Karlsruher Institut für Technologie

IRTG 2078
Project C2

Microstructure generation of carbon fiber reinforced polyamide 6 by a generative adversarial network (GAN) based on µCT data

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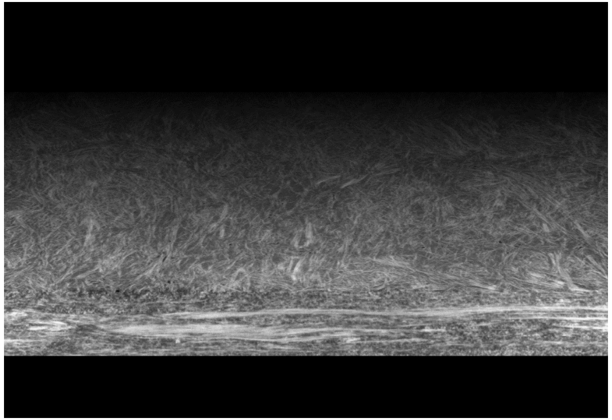
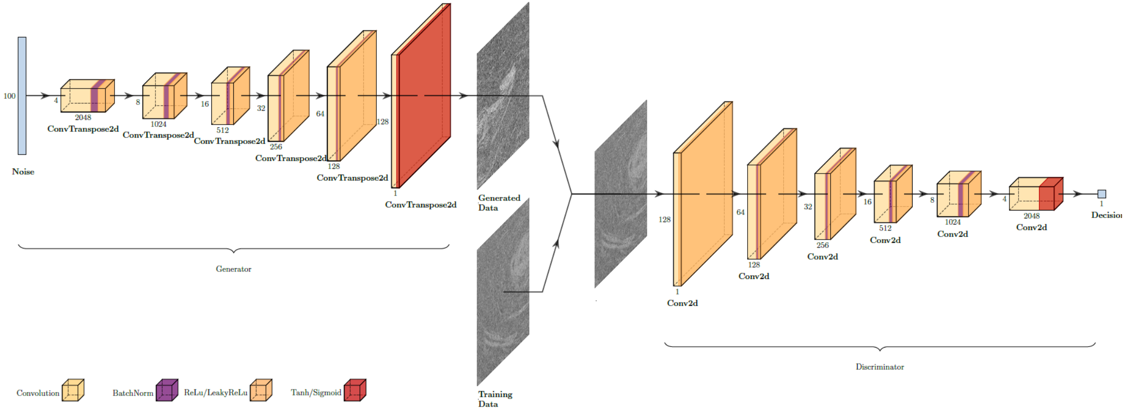
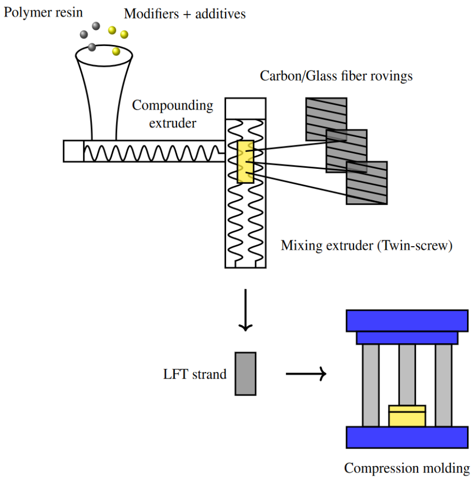
KIT, ICCM 2023, Belfast



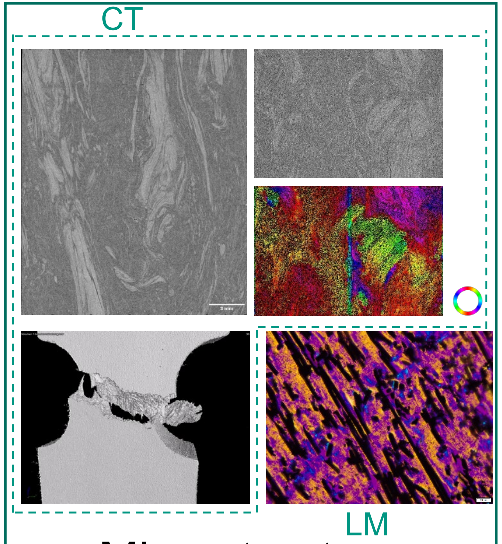


3rd generation IRTG 2078

Carbon fiber reinforced polyamide 6



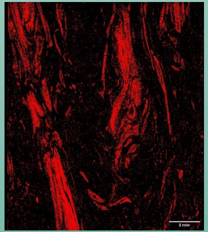
LFT-D-process



Microstructure characterization

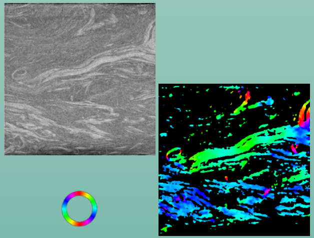
Microstructure characterization on volumetric images

Fiber volume content (FVC)



- Elastic properties
- Density

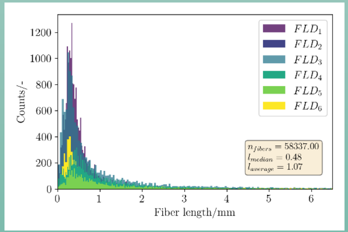
Fiber orientation distributions



- Elastic properties
- Creep behaviour

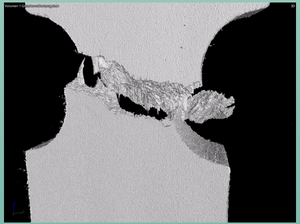
$$\begin{bmatrix} 0.105635 & -0.093760 & 0.008141 \\ -0.093760 & 0.859305 & -0.104421 \\ 0.008141 & -0.104421 & 0.035060 \end{bmatrix}$$

Fiber length distribution (FLD)



- Damage initiation
- Flow behaviour

In-situ tests



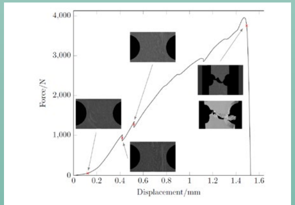
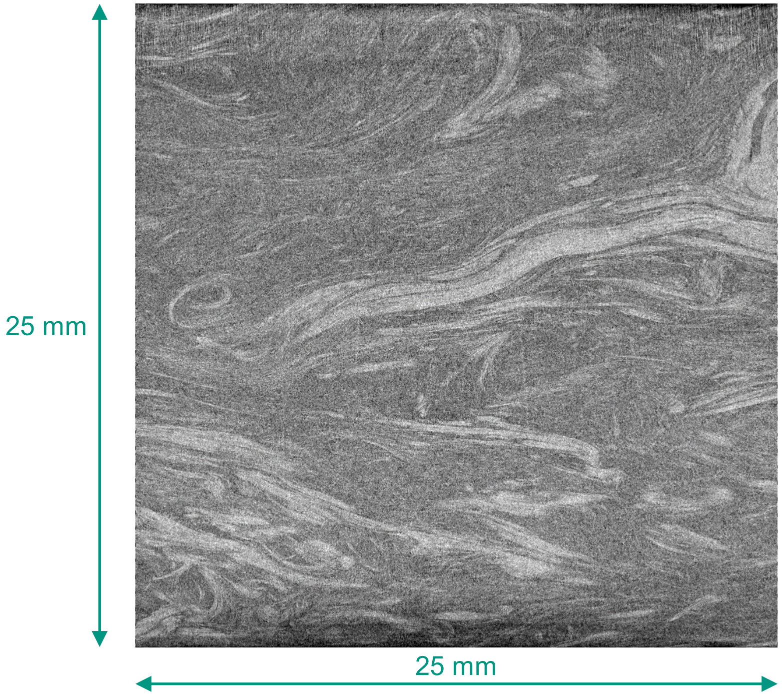


Figure 1: Force-displacement-curve for in-situ tensile test of PA6/CF sample

BUT: Low image quality of CFRP scans

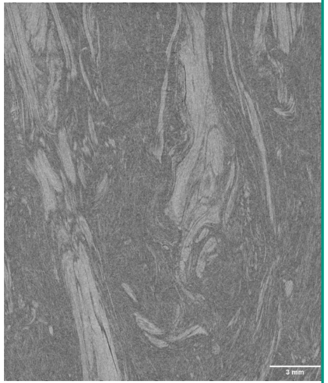
- **Low contrast** between carbon fiber and polymer
- High resolution needed due to **small diameter** of carbon fiber
- Both leads to high amount of salt and pepper **noise** in CT scans

→ Generate realistic microstructures in order to understand behavior better

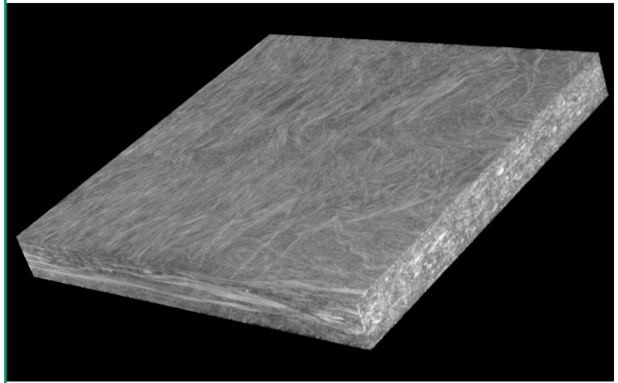


Institut für Angewandte Materialien – Werkstoffkunde

State of the art: Microstructure generation

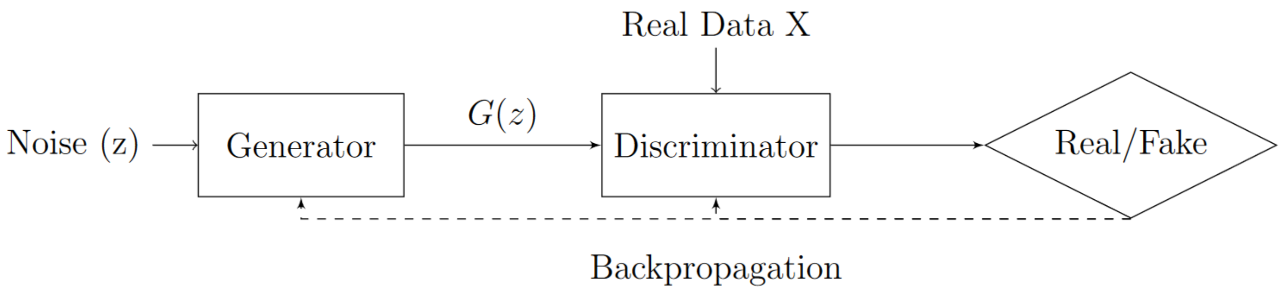


- Conventional approach:
  "sphere-packing algorithms" (RSA [1], Lubachevsky-Stillinger [2], mechanical contraction [3], Torquato-Jiao[4])
- Problems for higher FVC or fiber curvature
- Newer, improved approaches (Schneider 2022 [5])



- Alternative: AI-based approach
- Generative adversarial networks (GANs) introduced by Goodfellow et al. in 2014 [6]

Generative adversarial network (GAN)



$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D(\boldsymbol{x}^{(i)}) + \log(1 - D(G(\boldsymbol{z}^{(i)})))\right] . \tag{1}$$

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(1 - D(G(\boldsymbol{z}^{(i)}))). \tag{2}$$

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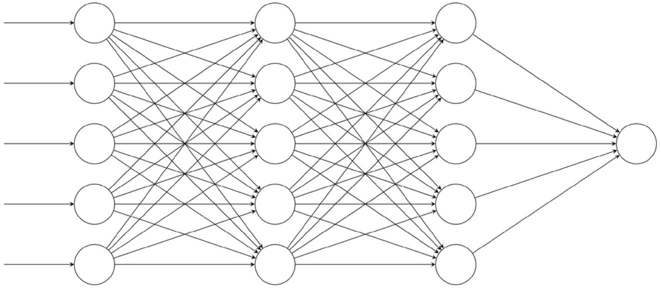
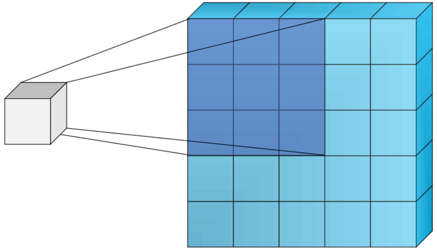
GAN vs. DCGAN

- Dense layers (feed-forward)



- Continuous convolution

$$(f * g)(x) := \int f(\tau)g(x - \tau)d\tau$$



10	10	10	0	0	0
10	10	10	0	0	0
10	10	10	0	0	0
10	10	10	0	0	0
10	10	10	0	0	0
10	10	10	0	0	0

Image

$*$

1	0	-1
1	0	-1
1	0	-1

3×3 filter

$=$

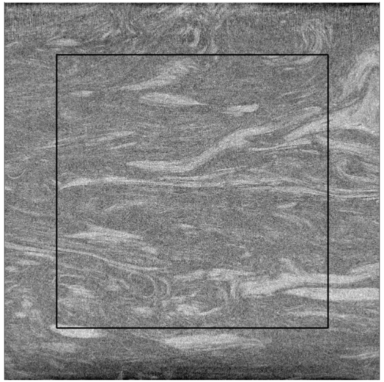
0	30	30	0
0	30	30	0
0	30	30	0
0	30	30	0

Feature map

Input data and pre-processing

1. Cutting

1024×1024



2. Resizing

128×128

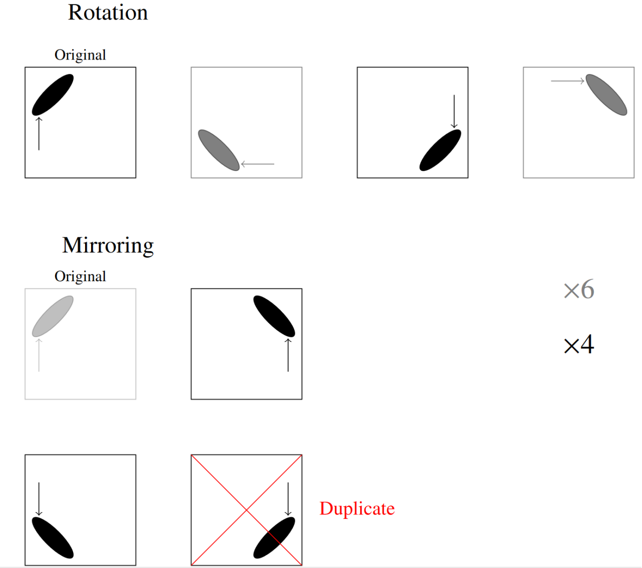
3. Normalization

$2^8 = 256\ values$

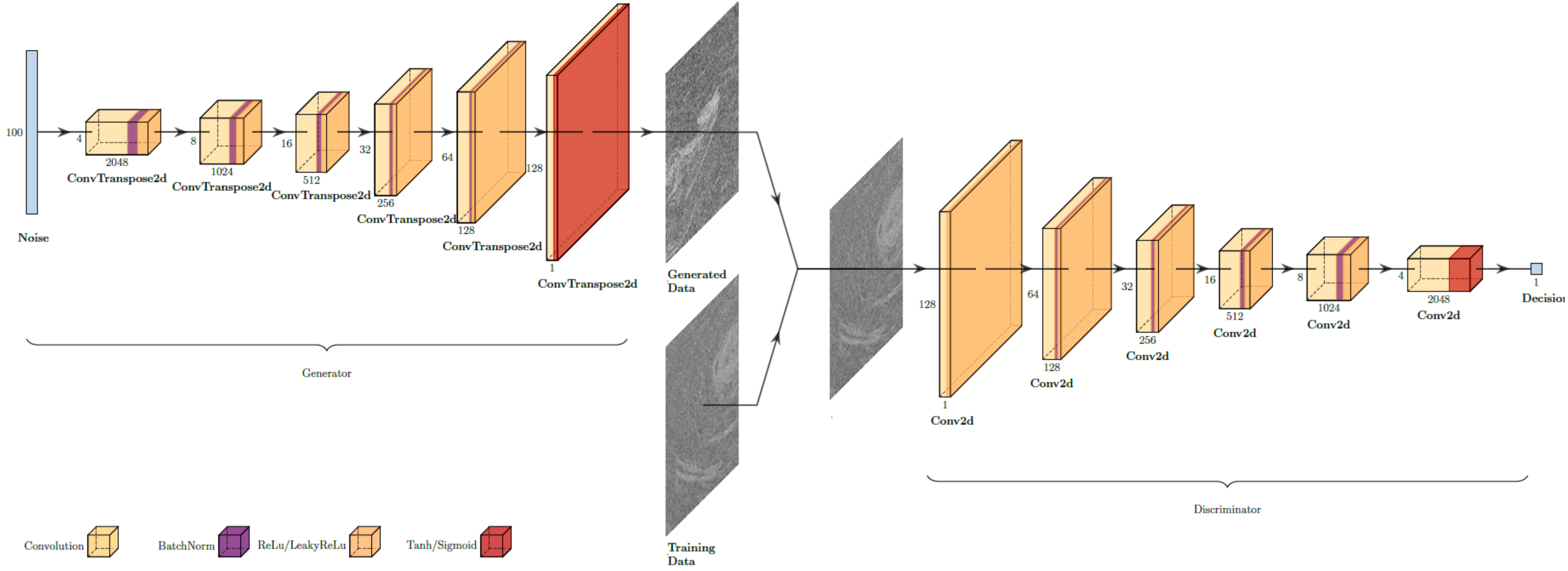
$\in [0,1] \rightarrow \in [-1,1]$

$$x_{train,new} = \frac{x_{train} - \mu_{train}}{\sigma_{train}}$$

4. Augmentation



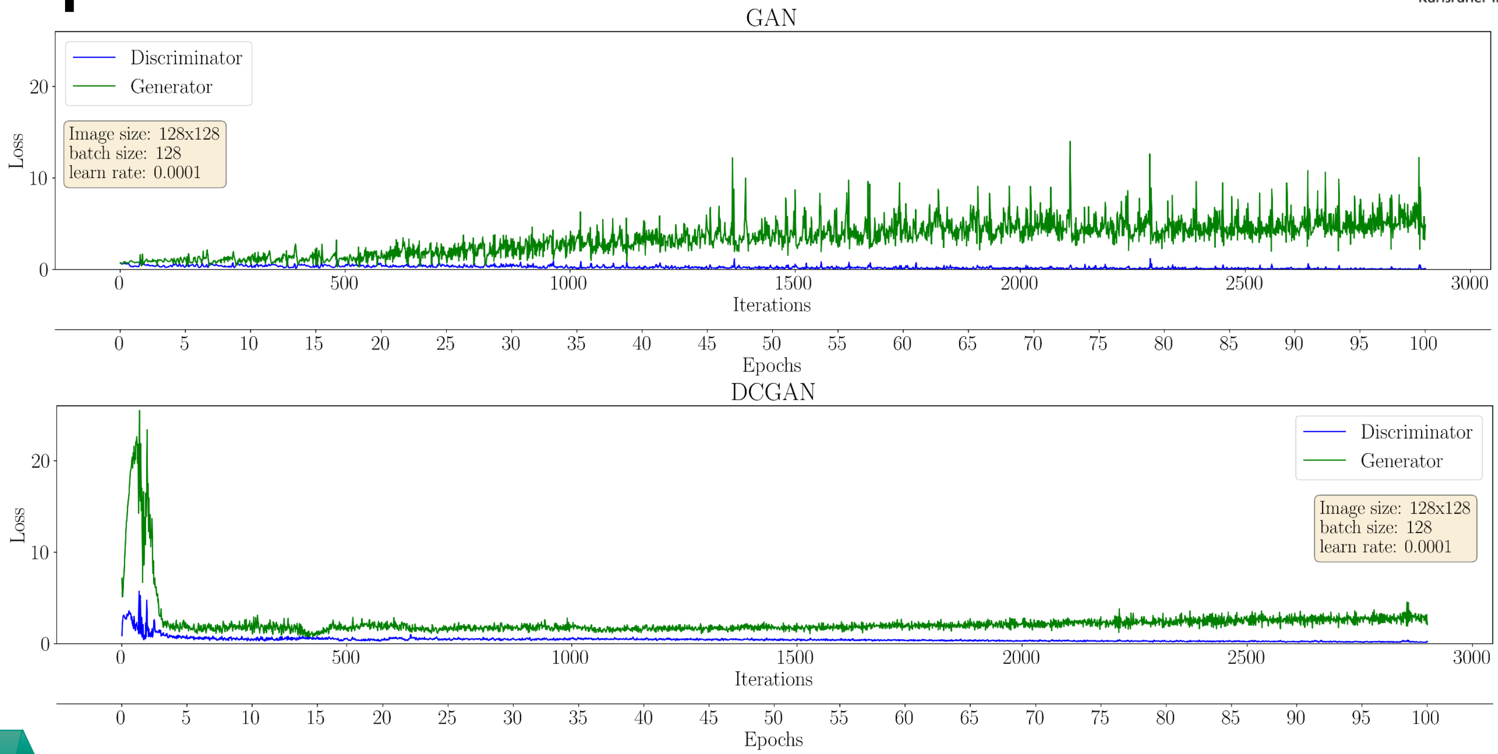
DCGAN network architecture



Additional parameters

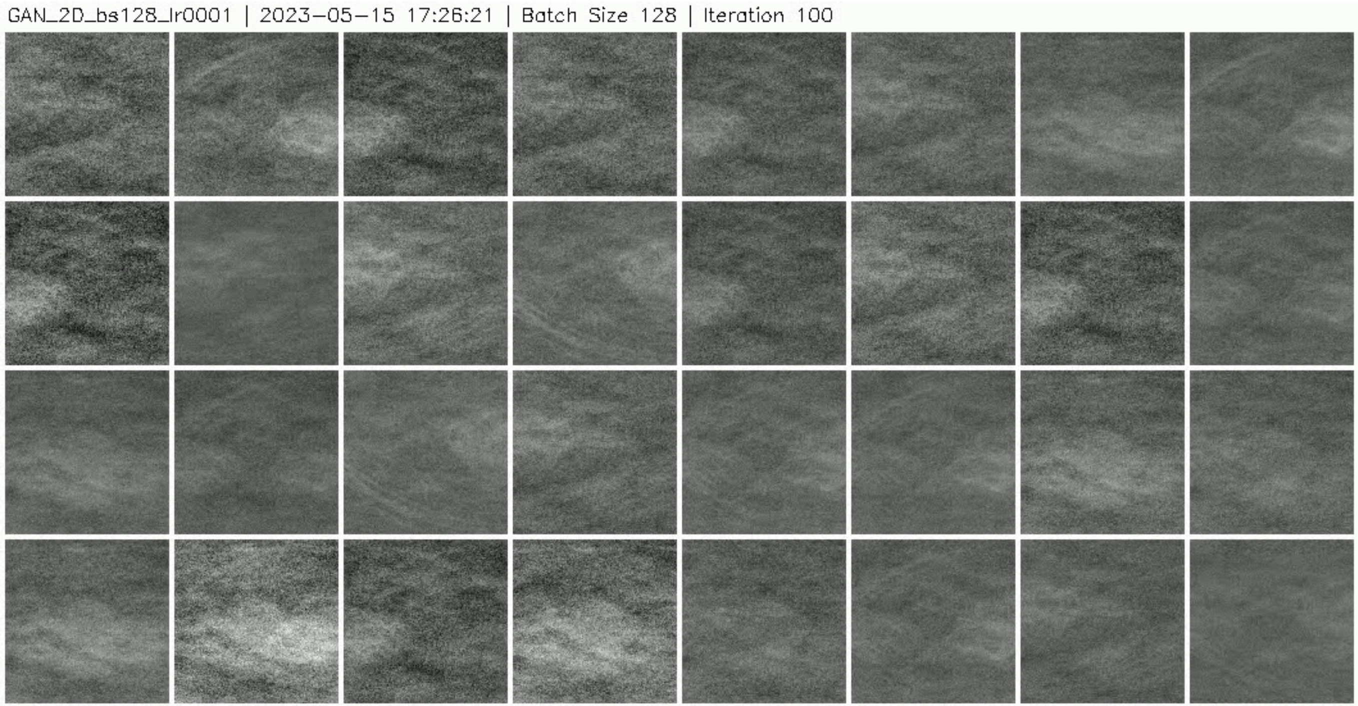
Parameter	Chosen value
Learning rate	**0.0001**, 0.0002, 0.0005
Optimizer	Adam
Loss function	**BCE**, Wasserstein
Batch size	32, 64, **128**
Epochs	50, **100**, 150
Kernel size (convolution)	4×4, 5×5

Loss plot

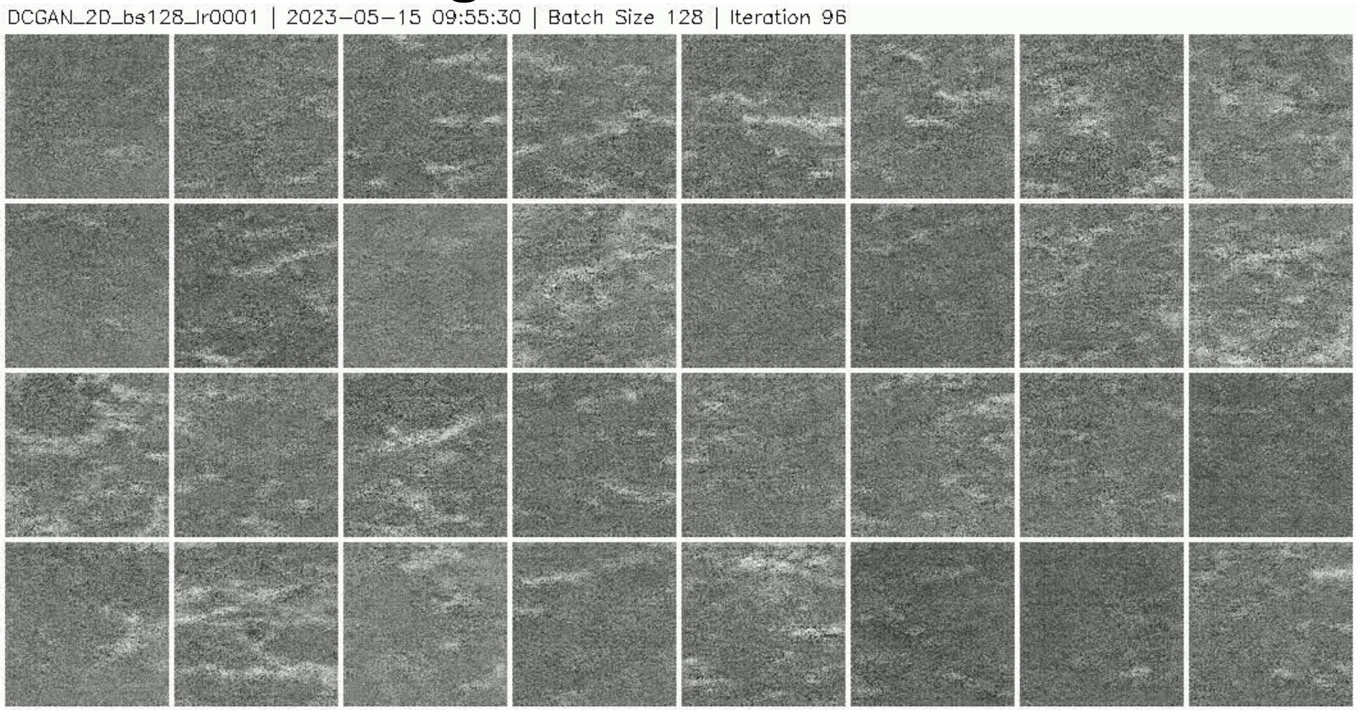


Motivation & state of the art | Methods | **Results** | Discussion | Further steps/questions

Generated images GAN



Generated images DCGAN



Frêchet Inception Distance (FID)

$d(X, Y) = (\mu_X - \mu_Y)^2 + (\sigma_X - \sigma_Y)^2$ "univariate"

FID = $||\mu_X - \mu_Y||^2 - Tr(\sum_X + \sum_Y - 2\sqrt{\sum_X \sum_Y})$ "multivariate"

X, Y: Real and fake embeddings (activation from Inception model)

μ_X and μ_Y: Magnitudes of vector X and Y

$\sum_X, \sum_Y$: Covariance matrix of the vectors

FID

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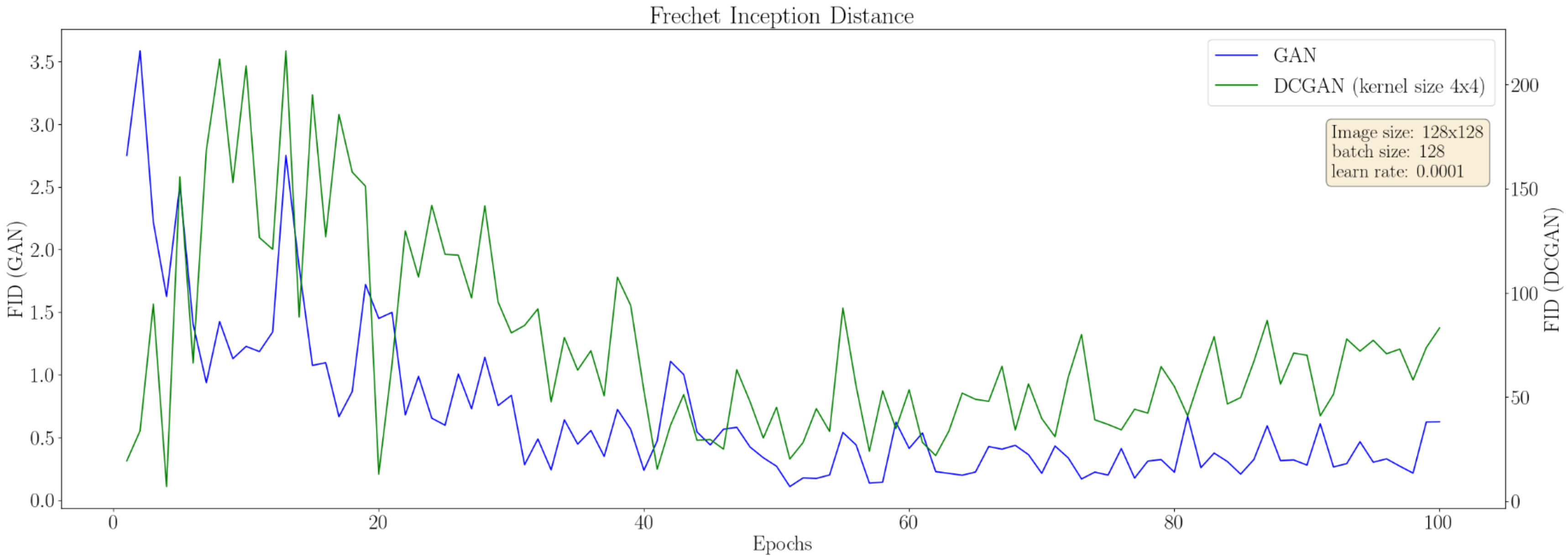
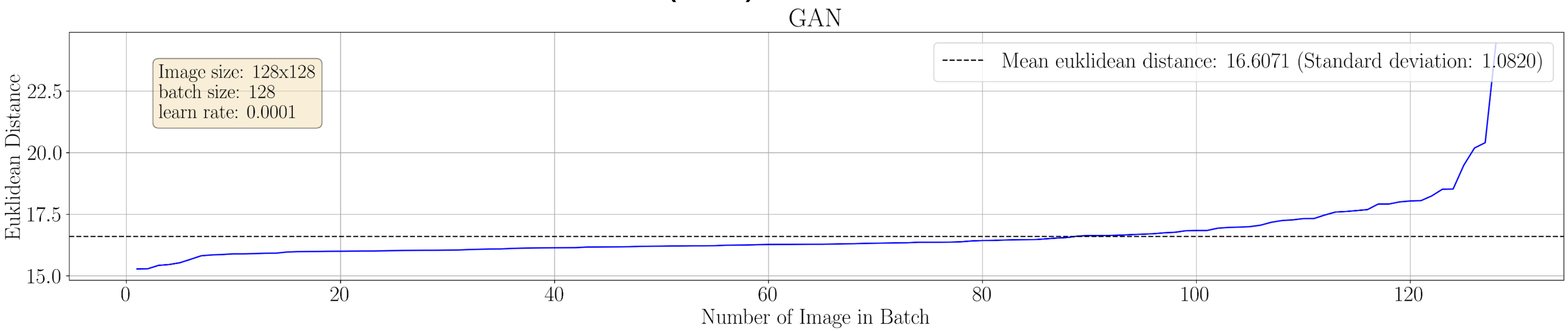
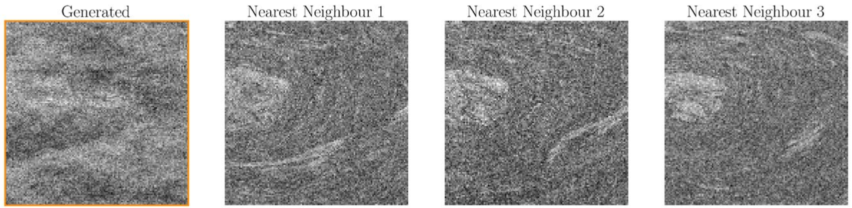


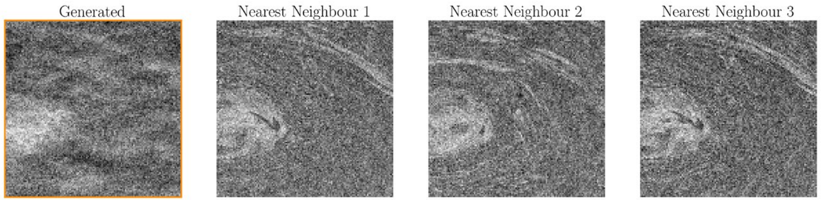
Motivation & state of the art | Methods | **Results** | Discussion | Further steps/questions

Nearest neighbor GAN

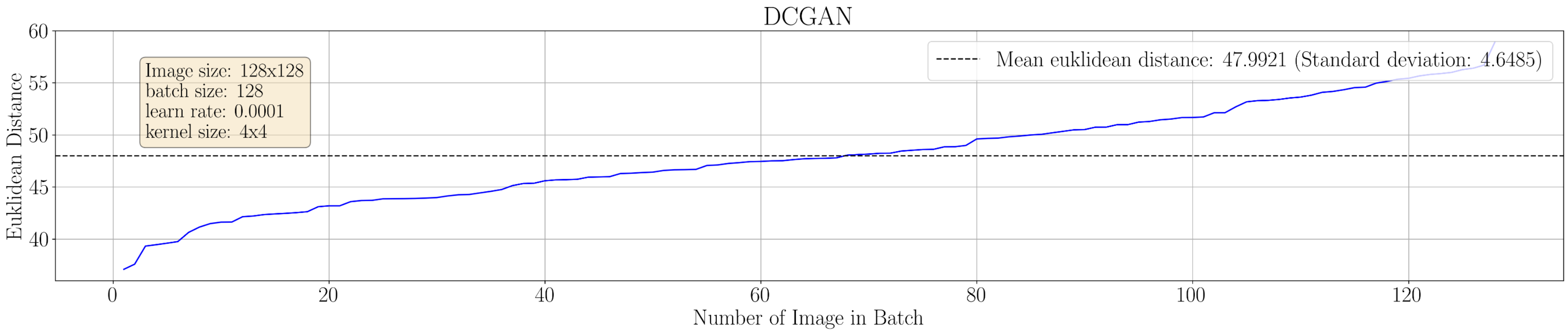
- Based on Euklidean distance (ED): $d(p,q) = \sqrt{(q_1 - p_1)^2 + (q_2 - p_2)^2}$

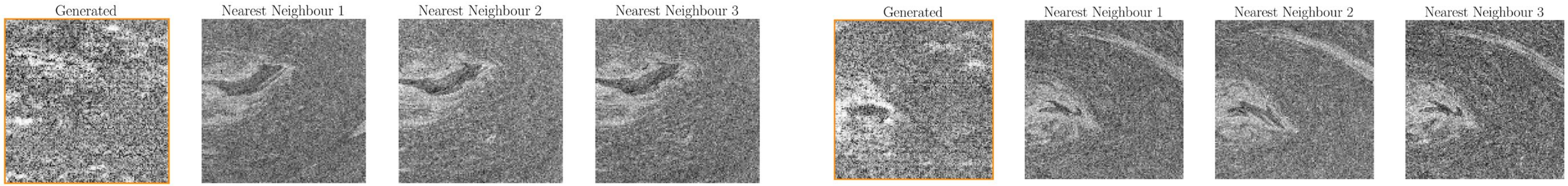






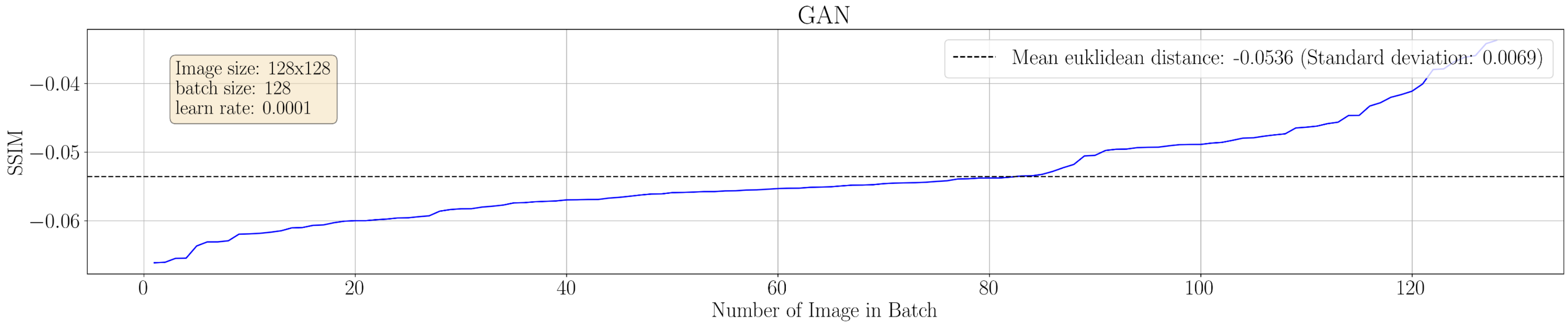
Nearest neighbor DCGAN

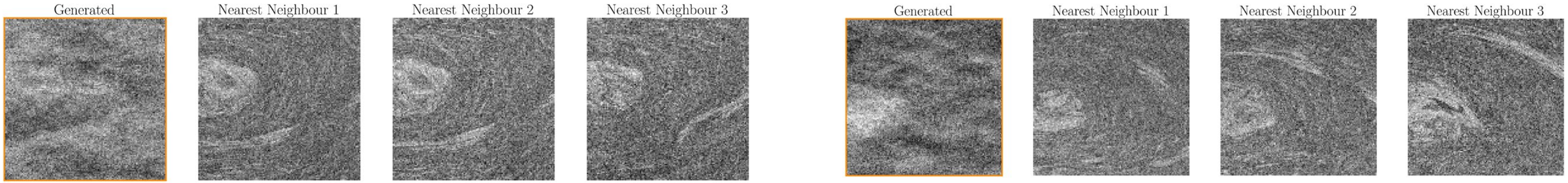




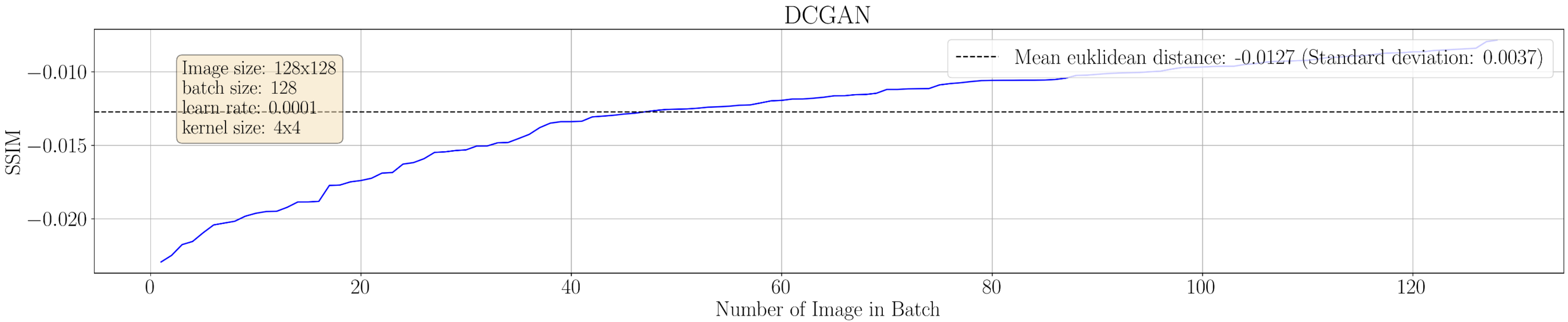
SSIM GAN

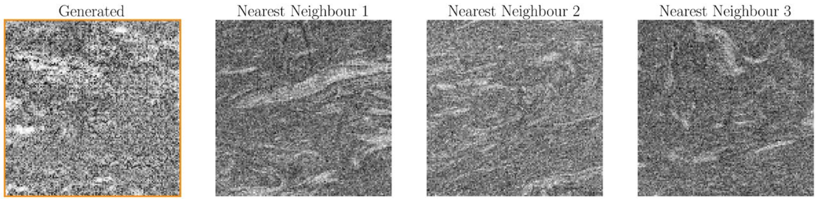
$$SSIM(x,y) = \frac{(2\mu_x\mu_y + c_1)(2\sigma_{xy} + c_2)}{(\mu_x^2 + \mu_y^2 + c_1)(\sigma_x^2 + \sigma_y^2 + c_2)}$$

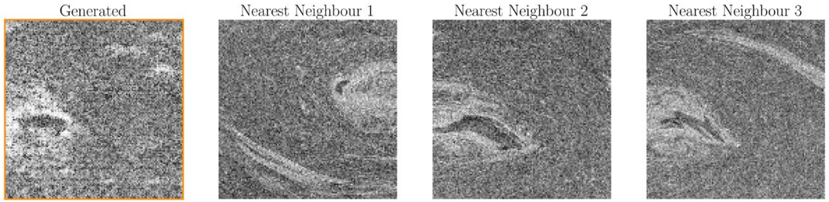




SSIM DCGAN


DCGAN
Image size: 128x128
batch size: 128
learn rate: 0.0001
kernel size: 4x4
Mean euklidean distance: -0.0127 (Standard deviation: 0.0037)
SSIM
−0.010
−0.015
−0.020
0
20
40
60
80
100
120
Number of Image in Batch


Generated
Nearest Neighbour 1
Nearest Neighbour 2
Nearest Neighbour 3


Generated
Nearest Neighbour 1
Nearest Neighbour 2
Nearest Neighbour 3

Discussion

- **DCGAN** reproduces **noise** more strongly
- **GAN** produces images very **close to training** data (structurally)
- Normal GAN: nearest neighbors determined with ED hardly differ from those determined with SSIM
- DCGAN: for images deviating more strongly from training data, more plausible nearest neighbors are found with SSIM (however, some results still out of line)
- SSIM value could become interesting again, especially at higher resolutions

Outlook

- Median filter for input data
- Higher resolution of input data
- More input data
- Texture quantification (Haralick entropy, etc.)
- Adaption of network for Wasserstein loss (e.g. RMS prop as optimizer)
- Binarization of input data?
- Super resolution network in front of GAN?

Thanks for your attention!



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Literature

[1] Feder J. Random Sequential Adsorption. Journal of Theoretical Biology 1980;87(2):237–54. https://doi.org/10.1016/0022-5193(80)90358-6.

[2] Lubachevsky BD, Stillinger FH. Geometric properties of random disk packings. Journal of Statistical Physics 1990;60(5/6):561–83. https://doi.org/10.1007/BF01025983.

[3] Williams SR, Philipse AP. Random packings of spheres and spherocylinders simulated by mechanical contraction. Phys Rev E Stat Nonlin Soft Matter Phys 2003;67(5 Pt 1):51301. https://doi.org/10.1103/PhysRevE.67.051301.

[4] Torquato S, Jiao Y. Robust algorithm to generate a diverse class of dense disordered and ordered sphere packings via linear programming. Phys Rev E Stat Nonlin Soft Matter Phys 2010;82(6 Pt 1):61302. https://doi.org/10.1103/PhysRevE.82.061302.

[5] Schneider M. An algorithm for generating microstructures of fiber-reinforced composites with long fibers. Numerical Meth Engineering 2022. https://doi.org/10.1002/nme.7110.

[6] Goodfellow IJ, Pouget-Abadie J, Mirza M, Xu B, Warde-Farley D, Ozair S et al. Generative Adversarial Networks; 2014.