

Generative Models: Part II

Advanced GAN Techniques & Application in Particle Physics

Wasserstein GANs

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RWTH Aachen

23.03.2022 Deep Learning Weeks, Uppsala

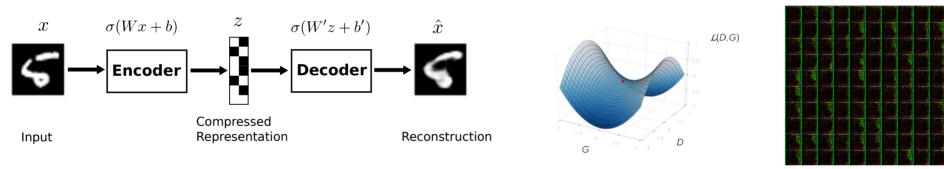


Recap – Generative Models



Variational Autoencoder

- Hidden representation follows low dimensional arbitrary prior distribution
- Trained decoder part can be used as generator to produce new samples



Generative Adversarial Networks

- Hand-coded loss is replaced by discriminator (tries to discriminate between fake samples and real samples)
- Adversarial training: generator and discriminator trained "against" each other
- Generator tries to fool discriminator

Outline



- I. Deep Learning Basics short hands-on
- II.Convolutional Neural Networks short hands-on **BREAK**
- III.Introduction to Generative Adversarial Networks (GANs)
- IV. Tutorial: Implementation of GANs

- V.Latest developments & advanced techniques
 - Wasserstein GANs
- VI.Application in physics research
 - Simulation acceleration, domain adaption

BREAK

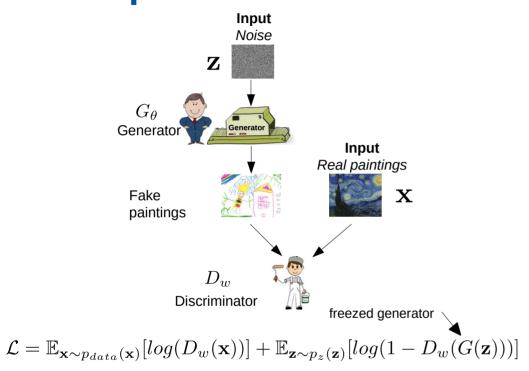
VII.Tutorial: Implementation of Wasserstein GANs

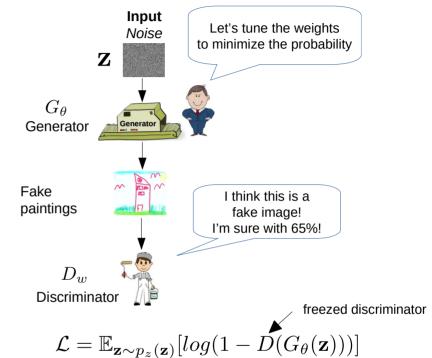


Feel free to ask questions during the seminar!
Just "raise" your hand...

Recap – Generative Adversarial Networks







Adversarial framework:

- Train generator to fool discriminator with fake samples, train discriminator to detect fake samples
- Iteratively (after each batch update) update generator and discriminator

Recap - Manifold Hypothesis

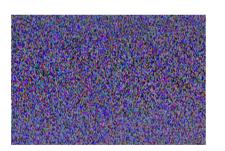


Idea: Manifolds of meaningful pictures are highly concentrated with very little volume and embedded in a very high dimensional space

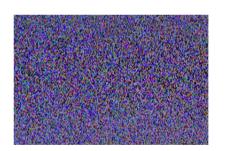
- Generation of images is a very challenging task
- Correlations / probability dimension are high dimensional
- **Example:** Try to generate images randomly:



Goal



Sample 1



Sample 100,000



You will even never reach this "neighborhood sample"

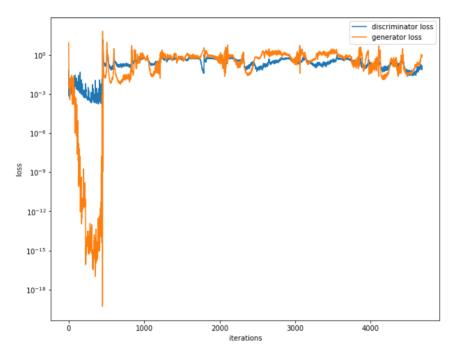
"To deal with a 14-dimensional space, visualize a 3-D space and say 'fourteen' to yourself very loudly.

Everyone does it." - G. Hinton

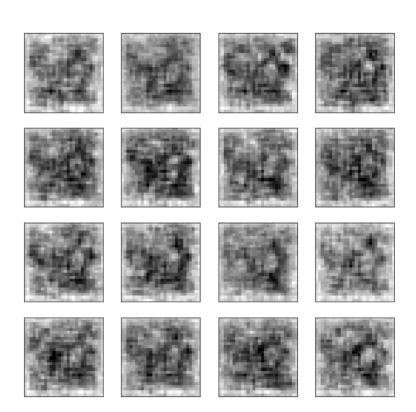
Results Fashion MNIST





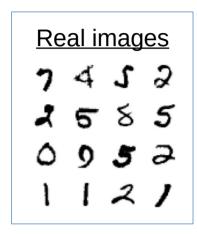


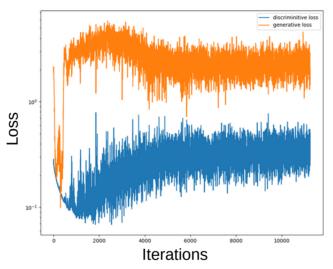
- Challenging training!
- "Weak convergence" after 3000 iterations
- Complex models show very instable training



Results







- GAN produces meaningful images after ~5 epochs
- Loss do not correlate with image quality
- Not stable training

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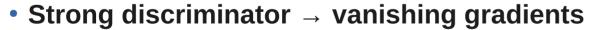
Interpreting the Adversarial Loss



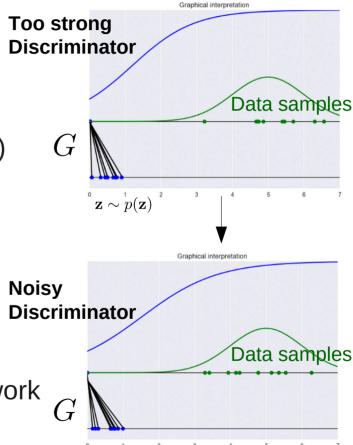
Emanuele Sansone: Tutorial on Generative Adversarial Networks (GANs) - GitHub

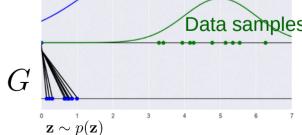
- GANs are hard to train → Nash equilibrium
 - generator ← → discriminator

- Loss is hard to interpret (depends on discriminator)
 - no correlation with image quality



- Best: generator and discriminator on same scale
 - Inexact noisy training → Rarely converging framework



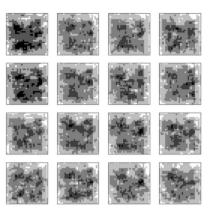


Mode Collapsing - Helvetica Scenario

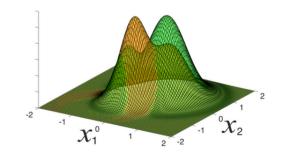


Problem: GANs often suffer from mode collapsing

- Many $\mathbf{z} \sim p(\mathbf{z})$ collapse towards restricted space in P_r
 - Generator produce samples of a limited phase space
 - Example: generate only digits 1 and 8



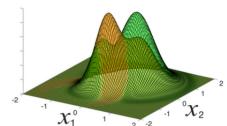
- Discriminator feedback is insensitive to complete phase-space
 - Will focus on point(s) of phase space the generator do not cover
- Discriminator will push generator to this mode → cycling behavior
- Need different (softer) metric to address these issues!



GAN Objective



• By fooling the discriminator the generator minimize distribution differences $\rightarrow P_{\theta} \approx P_{r}$



• GAN training similar to minimizing Jensen-Shannon divergence (assume optimal discriminator)

$$\mathcal{D}_{JS}(P_r||P_{\theta}) = \mathcal{D}_{KL}(P_r||P_m) + \mathcal{D}_{KL}(P_{\theta}||P_m) \qquad P_m = \frac{1}{2}(P_r + P_{\theta})$$

- Symmetrized and smoothed version of the Kullback-Leibler divergence
- * Fails to provide a meaningful value when two distributions are disjoint
 - In very high dimensional manifolds the distributions between generated and real samples are disjoint

Wasserstein Distance



Also known as Earth Mover's distance (EMD)

Ensures smallest cost

Traveling distance

$$\mathcal{D}_W(P_r||P_\theta) = \inf_{\gamma \in \Pi(P_r, P_\theta)} \mathbb{E}_{(x,y) \sim \gamma}[||x - y||]$$

Transportation plans

- Describes **minimal cost** to move distribution P_{θ} on P_{r} and vice versa
 - Cost: mass * distance



Distribution Similarity - Metrics



- Kullback-Leibler divergence
 - Not finite, not symmetric

$$\mathcal{D}_{KL}(P_r||P_{\theta}) = \mathbb{E}_{\mathbf{x} \sim P_r} log\left(\frac{P_r}{P_{\theta}}\right)$$

Jensen-Shannon divergence

$$\mathcal{D}_{JS}(P_r||P_{\theta}) = \mathcal{D}_{KL}(P_r||P_m) + \mathcal{D}_{KL}(P_{\theta}||P_m)$$

✓ Symmetric

- Wasserstein distance
 - ✓ Symmetric
 - Meaningful distance measure for disjoint distributions

$$P_m = \frac{1}{2}(P_r + P_\theta)$$

For disjoint distributions:

$$\mathcal{D}_{KL}(P_{\theta}||P_r) = \infty$$

$$\mathcal{D}_{KL}(P_r||P_\theta) = \infty$$

$$\mathcal{D}_{JS}(P_r||P_{\theta}) = \log(2)$$

In GAN training we are dealing with disjoint distributions!

Kantorovich-Rubinstein Duality

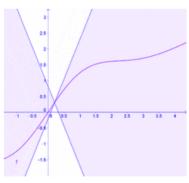


• Wasserstein distance (formal definition very intractable) can be expressed

$$\mathcal{D}_W(P_r||P_\theta) = \sup_{f \in Lip_1} \mathbb{E}_{x \sim P_r}[f(x)] - \mathbb{E}_{\tilde{x} \sim P_\theta}[f(\tilde{x})]$$

- supremum = least upper bound
- f = Set of 1-Lipschitz functions
- $\mathbb{E}_{x \sim P_r}[f(x)]$ Expectation value when applying set of 1-Lipschitz functions on samples from real samples
- ightharpoonup Approximate $fpprox f_w$ with neural network

1-Lipschitz functions



Slope everywhere less equal 1!

The WGAN Concept

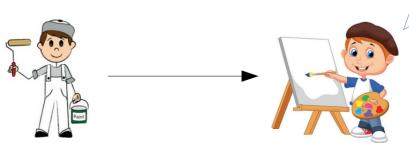


$$\mathcal{D}_W(P_r||P_\theta) = \sup_{f \in Lip_1} \mathbb{E}_{x \sim P_r}[f_w(x)] - \mathbb{E}_{\tilde{x} \sim P_\theta}[f_w(\tilde{x})]$$
 Real samples Generated samples $\tilde{x} = G_\theta(z)$

 f_w = neural network (discriminator \rightarrow critic)

- Neural network carries the Lipschitz continuity constraint
- Critic network estimate Wasserstein distance between generate and real samples

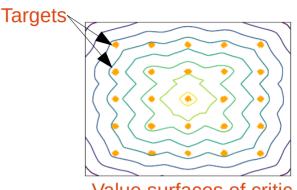
To paint more realistic images:
Just change your brush!



Discriminator

Gradient Penalty

- Implement Lipschitz constraint
- Build up space for meaningful discriminator feedback
- Without Lipschitz constrain
 - Critic will not converge → No Wasserstein!



Value surfaces of critic

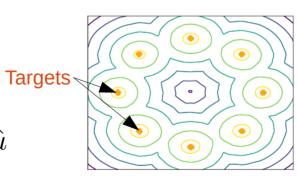
Extend objective with additional term:

Penalize gradients being different from 1

$$\mathcal{L}_{GP} = \underset{\text{hyperparameter}}{\lambda} \mathbb{E}_{\hat{u} \sim P_{\hat{u}}}[(||\nabla_{\hat{u}} f_w(\hat{u})||_2 - 1)^2]$$

ullet Sample gradients along line between event mixture \hat{u}

$$\hat{u} = \epsilon x + (1 - \epsilon)\tilde{x}$$
 $0 \le \epsilon \le 1$



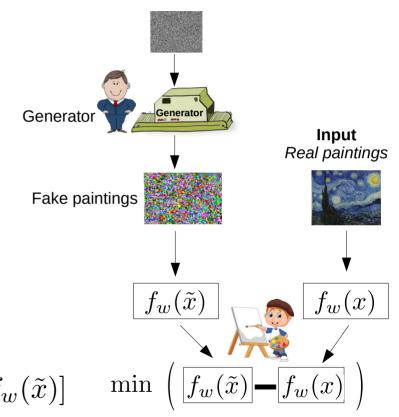
Value surfaces of critic

Critic



- Critic approximates Wasserstein distance
 - Carries Lipschitz constraint
 - Ensures meaningful and stable gradients
- No explicit formulation of loss function
 - Approximate loss function itself
 - Maximize difference $|f_w(\tilde{x}) f_w(x)|$
- Critic should be always trained to convergence
 - Usually ~ 5 10 iterations

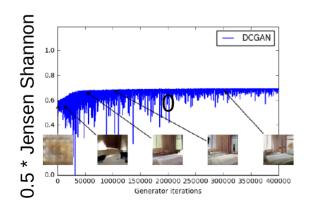
$$\mathcal{D}_W(P_r||P_\theta) = \sup_{f \in Lip_1} \mathbb{E}_{x \sim P_r}[f_w(x)] - \mathbb{E}_{\tilde{x} \sim P_\theta}[f_w(\tilde{x})]$$

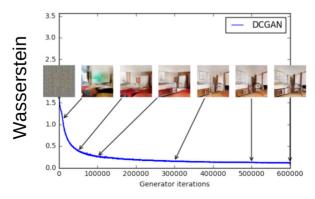


Advantages WGAN vs. GAN



- Train critic to convergence ensure quality gradients
- Insensitive to mode collapsing
- Meaningful metric / objective → allow for easy hyperparameter search
 - Convergence correlates with generation quality
- Change from Jensen Shannon divergence to Wasserstein-1
- We get feedback from an art expert!



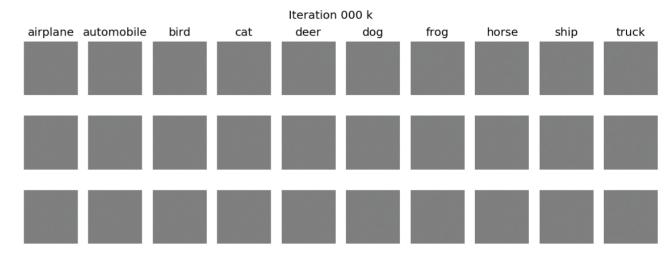




Results

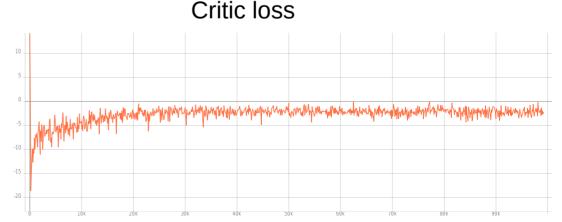
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- WGAN generates images with much better quality
- Critic loss converges
- Loss correlates with images quality



Wasserstein GANs

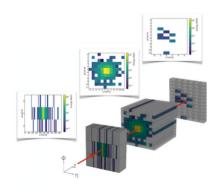
- Allow stable training of GANs
 - Train critic to convergence
 - Precise feedback for generator
- Prevent mode collapsing
- Provide meaningful loss

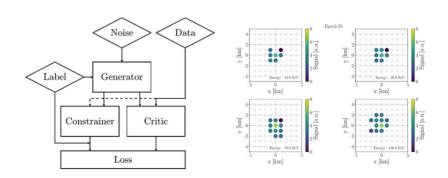


Application in Particle Physics



- Detector simulation are very time consuming
- Replace simulation programs like Geant4 with generative model
 - Reach speed-up of factor 10³ 10⁵
- Add constrainer networks to condition the generation process
 - Generator needs dependence (energy, particle type...)
 - Samples must comply with physics laws





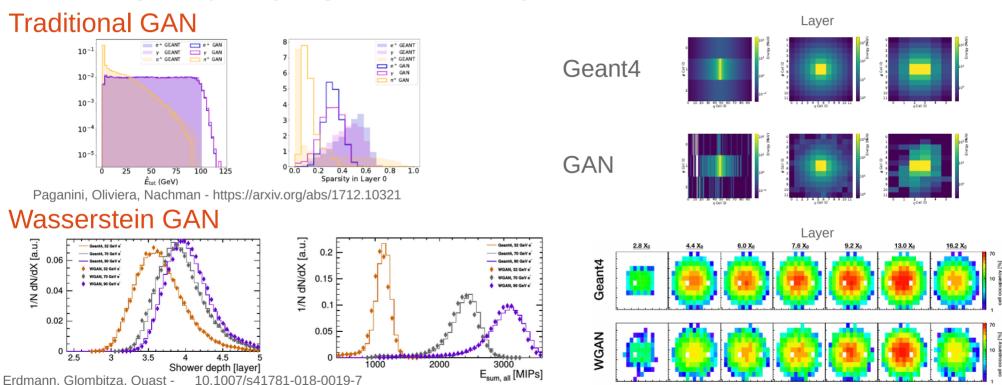
Paganini, Oliviera, Nachman - https://arxiv.org/abs/1712.10321

Erdmann, Geiger, Glombitza, Schmidt - https://arxiv.org/abs/1802.03325

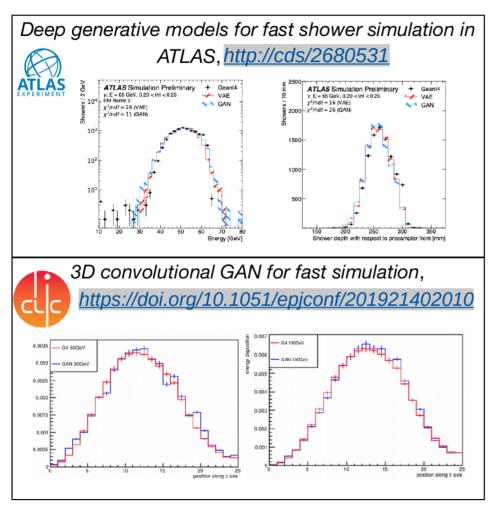
Generation of Calorimeter Images

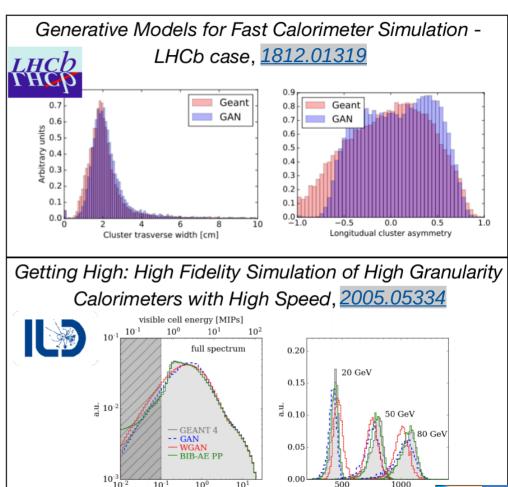


- Quality of images is crosschecked using physics observables
- Challenges: Sparsity, logarithmic intensity distribution



GAN applications for fast calorimeter simulation in other experiments 22





visible cell energy [MeV]

number of hits

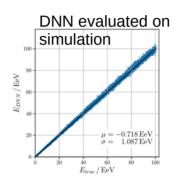
Simulation Refinement

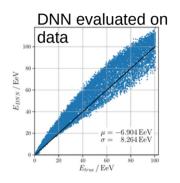


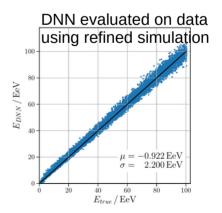
- Simulation data mismatches
- Predictive models can be sensitive to artifacts / mismatches existing in simulation

- Can lead to reconstruction errors
- Use adversarial networks with refinement constraint
- Train refiner to refine simulations





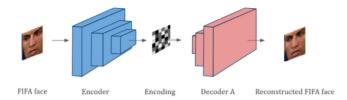


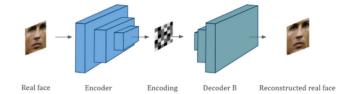


Simulation Refinement

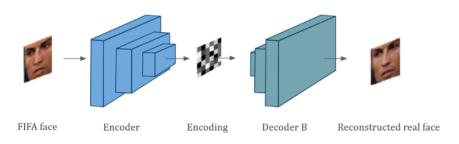


• Use auto encoder set up to mitigate data / simulation differences





- Simulation and data share encoder but different decoder (similar representation)
- After training: refine simulation with decoder trained to reconstruct data



Chintan Trivedi: Using Deep Learning to improve FIFA 18 graphics – Towards Data Science



Spectral Normalization for GANs



- Gradient penalty / regularization is most important for training GANs!
- WGAN-GP is state of the art
- Adapt Lipschitz constraint using Gradient "normalization" (penalty)
 - Also standard (NS-GAN) with gradient penalty performs well!

- Adapt Lipschitz constraint in the weights using the spectral norm
- Critic in WGAN-GP needs many iterations → slow training
- Spectral norm can be fast approximated using power iteration method
- Increased stability (high learning rates, high momentum rates)

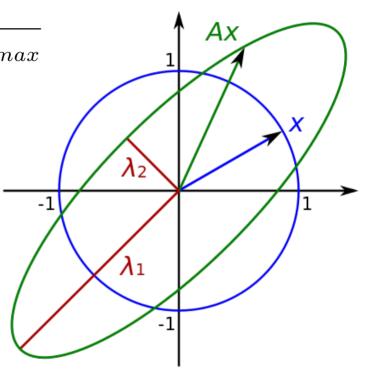
Spectral Norm



Spectral norm: "natürliche Matrixnorm"

$$||\mathbf{W}||_2 = \max_{x \neq 0} \frac{||\mathbf{W}x||_2}{||x||_2} = \max_{||x||_2 = 1} ||\mathbf{W}x||_2 = \sqrt{\lambda_{max}}$$

- Maximum stretch factor of unit vector after multiplication with matrix
- $\lambda_1 = \lambda_{max}$ = highest singular value ("Singulärwert") of the matrix



Spectral Normalization for GANs



- D(x) = discriminator
- Adapt WGAN-GP constraint (gradient wrt. x real and fake samples)
 - Use spectral normalization in each layer!
- Basic idea:

$$||D(x)||_{\text{Lip}} = \sup_{x} \sigma(\nabla_x D(x)) = \sup_{x} \sigma(\nabla_x Wx) = \sigma(W) \longrightarrow W_{\text{norm}} = \frac{W}{\sigma(W)}$$

- Cover Lipschitz constraint by normalizing the weights
- Gradient update:
 - Gradient penalizes updates in direction of highest singular value (in each layer)

SNGAN



discriminator

- discriminator weights cover Lipschitz constraint due to spectral norm
- "regularize" gradients → mode collapsing unlikely
- discriminator loss still meaningless → no critic / distance measure

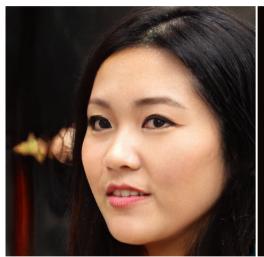
generator

- Also spectral normalization in generator improves stability
- enforce harmless mapping
- Framework trained with 1:1 discriminator / generator update ratio

Game: Which face is real?



http://www.whichfaceisreal.com/index.php

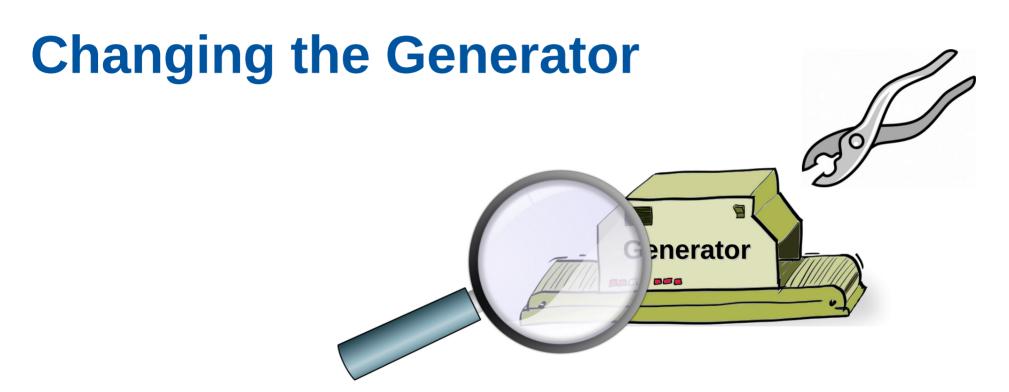








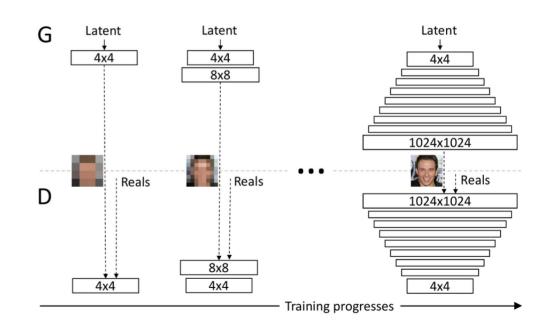




Progressive Growing

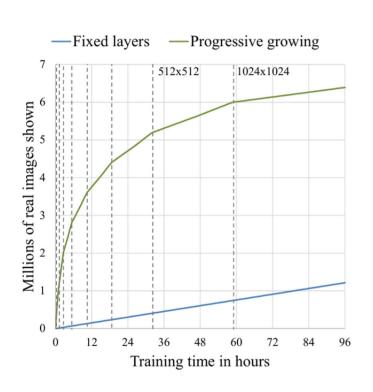


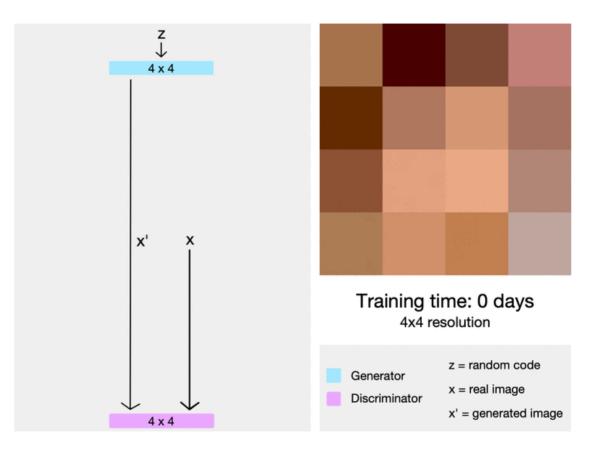
- Separation of training process in several steps
- Increase image resolution stepwise
- Beginning: (low resolution) data set has only few modes
 - small differences to be learned
- low resolution
 - learn large scale structure
- High resolution
 - learn fine details
- Speed up
 - Most iteration in the beginning



Progressive Training







Training on 8 Tesla V100!

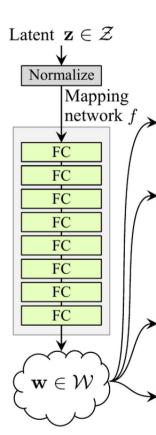
StyleGAN

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- Image contains of several style levels
- Change structure of generator
 - disentangle styles in architecture
 - Coarse (pose, face shape)
 - Medium (facial features, eyes closed)
 - Fine (finer hair details, exes)
 - Learning of high-level attributes
- Add additional noise
- Use medium representation of latent space
 - Use mapping network



High resolution: 1024 x 1024 pixels



StyleGAN

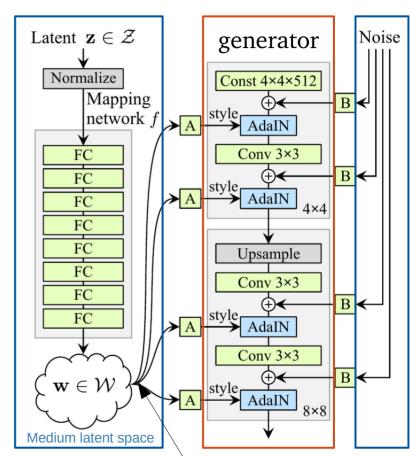


styles $\hat{=}$ $\mathbf{y} = (\mathbf{y}_s, \mathbf{y}_b)$

- Mapping network learns "medium" latent space
 - perceptually smoother latent space
- Generator input:
 - Styles control adaptive instance normalization

$$\mathbf{X}_i$$
 = feature map $AdaIN(\mathbf{x}_i,\mathbf{y}) = \mathbf{y}_{s,i} rac{\mathbf{x}_i - \mu(\mathbf{x}_i)}{\sigma(\mathbf{x}_i)} + \mathbf{y}_{b,i}$

- Styles re-scale features maps in generator at each representation level
- Add noise at each level of representation
 - Small image variations (natural images)
- Sample from restricted (truncated) phase space
 - Loss off variation → better quality



Tutorial on Generative Models Glombitza | RWTH Aachen | 03/22/22 | Deep Learning Weeks, Uppsala





https://www.youtube.com/watch?time continue=370&v=kSLJriaOumA

Summary



GANs

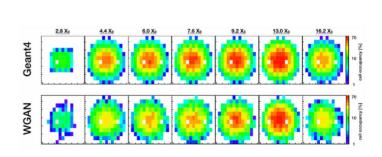
Delicate, hard to train (mode collapsing, vanishing gradients, meaningless loss)

Advanced techniques – WGAN, ProGAN, SNGAN

- Stabilize training process using smooth metric → meaningful distance measure
- Use regularization: penalize gradient, enforce spectral norm of the weights
- Imply prior on generator architecture (progressive growing, hierarchy control)

Generative Models in Physics Research

- Speed up simulations by factor 10³ − 10⁵
- Reduce data / simulation mismatches



References & Further Reading



- M. Erdmann, J. Glombitza, G. Kasieczka, U. Klemradt, Deep Learning for Physics Research, World Scientific, 2021, www.deeplearningphysics.org/
- Goodfellow et al.: Generative Adversarial Networks https://arxiv.org/abs/1406.2661
- Arjovsky, Chintala, Bottou: Wasserstein GAN https://arxiv.org/abs/1701.07875
- Gulrajani et al.: Improved Training of Wasserstein GANs https://arxiv.org/abs/1704.00028
- Paganini, Oliveira, Nachman: CaloGAN https://arxiv.org/abs/1712.10321
- Erdmann, Geiger, Glombitza, Schmidt https://arxiv.org/abs/1802.03325
- Erdmann, Glombitza, Quast: Calorimeter WGAN T. Comput Softw Big Sci (2019) 3: 4
- C. Trivedi: Using Deep Learning to improve FIFA 18 graphics Towards Data Science
- Emanuele Sansone: https://github.com/emsansone/GAN
- Miyato et al.: SNGAN- https://arxiv.org/abs/1802.05957
- T. Karras, S. Laine, T. Aila: A Style-Based Generator https://arxiv.org/abs/1812.04948



Tryout Deep Learning Yourself!

Find many physics examples at: http://www.deeplearningphysics.org/

For example:

- CNNs, RNNs, GCNs
- GANs and WGANs
- Anomaly detection, Denosing AEs
- Visualization & introspection and more



Generate Air Shower Footprints

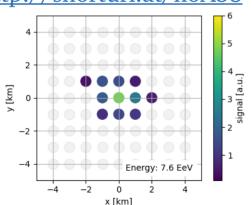




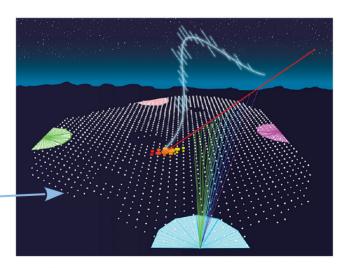
- Measurement of cosmic ray induced air showers
- Pierre Auger Observatory: Fluorescence (FD) and Surface Detector (SD)
 - FD: Telescopes measure light of excited nitrogen
 - SD: Water Cherenkov stations detect passage of charged particles
 - Simulation: 2D image sequence, Cartesian grid, 1-100 EeV protons

Open notebook:

http://shorturl.at/hoA38







https://physics.aps.org/articles/v9/125

Stay tuned...



Yang, Chou, Yang - https://arxiv.org/abs/1703.10847





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bicubic (21.59dB/0.6423) (23.53dB/0.7832) (21.15dB/0.6868) original

Figure 2: From left to right: bicubic interpolation, deep residual network optimized for MSE, deep residual generative adversarial network optimized for a loss more sensitive to human perception, original HR image. Corresponding PSNR and SSIM are shown in brackets. [4x upscaling]

Ledig et. al. - https://arxiv.org/abs/1609.04802



Isola, Zhu, Zhou, Efros - https://arxiv.org/abs/1611.07004

... there is much more going on!

Zhu, Park, Isola, Efros - https://arxiv.org/abs/1703.10593

The WGAN-GP Algorithm



Algorithm 1 WGAN with gradient penalty. We use default values of $\lambda = 10$, $n_{\text{critic}} = 5$, $\alpha = 0.0001$, $\beta_1 = 0$, $\beta_2 = 0.9$.

Require: The gradient penalty coefficient λ , the number of critic iterations per generator iteration n_{critic} , the batch size m, Adam hyperparameters α, β_1, β_2 .

Require: initial critic parameters w_0 , initial generator parameters θ_0 .

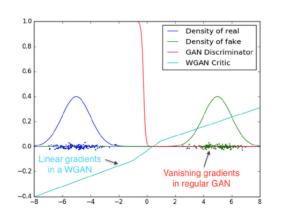
```
1: while \theta has not converged do
              for t = 1, ..., n_{\text{critic}} do
  3:
                     for i = 1, ..., m do
                            Sample real data x \sim \mathbb{P}_r, latent variable z \sim p(z), a random number \epsilon \sim U[0,1].
  4:
                            \tilde{\boldsymbol{x}} \leftarrow G_{\theta}(\boldsymbol{z})
                           \hat{\boldsymbol{x}} \leftarrow \epsilon \boldsymbol{x} + (1 - \epsilon)\tilde{\boldsymbol{x}}
 6:
                            L^{(i)} \leftarrow D_w(\tilde{x}) - D_w(x) + \lambda (\|\nabla_{\hat{x}} D_w(\hat{x})\|_2 - 1)^2
                     end for
 8:
                     w \leftarrow \operatorname{Adam}(\nabla_w \frac{1}{m} \sum_{i=1}^m L^{(i)}, w, \alpha, \beta_1, \beta_2)
 9:
              end for
10:
              Sample a batch of latent variables \{z^{(i)}\}_{i=1}^m \sim p(z).
11:
              \theta \leftarrow \operatorname{Adam}(\nabla_{\theta} \frac{1}{m} \sum_{i=1}^{m} -D_{w}(G_{\theta}(z)), \theta, \alpha, \beta_{1}, \beta_{2})
13: end while
```

Generator

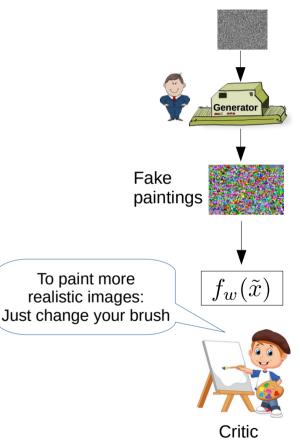
- Use critic feedback to increase generation quality
 - Minimize $\mathcal{D}_W(P_r, P_\theta)$ using gradient descent

$$\nabla_{\theta} \mathcal{D}_W(P_r, P_{\theta}) = -\mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} [\nabla_{\theta} f(G_{\theta}(\mathbf{z}))]$$

No vanishing gradients for the generator







Non Saturation GAN (NS-GAN)



- Use **label switching** to avoid vanishing gradients in discriminator
- Standard loss: minimize

$$Loss = \mathbb{E}_{\mathbf{z} \sim p_z(\mathbf{z})}[log(1 - D(G_{\theta}(\mathbf{z})))]$$

- But gradients vanish for $D(G_{\theta}(\mathbf{z})) \to 0$ (good discriminator)
- Replace loss and minimize instead

$$Loss = -\mathbb{E}_{\mathbf{z} \sim p_z(\mathbf{z})}[log(D(G_{\theta}(\mathbf{z})))]$$

- No vanishing gradient but very instable update
- But new loss has strange update behavior:

$$\mathbb{E}_{z \sim p(z)} \left[-\nabla_{\theta} \log D^*(g_{\theta}(z)) |_{\theta = \theta_0} \right] = \nabla_{\theta} \left[KL(\mathbb{P}_{g_{\theta}} || \mathbb{P}_r) - 2JSD(\mathbb{P}_{g_{\theta}} || \mathbb{P}_r) \right] |_{\theta = \theta_0}$$

Distribution Similarity - Metrics



$$\theta = 0$$

$$\mathcal{D}_{KL} = 0$$

$$\mathcal{D}_{LS} = 0$$

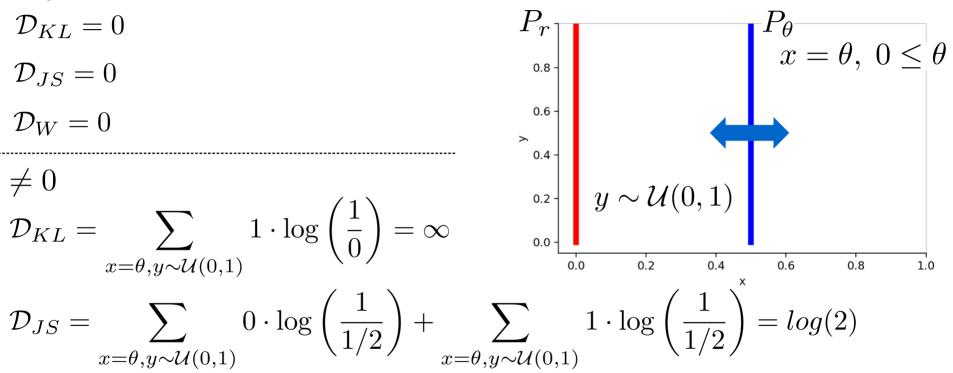
$$\mathcal{D}_W = 0$$

 $\theta \neq 0$

$$\mathcal{D}_{KL} = \sum_{x=\theta} \sum_{u \in \mathcal{U}(0,1)} 1 \cdot \log\left(\frac{1}{0}\right) = \infty$$



Parametrized approximation



$$\mathcal{D}_W = |\theta|$$

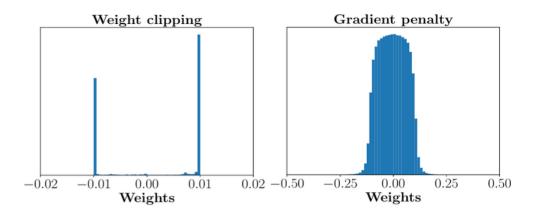
 \triangleright Only \mathcal{D}_W provides meaningful distance measure even for disjoint distributions!

Tutorial on Generative Models Glombitza | RWTH Aachen | 03/22/22 | Deep Learning Weeks, Uppsala

Weight Clipping vs. WGAN-GP



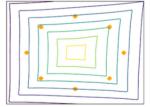
- Weight Clipping:
 - Constraints the weights to lie on a compact space
 - Clip weights after each gradient update eg. to [-0,001; 0,001]
- Heavily constraints the discriminator
- Gradient Penalty allows for a much more complex approximation



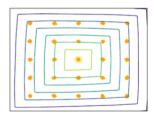
Weight clipping

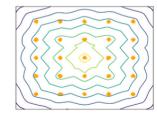
Gradient

Penalty





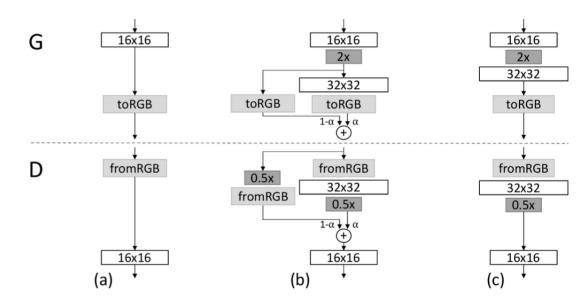




Progressive Growing



- RGB Layer: project feature maps to RGB colors (1 x 1 convolution)
- Upscaling using nearest-neighbor interpolation
- New layer act as "residual block"
 - In generator & discriminator
- During transition:
 - New block is slowly faded in
 - α increases linear from 0 to 1



- Training samples:
 - down-scaled and interpolated during transition between resolutions