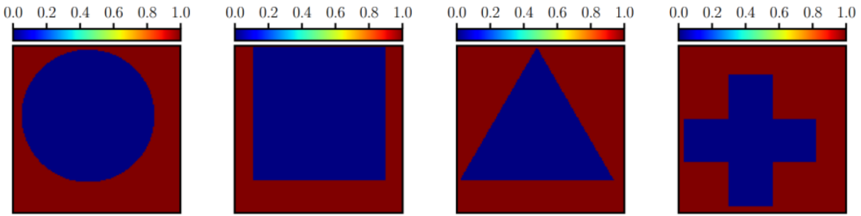
- Cost function

$$C = \left\| d(e(x)) - x \right\|^2$$

This is a dimensionality reduction technique (and not a generative model):
Generation is theoretically possible by randomly sampling the latent space & decoding it

- Autoencoders are problematic for generation, due to discontinuities between different objects in the latent space





8.2 Variational Autoencoder

Variational autoencoders (**VAEs**) are a variation of an autoencoder for generative modelling

- After training the autoencoder, the latent space $h \sim \mathcal{N}(\mu, \sigma^2)$ is sampled randomly and decoded $\hat{x} = d(h)$
- Discontinuities in the latent space are overcome

μ is the mean and σ the standard deviation of a normal distribution

  - By mapping to $\mu(x), \sigma(x)$ instead of a deterministic h (and sampling $h \sim \mathcal{N}(\mu, \sigma^2)$ during training)
  - The probabilistic framework is trained with the Kullback-Leibler (KL) divergence

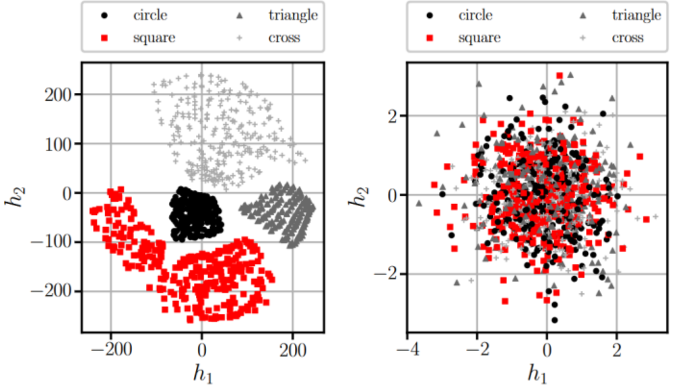
$$\mathrm{KL}(\mathcal{N}(\mu, \sigma^2) || \mathcal{N}(0, I)) = \frac{1}{2} \sum_{i=1}^{d} (\sigma_i^2 + \mu_i^2 - \ln \sigma_i^2 - 1)$$

Penalizes distribution $p(h|x)$ for deviating from the standard normal distribution $\mathcal{N}(0, I)$: avoids μ being large and σ being small

  - Sampling operations are non-differentiable → reparametrization

$$h = \mu(x) + \sigma(x)\epsilon, \qquad \epsilon \sim \mathcal{N}(0, I)$$

Trained with reconstruction loss



Trained with Kullback-Leibler divergence

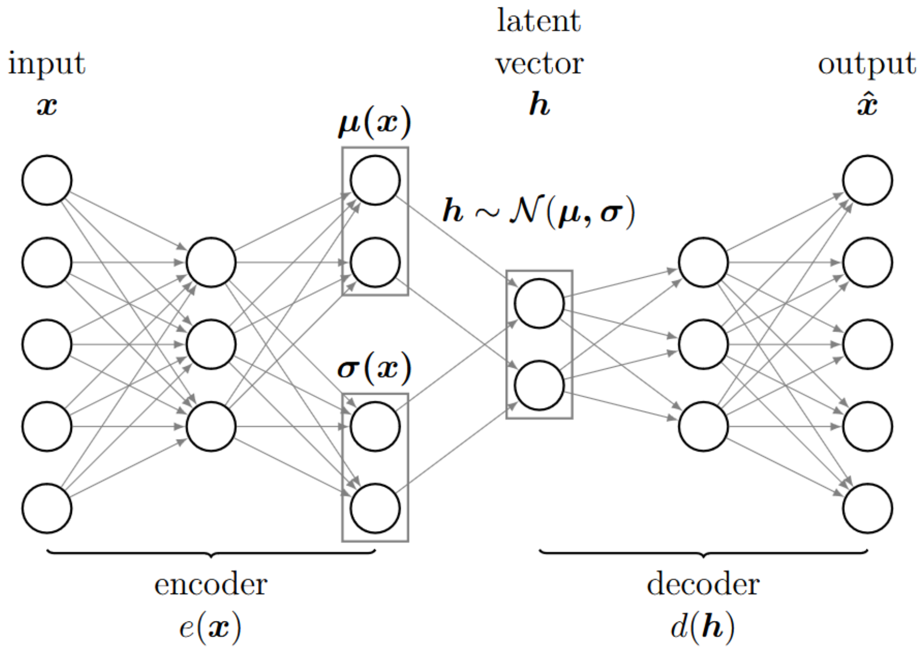
Encodings are distributed randomly around zero (and entangled)

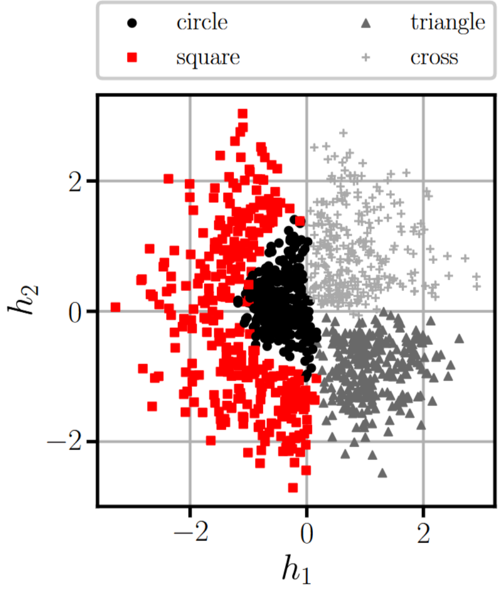
8.2 Variational Autoencoder

Cost function of variational autoencoder as combination between reconstruction loss & Kullback-Leibler divergence

$$C = \|x - \hat{x}\|^2 + \mathrm{KL}(\mathcal{N}(\mu(x), \sigma), \mathcal{N}(0, I))$$

where the latent space prediction is made as $h = \mu(x) + \sigma(x)\epsilon, \quad \epsilon \sim \mathcal{N}(0, I)$





Disentangled and continuous latent space (with meaningful clusters centered around zero)

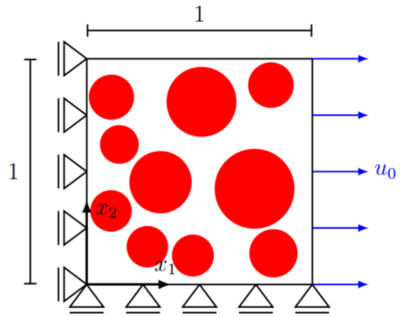
8.4 Autoencoders in Computer Vision: U-Net

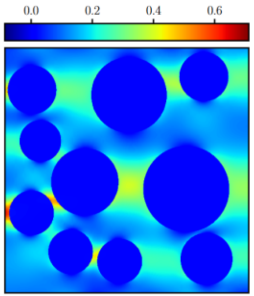
U-Net: Convolutional Networks for Biomedical Image Segmentation, Ronneberger et al. 2015

Autoencoders for surrogate modeling

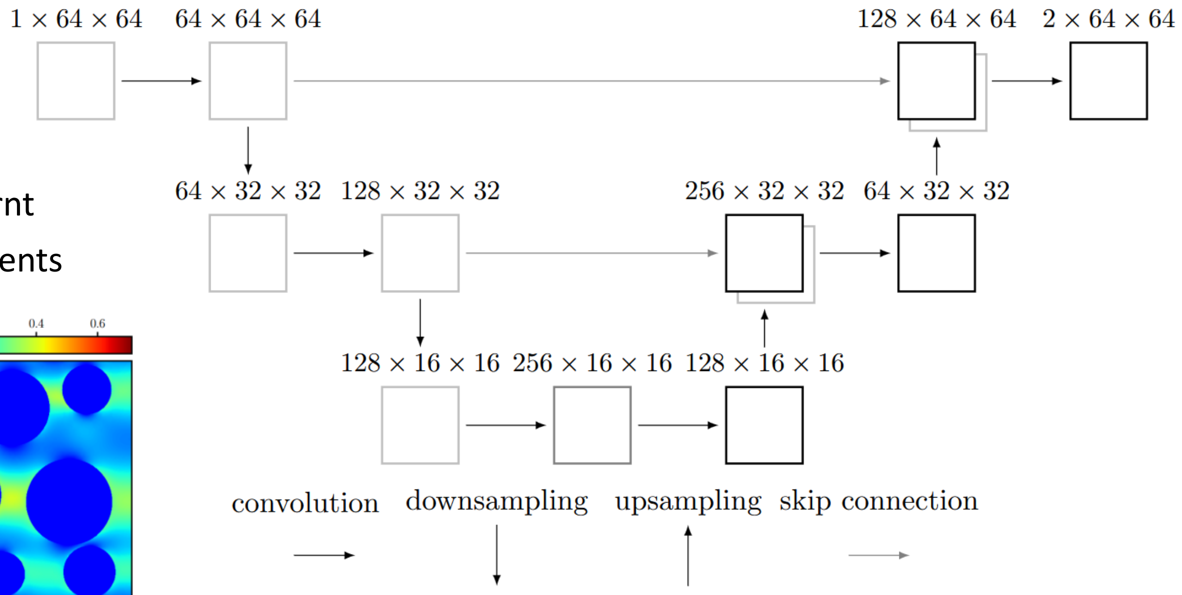
- Extract the essence of the input
- (Potentially) have to reconstruct important features

- **U-Net**
  - Encodes the input to a latent space
  - Adds skip connections
    - Features do not have to be relearnt
    - Avoids vanishing/exploding gradients





ε_{11}



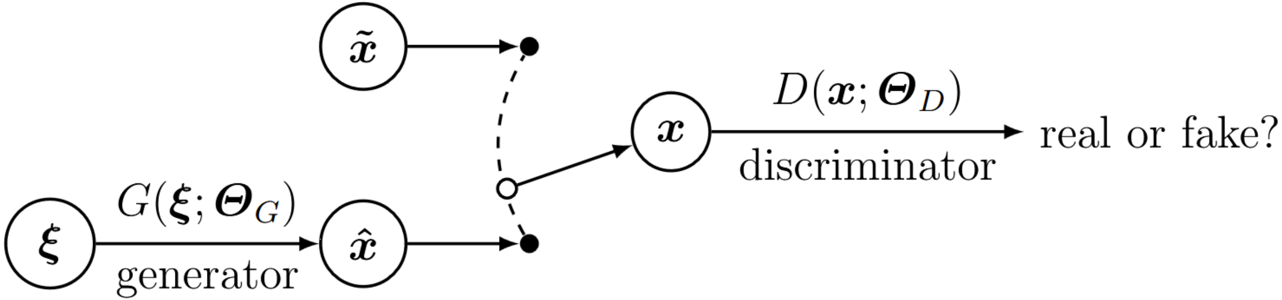
Example (learning strain distributions) from Chapter 3

8.3 Generative Adversarial Networks

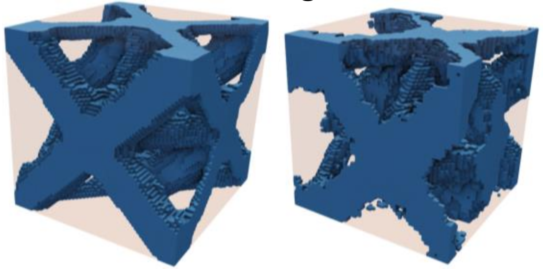
Generative Adversarial Nets, Goodfellow et al. 2014

Generative adversarial networks (**GANs**) learn to generate data through a two-player game

- The generator $G_{NN}(\boldsymbol{\xi}; \boldsymbol{\Theta}_G)$ creates fake samples $\hat{\boldsymbol{x}}$ from random noise $\boldsymbol{\xi}$
- The discriminator $D_{NN}(\boldsymbol{x}; \boldsymbol{\Theta}_D)$ assesses if a sample x is real or fake (i.e., generated by G_{NN})
  - This is quantified by the predicted probability score $\hat{p} = D_{NN}(\boldsymbol{x}; \boldsymbol{\Theta}_D)$



Reference cell & generated cell



- Thus: the generator aims to fool the discriminator
- The two-player game is formulated with the cost function

$$C = \frac{1}{m_D} \sum_{i=1}^{m_D} \log\left(D_{NN}(\tilde{\boldsymbol{x}}_i; \boldsymbol{\Theta}_D)\right) + \frac{1}{m_G} \sum_{i=1}^{m_G} \log(1 - D_{NN}(G_{NN}(\boldsymbol{\xi}_i; \boldsymbol{\Theta}_G); \boldsymbol{\Theta}_D))$$

- Handled with a minimax optimization $\min_{\boldsymbol{\Theta}_G} \max_{\boldsymbol{\Theta}_D} C$

Convergence is reached when $\hat{p} = 0.5$ for all samples

8.5 Diffusion Models

Diffusion models learn to reverse a gradual noising procedure

- A forward diffusion process q (slowly adds random noise to data x)

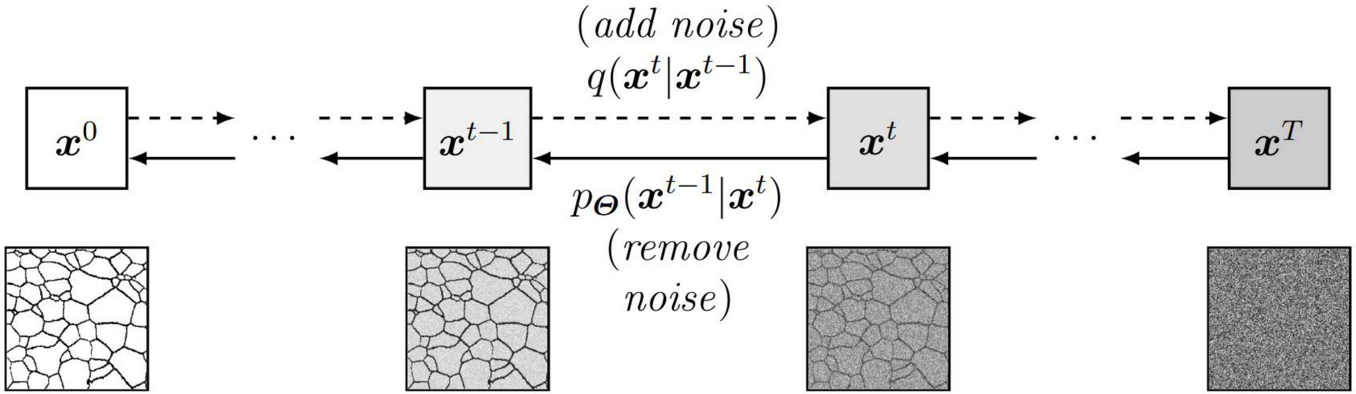
$$q(x^t|x^{t-1}) = \mathcal{N}(x^t; \sqrt{1-\beta^t}x^{t-1}, \beta^t I)$$

- A reverse denoising diffusion process p_Θ (a neural network learns to reverse the diffusion process)

$$p_\Theta(x^{t-1}|x^t) = \mathcal{N}\left(x^{t-1}; \mu_\Theta(x^t,t), \Sigma_\Theta(x^t,t)\right)$$

$\mu_\Theta, \Sigma_\Theta$ can be described by neural networks

$$p_\Theta(x^{0:T}) = p(x^T)\prod_{t=1}^{T} p_\Theta(x^{t-1}|x^t)$$

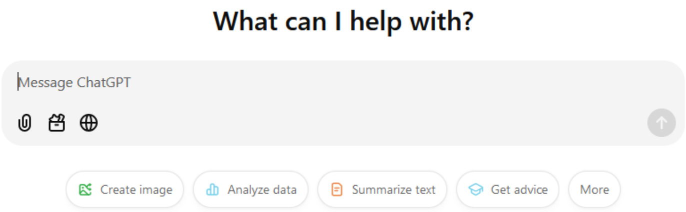


8.6 Transformers

Attention Is All You Need, Vaswani et al. 2017

Transformers operate on sequential data (typically text in natural language processing, e.g., ChatGPT):

- Text classification
- Text generation
- Summarization
- Question Answering
- Machine translation



Key ingredients

- Self-attention (to understand the context in long sequences)
- Positional encoding (enables parallelism, despite sequential input)
- Pretraining (cheaper applications to new tasks, e.g., GPT: Generative pre-trained transformer)

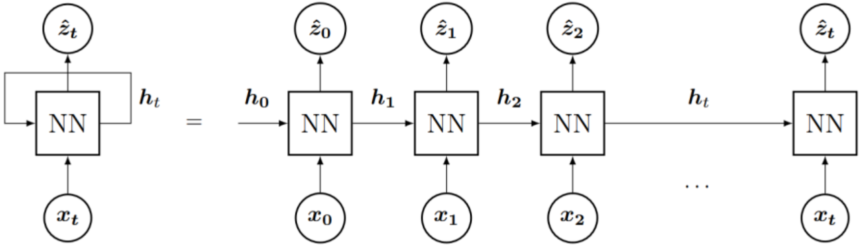
Let‘s understand how transformers work on the following translation task

In winter, it snows.	→	*Im Winter schneit es.*

8.6 Transformers

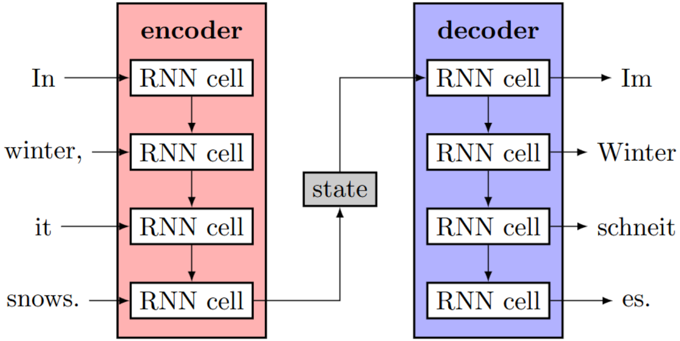
Natural Language Processing with Transformers, Tunstall et al. 2022

In natural language processing, the state-of-the-art before transformers were recurrent neural networks (& variants)



$\hat{z}$ can be the final output or an intermediate (hidden) state

The translation task could be handled by an encoder-decoder architecture (using two RNNs)



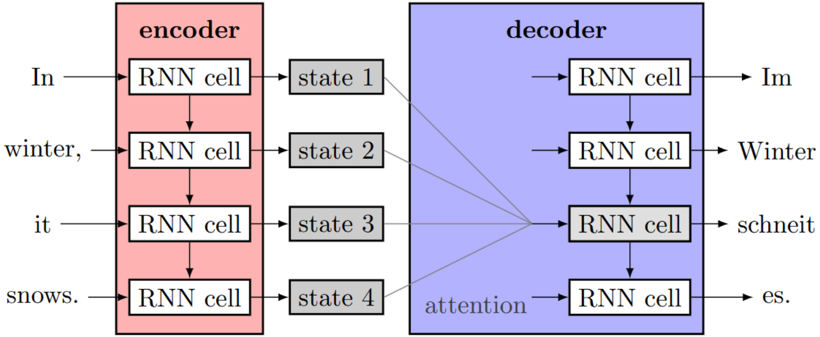
Problems:

- For long inputs, the hidden state cannot capture the meaning of the entire sequence
- The forward propagation cannot be parallelized

8.6 Transformers

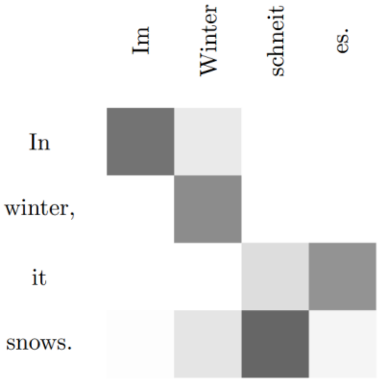
Natural Language Processing with Transformers, Tunstall et al. 2022

To handle long-range dependencies, attention is introduced within the decoder



An attention map is applied between every hidden state (each token, i.e., word) and each RNN cell of the output

Exemplary attention map between input and output



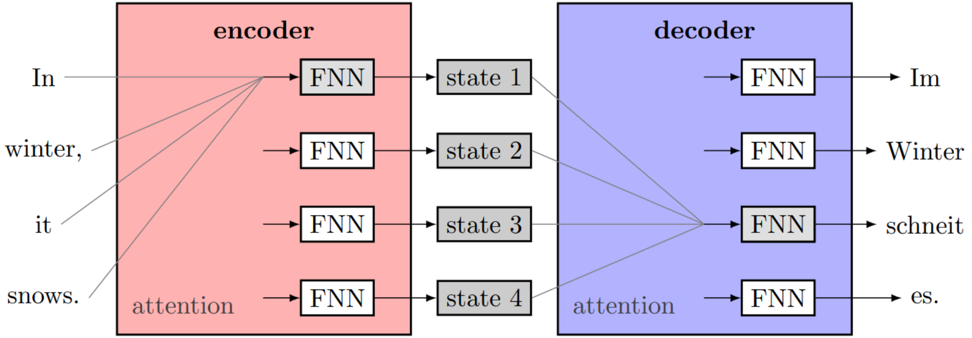
Problem:

- The forward propagation cannot be parallelized

8.6 Transformers

Natural Language Processing with Transformers, Tunstall et al. 2022

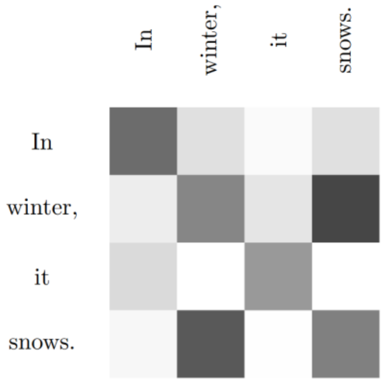
An additional attention mechanism in the encoder enables parallelism



Because each output token (decoder) attends to every input token (encoder), this mechanism is known as cross-attention.

But what about self-attention?

In self-attention, each token attends to every other token in the same sequence, capturing context and relationships between them.



8.6 Transformers

Implementation of self-attention in transformers

- Each input $\boldsymbol{x}_i \in \mathbb{R}^{N_e}$ is queried and compared to a key, i.e., other inputs $\boldsymbol{x}_j \in \mathbb{R}^{N_e}$
- The query $\boldsymbol{Q}$ and key $\boldsymbol{K}$ are obtained through linear transformations on $\boldsymbol{X} \in \mathbb{R}^{N_w \times N_e}$

$$\boldsymbol{Q} = \boldsymbol{X}\boldsymbol{W}^q \in \mathbb{R}^{N_w \times N_s}$$
$$\boldsymbol{K} = \boldsymbol{X}\boldsymbol{W}^k \in \mathbb{R}^{N_w \times N_s}$$

If key and query act on the same sequence: self-attention
Else: attention

- The similarity $\boldsymbol{S}$ describes the self-attention

$$\boldsymbol{S} = \boldsymbol{Q}\boldsymbol{K}^T \in \mathbb{R}^{N_w \times N_w}$$

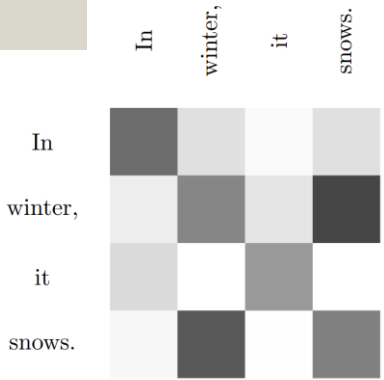
- The similarity is applied to values $\boldsymbol{V}$, i.e., transformed inputs $\boldsymbol{x}_i$

$$\boldsymbol{V} = \boldsymbol{X}\boldsymbol{W}^v \in \mathbb{R}^{N_w \times N_V}$$

- Through a normalization

Without softmax: unbounded
Softmax transforms $\boldsymbol{S}$ into a probability distribution

$$\tilde{\boldsymbol{z}} = \text{softmax}\left(\frac{\boldsymbol{S}}{\sqrt{N_s}}\right)\boldsymbol{V} \in \mathbb{R}^{N_w \times N_V}$$



Similarity matrix $\boldsymbol{S}$

- Can be applied multiple times, yielding $\tilde{\boldsymbol{Z}} = \{\tilde{\boldsymbol{z}}_0, \tilde{\boldsymbol{z}}_1, \dots, \tilde{\boldsymbol{z}}_h\}$, which can be transformed to

$$\boldsymbol{z} = \tilde{\boldsymbol{Z}}\boldsymbol{W}^z \in \mathbb{R}^{N_w \times N_z}$$

- As the attention mechanism is used multiple times within one layer, it is called multi-headed attention
- Learnable parameters are $\boldsymbol{W}^q, \boldsymbol{W}^k, \boldsymbol{W}^v, \boldsymbol{W}^z$

8.6 Transformers

Attention Is All You Need, Vaswani et al. 2017

Multi-headed self-attention layers are combined with

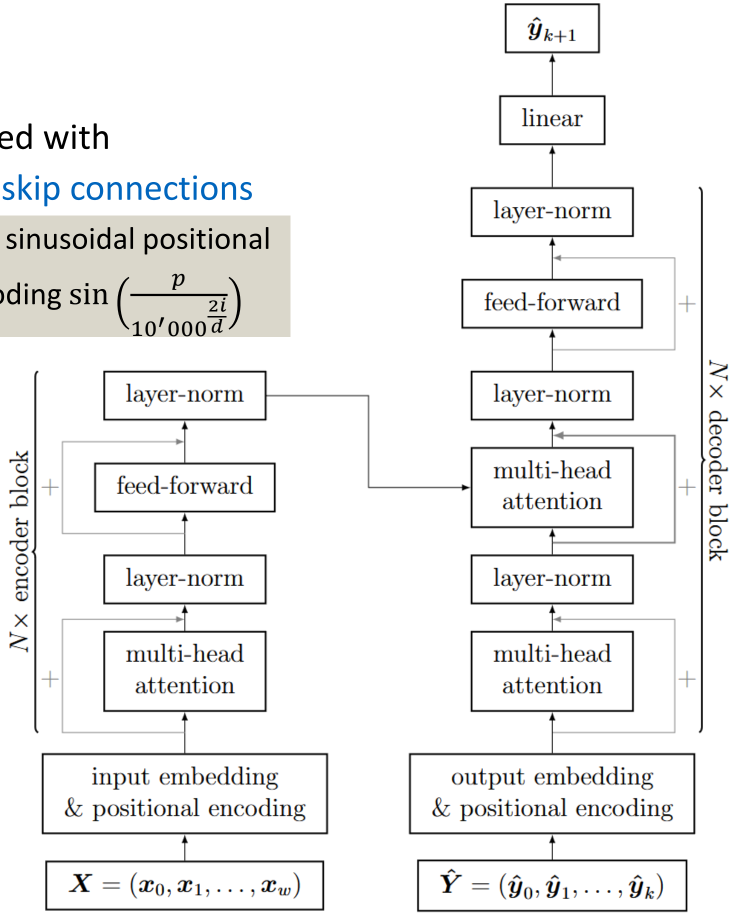
- Normalization layers, feed-forward layers, skip connections
- Positional encoding:
  - Extends input/output with unique positional identifier

e.g., sinusoidal positional encoding $\sin\left(\frac{p}{10'000^{\frac{2i}{d}}}\right)$

- Input embedding (how to encode words):
  - Word2Vec, learnable

In the original transformer formulation an encoder-decoder architecture was proposed:

- Encoder-only: text classification, extractive question answering
- Decoder-only: text generation, auto-regressive question answering
- Encoder-decoder: machine translation, speech processing, data to text



8.6 Transformers

https://github.com/meta-llama/llama/blob/main/MODEL_CARD.md

Pretraining: Perform a training on a larger and more general dataset

- e.g., predict next word from previous words (get text from internet)

Domain adaption: Perform a second training on specific dataset

- e.g., (hand-crafted) Q&A texts to build a chatbot, or adaption to another language

Fine-tuning: combination with additional neural networks for specific task

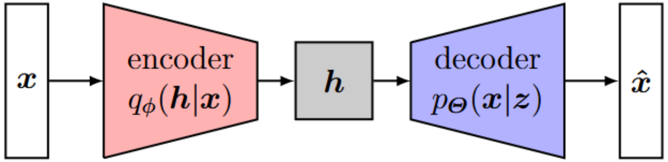
- e.g., classification layer appended to the hidden state, or using only the decoder for chatbots

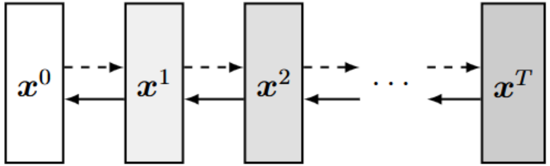
Pretraining is the most expensive part

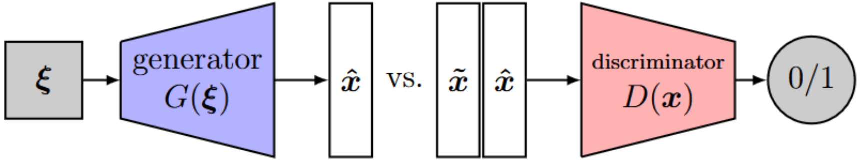
	parameters	**model size**	**training time** (on 2048 GPUs)	**training cost**
Llama 7B	7B	28 GB	4 days	0.1 M $
Llama 13B	13B	52 GB	8 days	0.2 M $
Llama 70B	70B	280 GB	35 days	1.1 M $
GPT-3	165B	700 GB	17 days	4.6 M $
GPT-4	100B-10T?	400 GB-40 TB	?	?

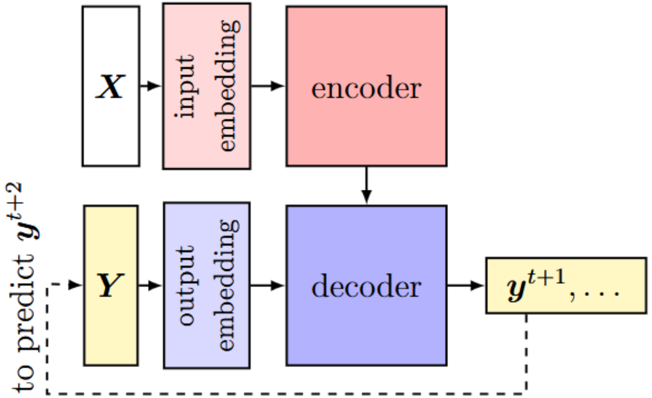
8 Generative Artificial Intelligence

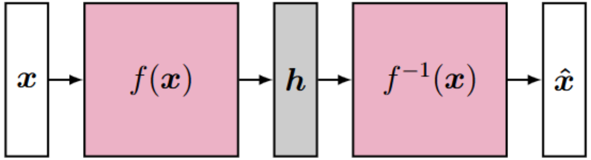
What is what?



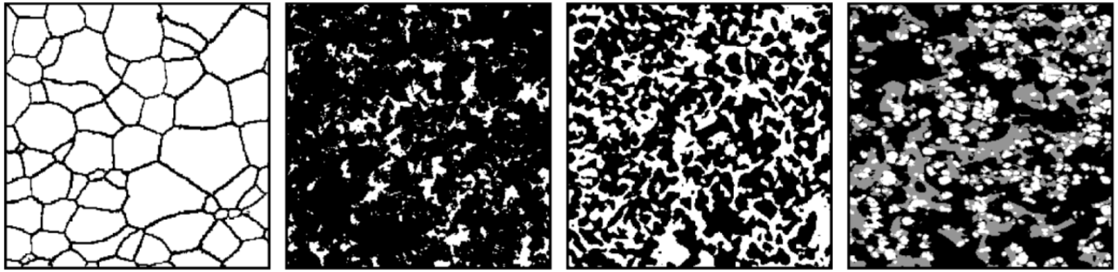




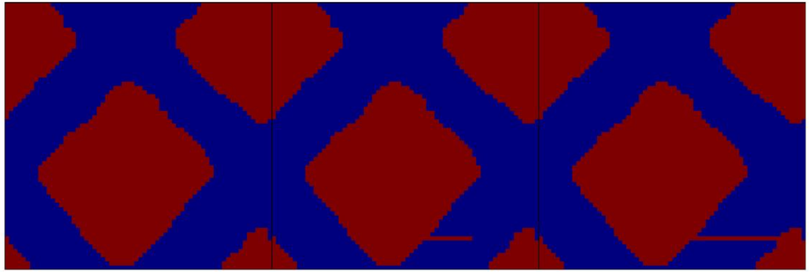




8.7 Applications in Computational Mechanics

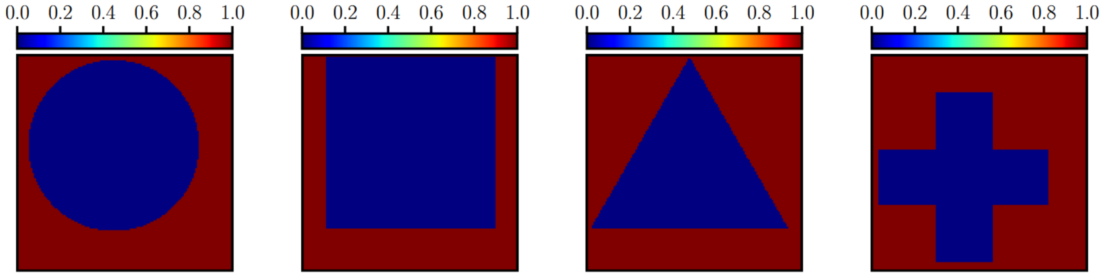


- 8.7.1 **Data Generation**
  - For surrogate models
  - As surrogate models
- 8.7.2 **Generative Design & Design Optimization**
  - Nonlinear dimensionality reduction (optimization on latent vectors)
  - Enforcement of exotic constraints
    - Novelty, aesthetics, manufacturability, creativity, …
  - Inverse design
- 8.7.3 **Anomaly Detection**
  - If generation is not possible, it must be an anomaly!
- 8.7.4 **Conditional Generation**
  - Additional inputs to generative models (but still multiple outputs)
- 8.7.5 **Surrogate Modeling**
  - Transformer architectures as surrogates
  - U-Net



8.7.1 Data Generation

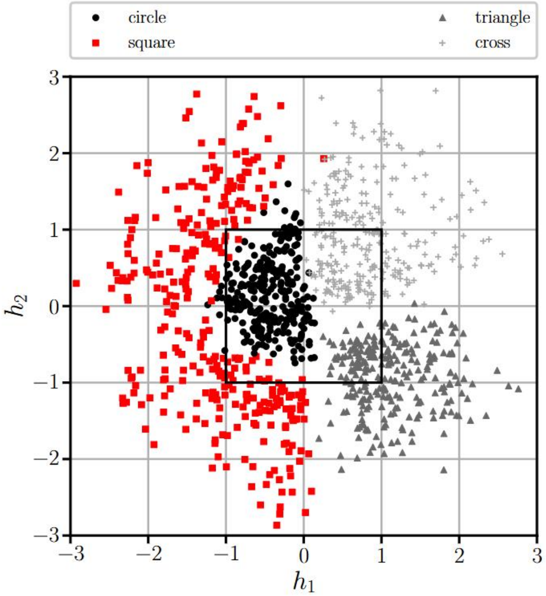
Shape generation with variational autoencoders

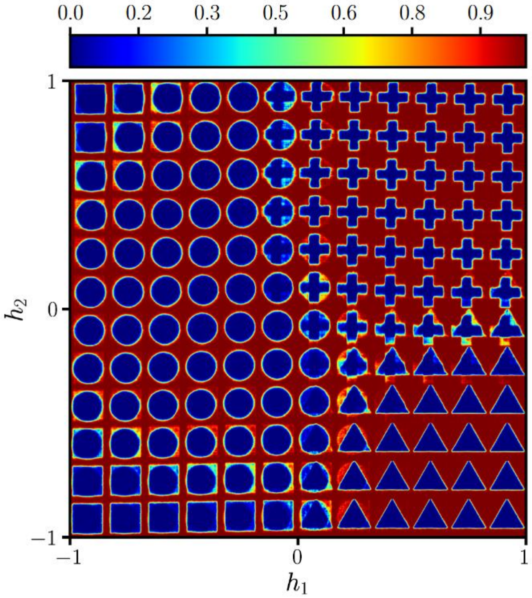


Training with

- Reconstruction loss
- Kullback-Leibler divergence

Latent space





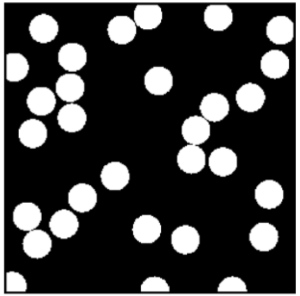
Interpolation of the latent space

Exercises

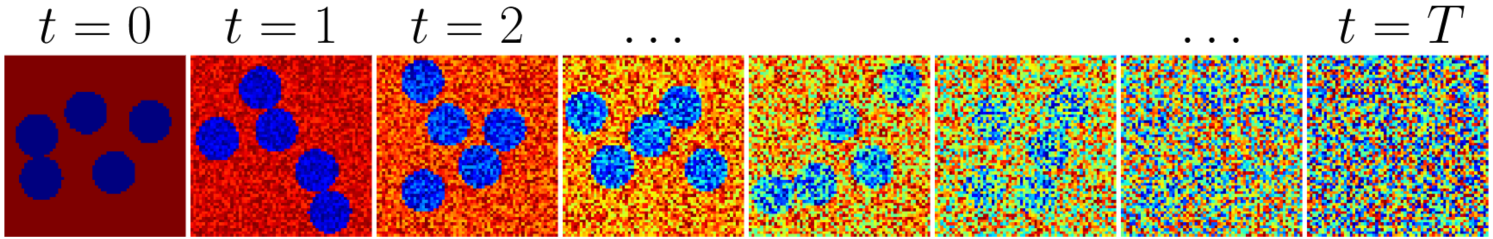
- E.28 Variational Autoencoder (C)
  - Apply a variational autoencoder to a simple data generation task. The task consists of generating basic shapes; circles, triangles, squares and crosses. Explore the latent space distribution and the effect of the Kullback-Leibler divergence.

8.7.1 Data Generation

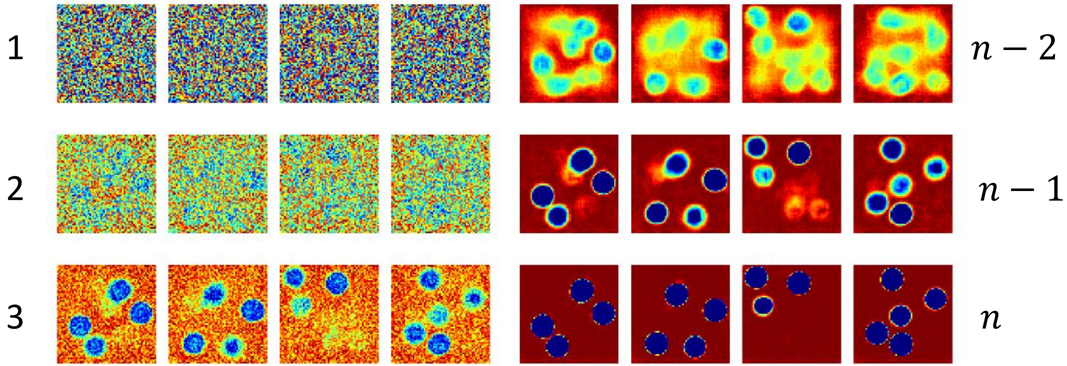
Fiber distribution generation with diffusion model



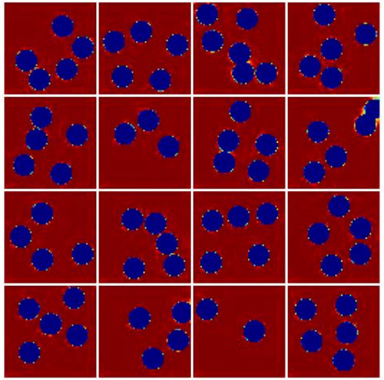
Forward diffusion process



Learned reverse denoising process



After 40 denoising steps

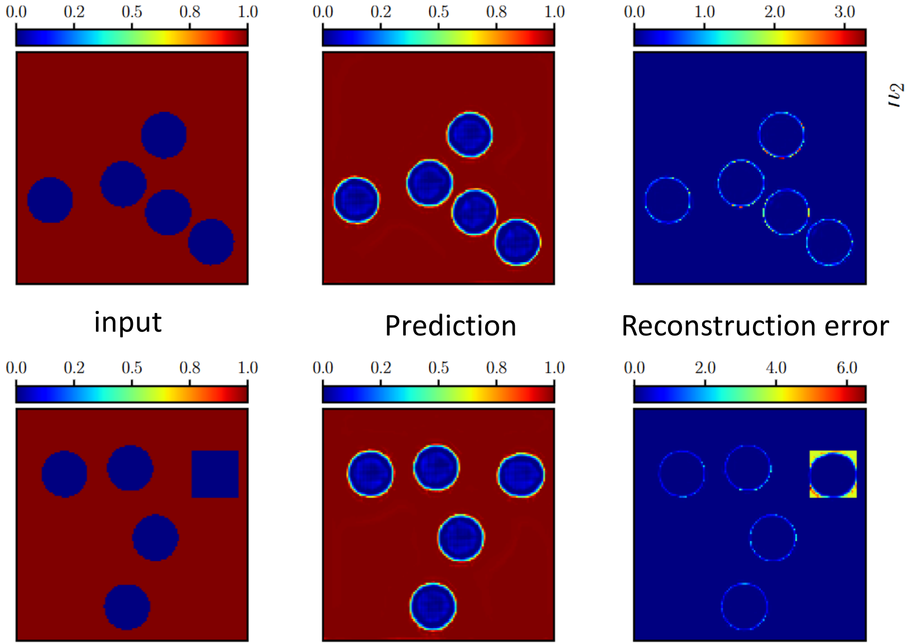


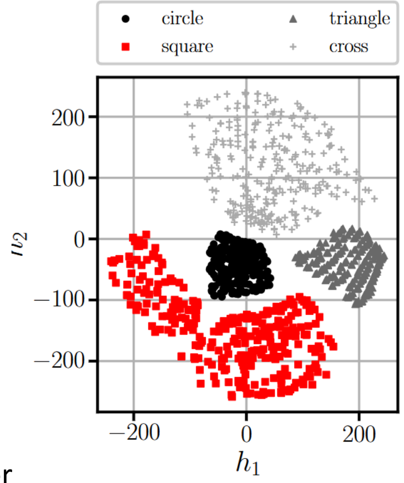
Exercises

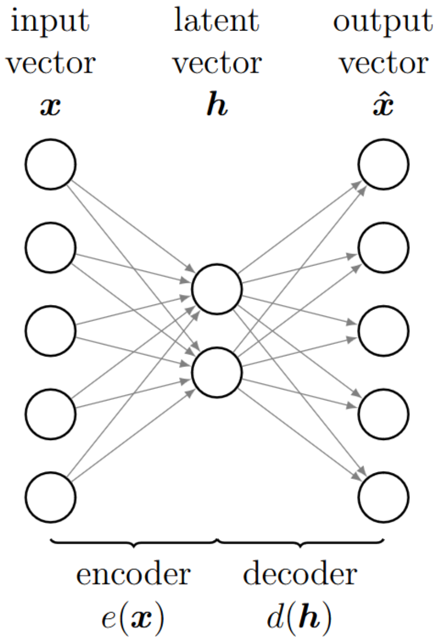
- E.30 Diffusion models (C)
  - Apply a diffusion model to a simple data generation task. The task consists of generating simple fiber matrix microstructures.

8.7.3.1 Autoencoders for Anomaly Detection

- Training of autoencoder on ”normal data”, i.e., without anomalies
- Detection of outliers
  - In latent space
  - By inability to reconstruct the input image

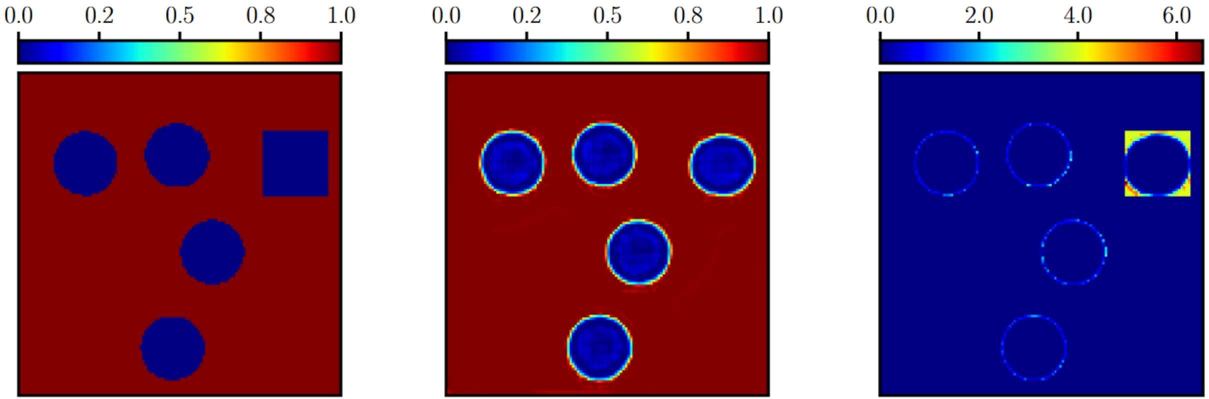




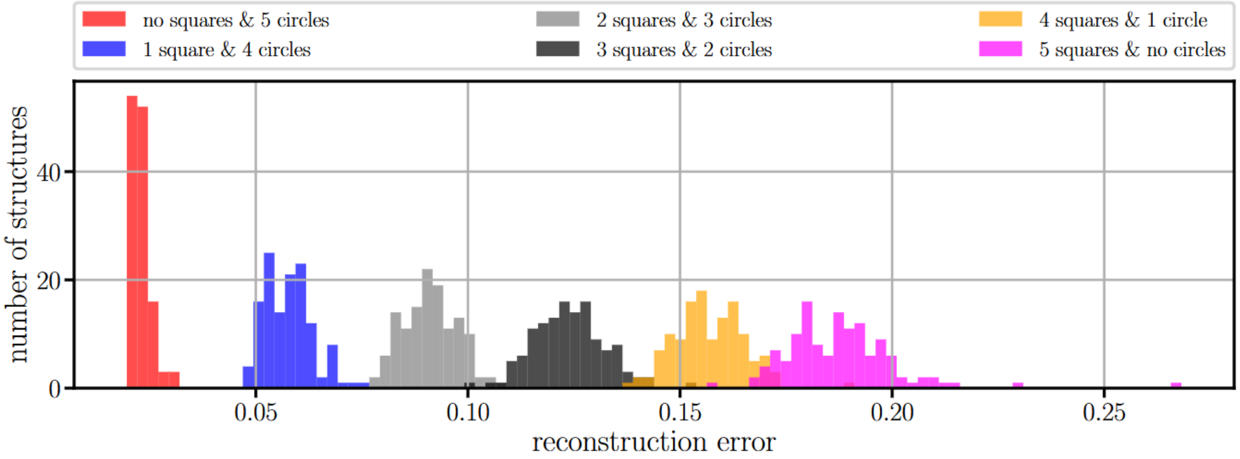


Deep Learning for Anomaly Detection: A Review, Pang et al. 2021

8.7.3.1 Autoencoders for Anomaly Detection



Statistical evaluation



Exercises

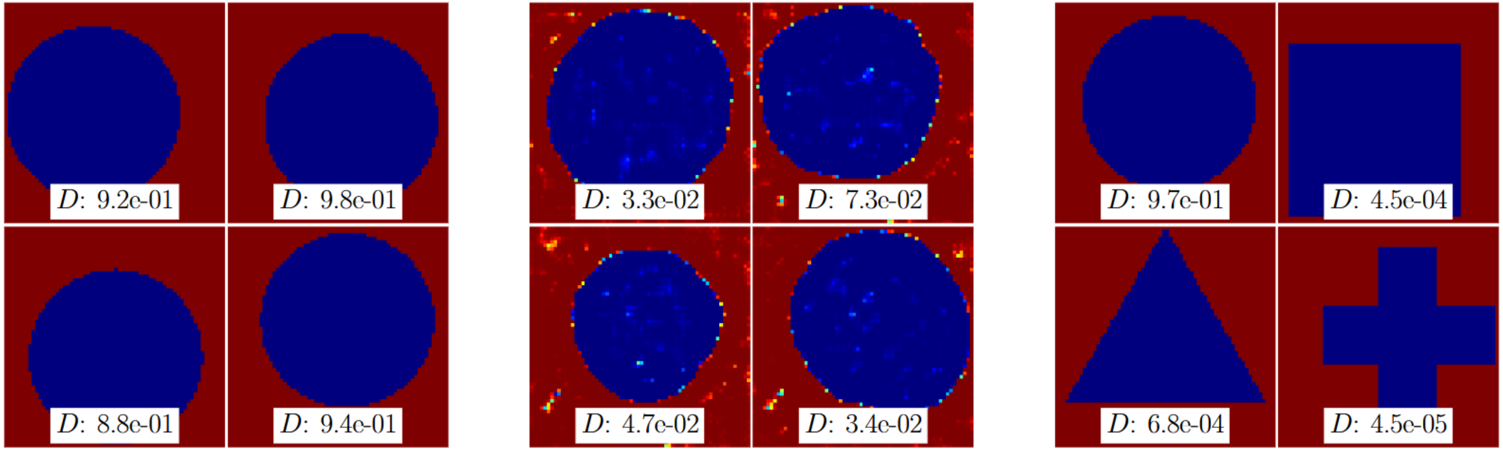
- E.27 Autoencoder (C)
  - Apply an autoencoder as an anomaly detector. First train the autoencoder on normal data (using a dataset consisting of randomly distributed circles). Next apply the autoencoder to anomolous data (using a dataset consisting of randomly distributed circles and squares). Compare the reconstruction errors with those obtained with normal data.

8.7.3.2 Generative Adversarial Networks for Anomaly Detection

Generative adversarial networks enable outlier detection and property monitoring for additive manufacturing of complex structures, Henkes et al. 2024

- Training of generative adversarial network on ”normal data”, i.e., without anomalies
- Detection of outliers
  - By inability to reconstruct the input image from noise (requires optimization with respect to input)
  - <u>Through the discriminator</u>
    - Discriminator cannot distinguish between real & fake ”normal data”
    - Anomalies outside of ”normal data” distribution are detectable

Diffusion models can be used similarly



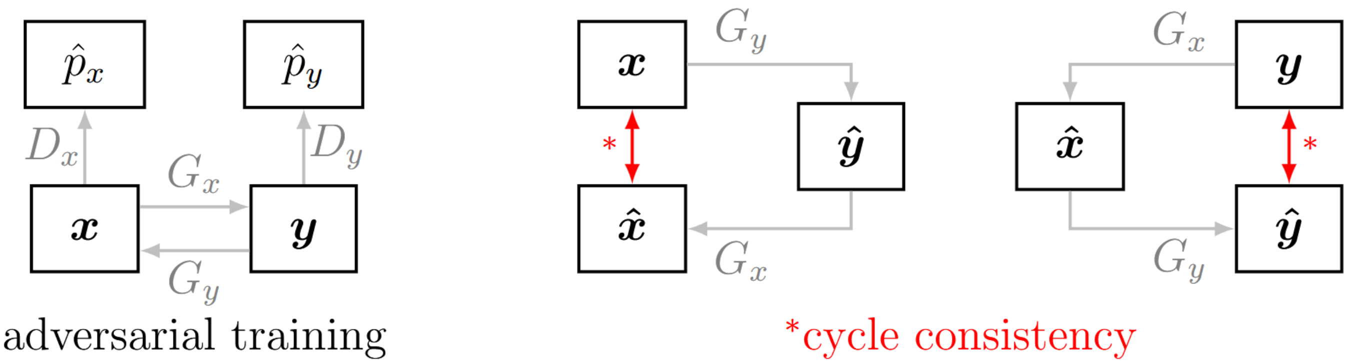
Real ”normal data” Fake ”normal data” Anomoulous data

Exercises

- E.29 Generative Adversarial Network (C)
  - Apply a generative adversarial network as an anomaly detector. First train the generative adversarial network on normal data (using a dataset consiting of circles). Next apply the trained discriminator to anomalous data (using a dataset consisting of squares, triangles, and crosses). Compare the discriminator score to the scores obtained with normal data.

8.7.4 Conditional Generation

- Conditional adversarial networks
  - Include inputs & labeled outputs (supervised)
- InfoGANs
  - Include latent code as input & disentanglement loss term (unsupervised)
- Variational autoencoder generative adversarial networks
  - Autoencoder architecture for the GAN generator
- CycleGANs



- tempoGAN (for temporal data, e.g., video)
  - Temporal coherence is assessed by second discriminator

Contents

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Deep Learning in Computational Mechanics – an introductory course, Herrmann et al. 2025

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book