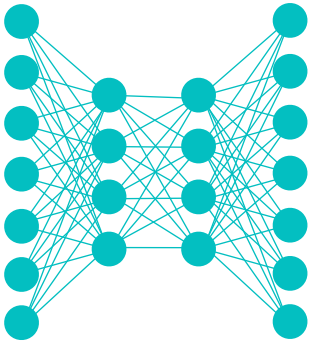
Lecture Notes for

Neural Networks and Machine Learning

Wasserstein GANs



Logistics and Agenda

- Logistics
  - **Student Presentation**: None
- Agenda
  - Quick revisiting: GAN Optimality
  - Wasserstein GAN
  - WGAN-GP
  - Demo
  - BigGAN

Last Time: The Optimal Discriminator

- Discriminator is maximizing:

$$\max_d \mathbf{E}_{x \leftarrow p_{data}} \left[\log d(x)\right] + \mathbf{E}_{x \leftarrow g(z)} \left[\log(1 - d(x))\right]$$

… math …

$$d(x) = \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}$$

-**Conclusion**: Discriminator is optimal when this condition occurs

In principle, it would seem like training the discriminator fully for each update of the generator is what we need. Then the generator could simply find a good update to itself based on the optimal discriminator…
…but that is not what we observe. Subsequent updates to the generator (as discriminator is better) do not seem to keep up… why?

Well, as the discriminator gets more and more confident (i.e., more optimal), it causes the generator gradients to vanish with this formulation of objective functions.

Last Time: What this means for the Generator

- It can be shown that the generator objective function (according to the Goodfellow loss) is optimal when it minimizes this:

$$C(G) = -\log(4) + KL\left(p_{data} \parallel \frac{p_{data} + p_g}{2}\right) + KL\left(p_g \parallel \frac{p_{data} + p_g}{2}\right)$$

$$C(G) = -\log(4) + 2.JSD(p_{data} \parallel p_g)$$ Jenson-Shannon Divergence

- Which helps explain the **Vanishing gradients**: if $p_{data} \| p_g \approx 0$ then JSD saturates and the gradient is basically zero. Optimization has no idea what direction to move in…
  - **Direct Solution**: we need to get rid of the loss function from Goodfellow
    - e.g., LS-GAN (tried to reformulate, but it wasn't so great)
  - **Indirect Solution:** Perhaps we can just use tips/tricks to get around the vanishing gradient problem?

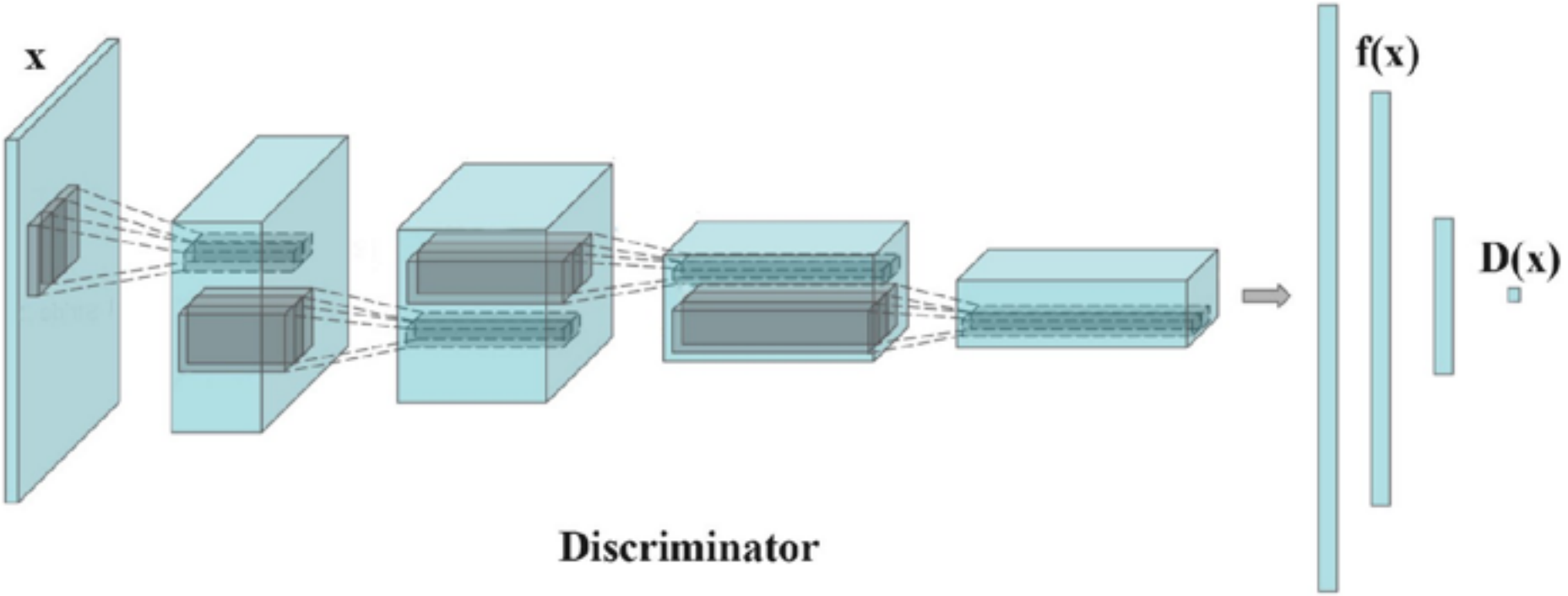
GAN Tricks

The Art of Science: Using tricks

- From Salimans, Goodfellow, et al., :
  - *In this work, we introduce several techniques intended to encourage convergence of the GANs game. These techniques are motivated by a heuristic understanding of the non-convergence problem. They lead to improved semi-supervised learning performance and improved sample generation. We hope that some of them may form the basis for future work, providing formal guarantees of convergence.*
- A collection of Heuristics and Observations that is more Alchemy than Science
  - Feature Matching loss
  - Mini-batch discrimination (*we will skip this*…)
  - Historical averaging
  - Virtual Batch normalization
  - Experience Replay
  - Manipulating the Loss Function

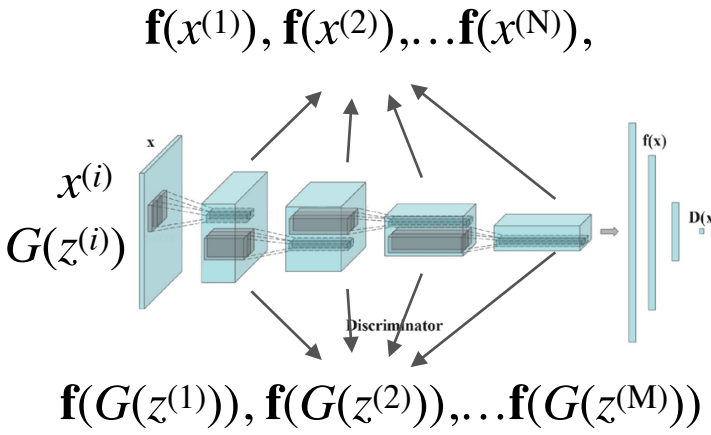
Salimans, Tim, **Ian Goodfellow**, Wojciech Zaremba, Vicki Cheung, Alec Radford, and Xi Chen. "Improved techniques for training gans." In *Advances in neural information processing systems*, pp. 2234-2242. 2016.

Before we go too far



Feature Matching

- Loss function for generator is really difficult as only means to "peek" inside (even with Leaky ReLU)
- Give generator a way to statistically match features inside the discriminator (ideally, to fool it)



1 … N are 1 … M
one turn of real/fake data
usually, N==M

$$\left\| \mathbf{E}_{x \leftarrow data}[\mathbf{f}(x)] - \mathbf{E}_{x \leftarrow q(z)}[\mathbf{f}(G(z))] \right\|^2$$

mean discriminator activations from **real** data

mean discriminator activations from **fake** data

```
real_mean  = K.reduce_mean(real_features, axis = 0)
fake_mean  = K.reduce_mean(fake_features, axis = 0)
feat_match = K.reduce_mean(tf.square(real_mean-fake_mean))
```

Caveat: too small batch size makes unstable…

Salimans, Tim, **Ian Goodfellow**, Wojciech Zaremba, Vicki Cheung, Alec Radford, and Xi Chen. "Improved techniques for training gans." In *Advances in neural information processing systems*, pp. 2234-2242. 2016.

Historical Averaging

- Since generator is not good to start, parameters should constantly be exploring different solutions and, later on, exploiting best found solutions
- **Solution**: Add explore/exploit tradeoff directly in loss function

$$\mathscr{L}(w)_{orig} - \lambda_T \left\| w[T] - \frac{1}{n} \sum_{i=T-n}^{T-1} w[t] \right\|^2$$

current weights

average weights of model over window, T

start: incentivize new weights to be different. Large value.

end: reduce term to zero so that we exploit current solutions.

Salimans, Tim, **Ian Goodfellow**, Wojciech Zaremba, Vicki Cheung, Alec Radford, and Xi Chen. "Improved techniques for training gans." In *Advances in neural information processing systems*, pp. 2234-2242. 2016.

Review: Batch Normalization

- Normalize and rescale activations before going to new layer

One Batch: $\mu_B = \frac{1}{m}\sum_{i=1}^{m} \underbrace{x_i}_{\text{input}}$ $\sigma_B = \frac{1}{m}\sum_{i=1}^{m}(\mu_B - x_i)^2$

Normalized x: $\hat{x}_i = \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$

Scaled activations with trainable parameters: $y = \gamma\hat{x} + \beta$

During inference: μ_B and σ_B are fixed based on the training set population

Virtual Batch Normalization

- Batch normalization is really swell
- But for GANs, it makes current $f(x)$'s dependent on other generated $f(x_{batch})$ 🤢
- Why not use a reference batch for statistics? And just use statistics of the reference batch activations for normalizing?
  - Periodically we need to recompute the statistics for the reference batch (usually real data)
  - *That's it!*

$$\mu^{ref} = \frac{1}{M}\sum_i a_i^{ref} \quad \sigma^{ref\,2} = \frac{1}{M}\sum_i (a_i^{ref} - \mu^{ref})^2 \quad z_i = \gamma \cdot \frac{(a_i - \mu^{ref})}{\sqrt{\sigma^{ref\,2} + \epsilon}} + \beta$$

Salimans, Tim, **Ian Goodfellow**, Wojciech Zaremba, Vicki Cheung, Alec Radford, and Xi Chen. "Improved techniques for training gans." In *Advances in neural information processing systems*, pp. 2234-2242. 2016.

Experience Replay

- The discriminator can overpower the generator quickly and this causes vanishing gradients
- **Solution**: feed older batches from generator with the current epoch
- Save previous epochs and randomly grab from them when updating the discriminator!
- The term *experience replay* comes form the usage of this technique in reinforcement learning
  - here we are just throwing a wrench into the optimization of discriminator by giving some easy examples to learn

Salimans, Tim, **Ian Goodfellow**, Wojciech Zaremba, Vicki Cheung, Alec Radford, and Xi Chen. "Improved techniques for training gans." In *Advances in neural information processing systems*, pp. 2234-2242. 2016.

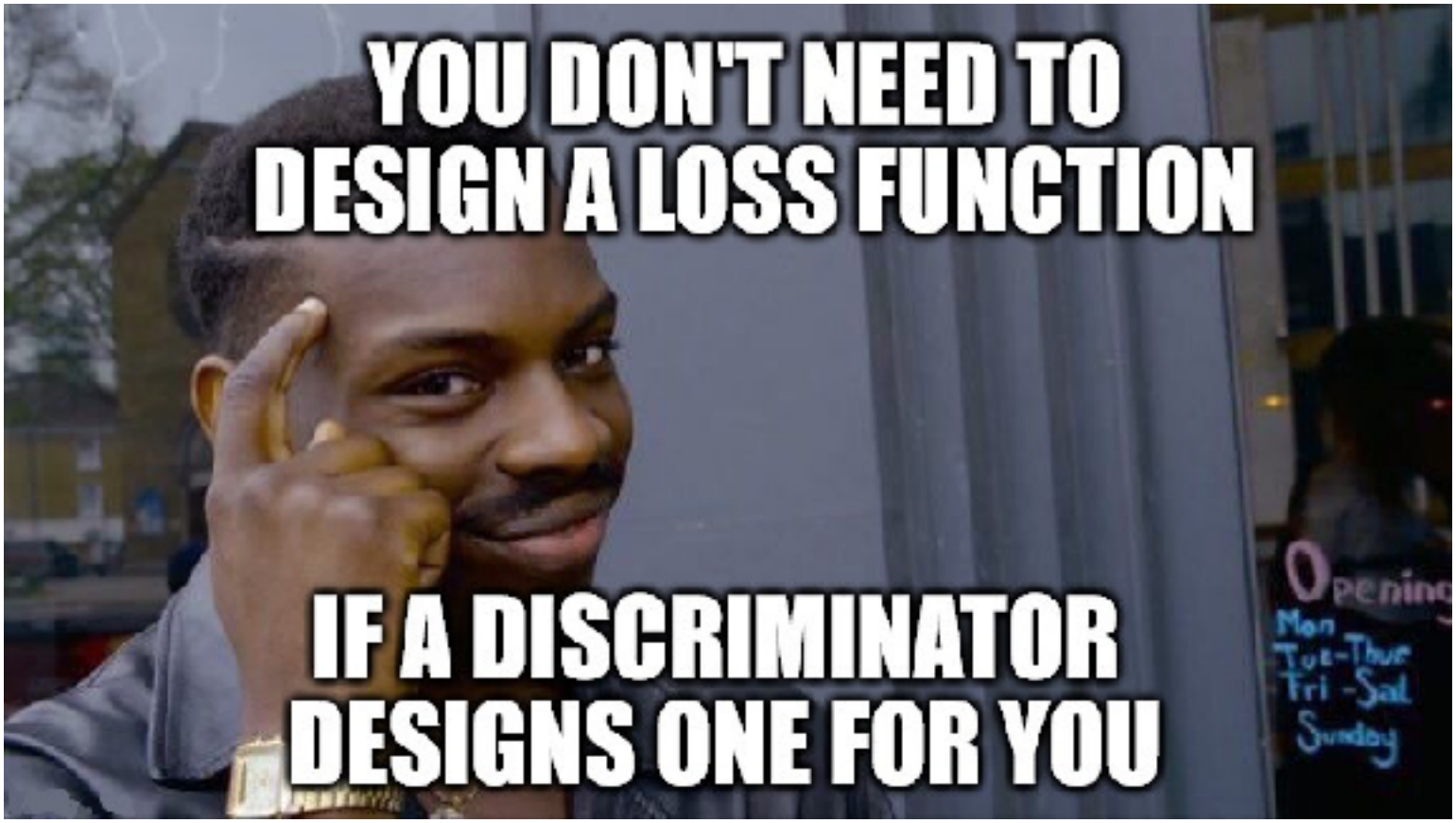
Figure 4: Samples generated during semi-supervised training on CIFAR-10 with feature matching (Section 3.1, *left*) and minibatch discrimination (Section 3.2, *right*).

Salimans, Tim, **Ian Goodfellow**, Wojciech Zaremba, Vicki Cheung, Alec Radford, and Xi Chen. "Improved techniques for training gans." In *Advances in neural information processing systems*, pp. 2234-2242. 2016.

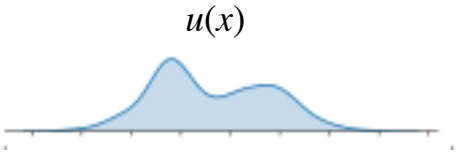
The Direct Solution

- All of the things we have discussed help to move the optimization along even when **the output distribution does not overlap with the actual data distribution**
- There must be a better objective function
  - There is! The Wasserstein distance!

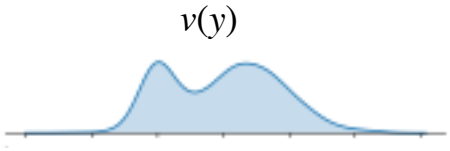
Wasserstein GANs

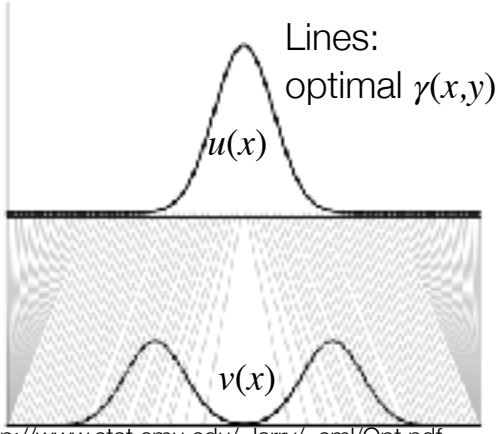


Wasserstein Distance (Earth Mover)



how to move dirt from u to v ?

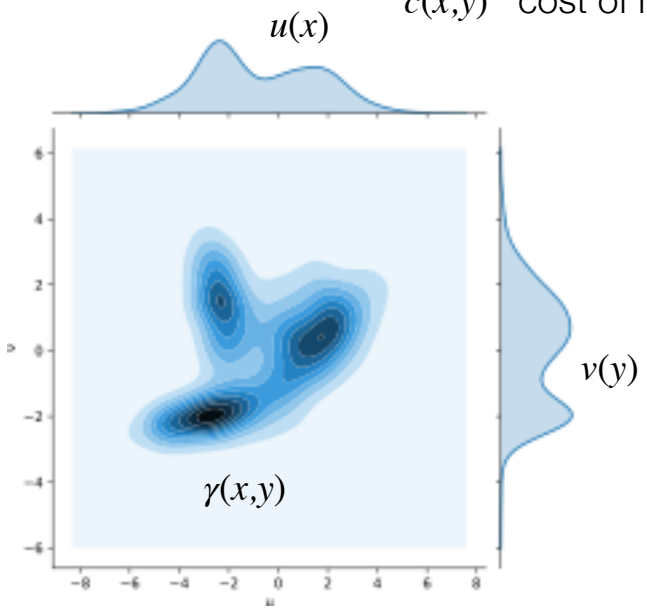




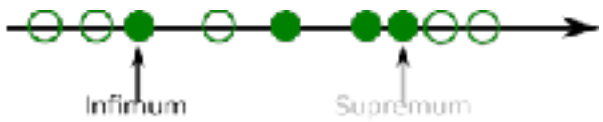
http://www.stat.cmu.edu/~larry/=sml/Opt.pdf

$\gamma(x,y)$ one plan to move u to v

$c(x,y)$ cost of moving u to v



$$\int\int c(x,y)\cdot\gamma(x,y)\,\partial x\partial y$$ Total cost of plan γ

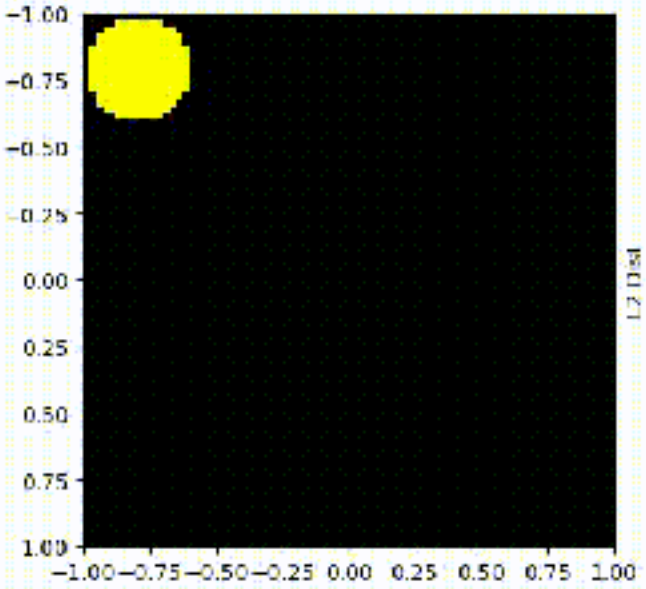


$$\inf_{\gamma\in\Pi}\int\int c(x,y)\cdot\gamma(x,y)\,\partial x\partial y$$ Optimal plan has greatest lower bound (minimum cost in set Π)

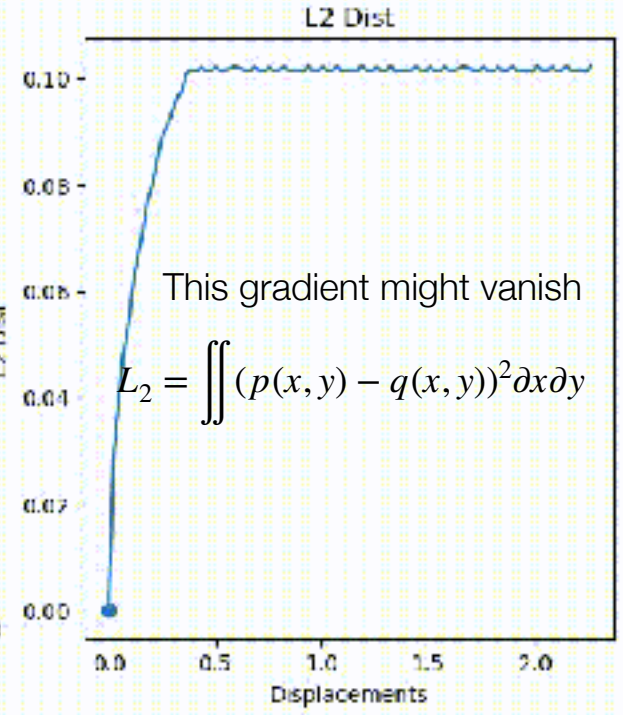
$$\inf \mathbf{E}_{x,y\leftarrow\gamma}\left[|x-y|\right] = \inf_{\gamma\in\Pi}\int\int |x-y|\cdot\gamma(x,y)\,\partial x\partial y$$ If cost is difference to move from x to y

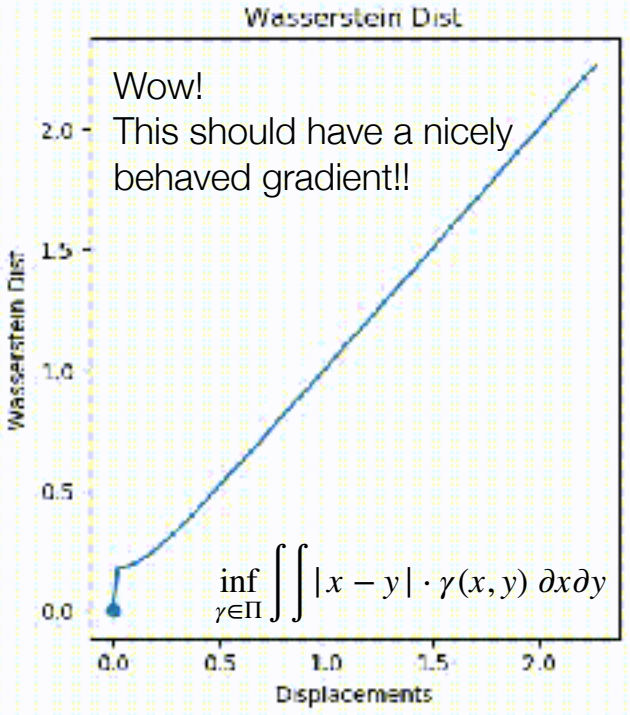
image: wikipedia

Wasserstein Distance



Two 2D Normal Distributions





- *Wasserstein GAN adds few tricks to allow the Discriminator to approximate Wasserstein (aka Earth Mover's) distance between real and model distributions. Wasserstein distance roughly tells "how much work is needed to be done for one distribution to be adjusted to match another" and is remarkable in a way that it is defined even for non-overlapping distributions.*

https://gist.github.com/ctralie/66352ae6ab06c009f02c705385a446f3

https://medium.com/@jonathan_hui/gan-wasserstein-gan-wgan-gp-6a1a2aa1b490

Wasserstein Distance

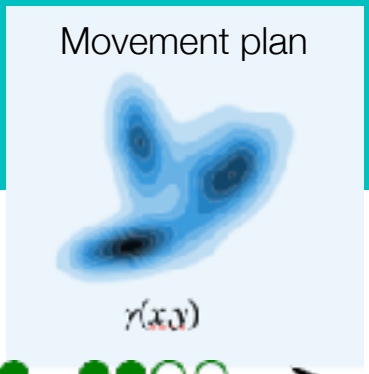
- How much do I need to change one distribution to get it to match another?
- Also, we will only have **samples** from the distributions (not the actual equations)
- **Wasserstein Distance** for continuous probabilities:

$$W(p_{data}, p_g) = \inf_{\gamma \in \prod(p_{data}, p_g)} \mathbf{E}_{x,y \leftarrow \gamma} \left[\|x - y\| \right]$$

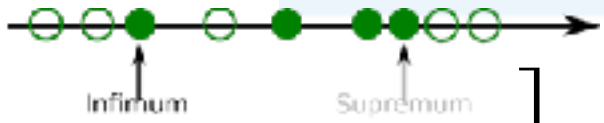
- $\inf$ is greatest lower bound (min of a set)
- γ is completely and utterly

intractable to **compute**

Wasserstein Duality, Critic



$$W(p_{data}, p_g) = \inf_{\gamma \in \prod(p_{data}, p_g)} \mathbf{E}_{x,y \leftarrow \gamma} \left[\|x - y\| \right]$$



$$= \inf_{\gamma} \mathbf{E}_{x,y \leftarrow \gamma} \left[\|x - y\| + \underbrace{\sup_{f} \mathbf{E}_{x \leftarrow p_{data}}[f(x)] - \mathbf{E}_{x \leftarrow p_g}[f(x)] - \left(f(x) - f(y)\right)}_{\text{enforce constraint = finite, if } \gamma \in \Pi, \text{ else } +\infty} \right]$$

$$= \inf_{\gamma} \sup_{f} \mathbf{E}_{x,y \leftarrow \gamma} \left[\|x - y\| + \mathbf{E}_{x \leftarrow p_{data}}[f(x)] - \mathbf{E}_{x \leftarrow p_g}[f(x)] - \left(f(x) - f(y)\right) \right]$$

$$= \sup_{f} \mathbf{E}_{x \leftarrow p_{data}}[f(x)] - \mathbf{E}_{x \leftarrow p_g}[f(x)] - \inf_{\gamma} \underbrace{\mathbf{E}_{x,y \leftarrow \gamma} \left[\|x - y\| + \left(f(x) - f(y)\right) \right]}_{\text{new constraint = finite, if } |f| \leq 1, \text{ else } -\infty}$$

$$= \sup_{|f| \leq 1} \mathbf{E}_{x \leftarrow p_{data}}[f(x)] - \mathbf{E}_{x \leftarrow p_g}[f(x)]$$

what have we done here????

read this: https://vincentherrmann.github.io/blog/wasserstein/

Wasserstein (Kantorovich-Rubinstein) Duality

- 1-Lipschitz constraint, critic: $|f(x_1) - f(x_2)| \leq |x_1 - x_2|$
- Wasserstein Duality Formula (approx. for samples):

$$\mathscr{L}_{wass} = \sup_{|f| \leq 1} \mathbf{E}[f(x_{real})] - \mathbf{E}[f(x_{fake})] \approx \frac{1}{m}\sum_{i=1}^{m} f(x_{real}^{(i)}) - \frac{1}{n}\sum_{j=1}^{n} f(g(z^{(j)}))$$

- where sup is least upper bound (max within set $|f|<1$, same as valid movement plans set)
- f will be the critic, learned as a neural network, $m=n$

$$\frac{1}{m}\sum_{i=1}^{m} f(x_{real}^{(i)}) - f(g(z^{(i)}))$$ Maximize f (called critic), freeze generator weights

$$\frac{1}{m}\sum_{i=1}^{m} f(g(z^{(i)}))$$ Maximize g, freeze weights of critic

Sometimes we use this, minimizes hinge loss:

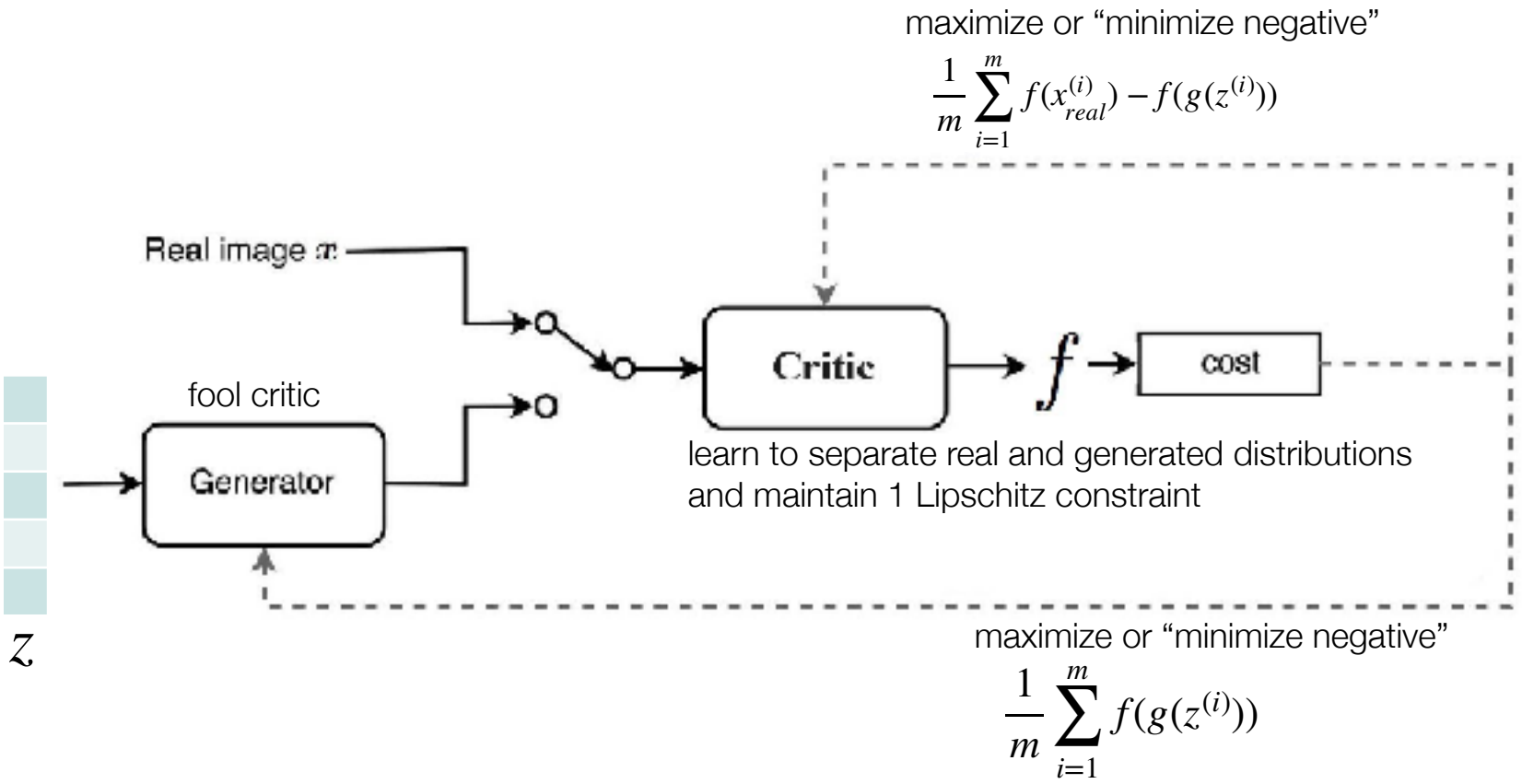
$$\frac{1}{m}\sum_{i=1}^{m} f(x_{real}^{(i)}) \cdot f(g(z^{(i)}))$$

when *values* are -1 to 1

f( )	*f*(*g*( ))	*f*-*f*(*g*)	*f* x *f*(*g*)
-1	-1	0	1
-1	1	-2	-1
1	-1	2	-1
1	1	0	1
		max	min

https://medium.com/@jonathan_hui/gan-wasserstein-gan-wgan-gp-6a1a2aa1b490

Wasserstein Architecture



https://medium.com/@jonathan_hui/gan-wasserstein-gan-wgan-gp-6a1a2aa1b490

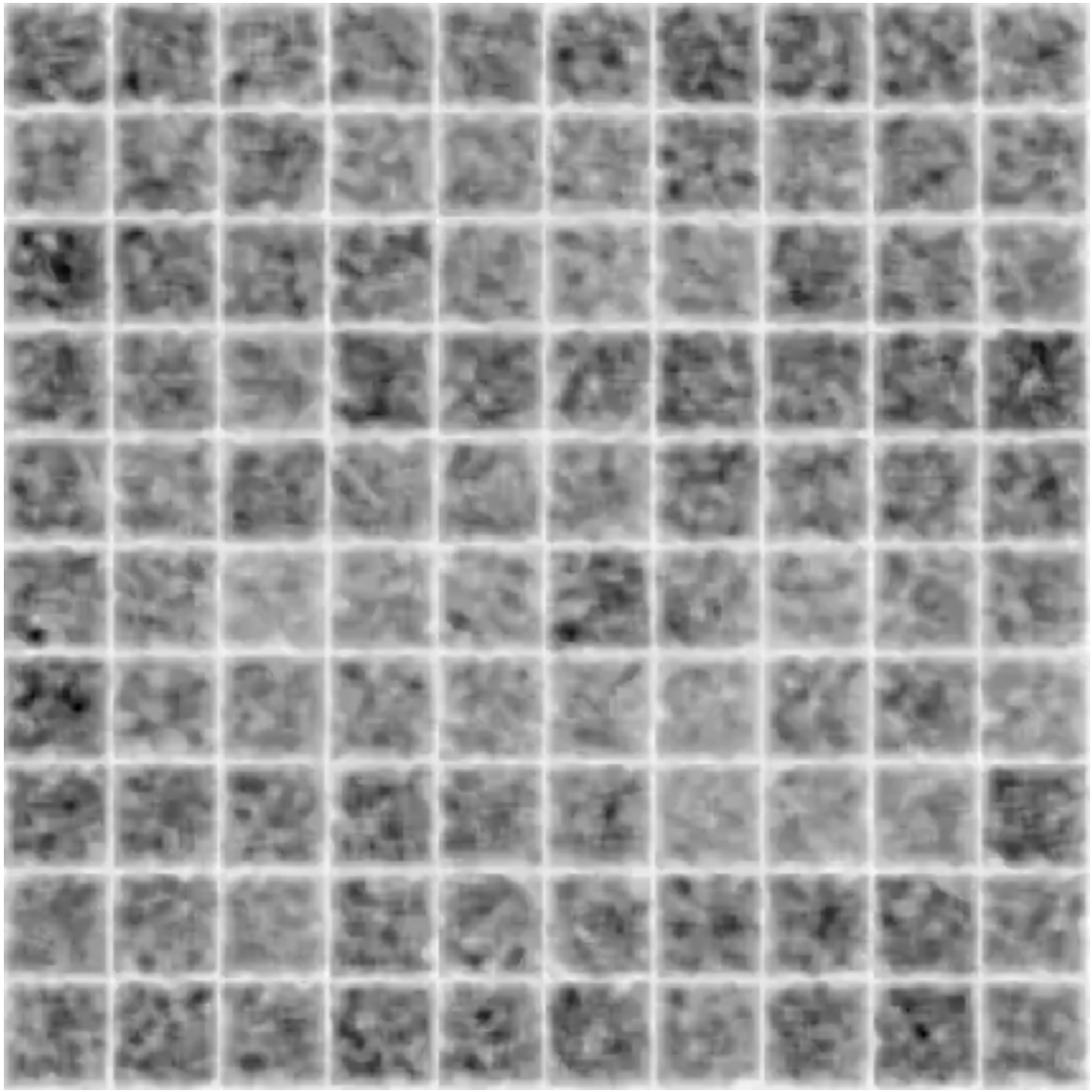
Practical Wasserstein Loss

- Discriminator (now critic) becomes **f**, and its output can be Lipschitz if all weights are small (squashes inputs)
  - so we clip them to (-c to c) (where c~0.01)
  - critic output should be linear

```
# define the standalone critic model
def define_critic(in_shape=(28,28,1)):
    # weight initialization
    init = RandomNormal(stddev=0.02)
    # weight constraint
    const = ClipConstraint(0.01)
    # define model
    model = Sequential()
    # downsample to 14x14
    model.add(Conv2D(64, (4,4), strides=(2,2), padding='same'
    model.add(BatchNormalization())
    model.add(LeakyReLU(alpha=0.2))
    # downsample to 7x7
    model.add(Conv2D(64, (4,4), strides=(2,2), padding='same'
    model.add(BatchNormalization())
    model.add(LeakyReLU(alpha=0.2))
    # scoring, linear activation
    model.add(Flatten())
    model.add(Dense(1))
```

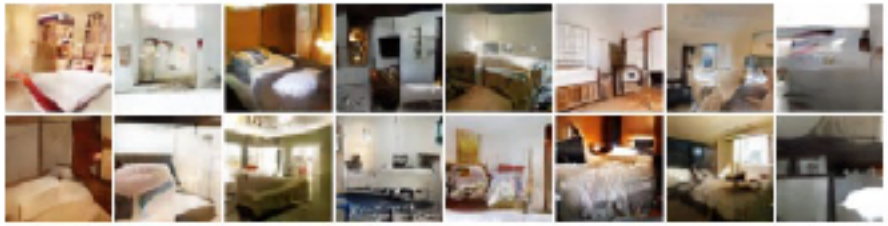
https://machinelearningmastery.com/how-to-code-a-wasserstein-generative-adversarial-network-wgan-from-scratch/

WGAN Example from Keras (MNIST)

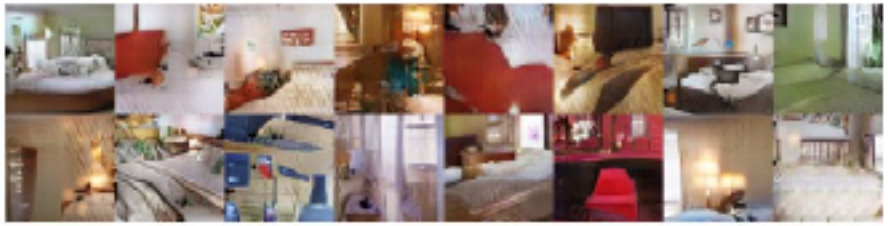


This is a conditional GAN, which like the LSGAN, adds some control over the class being generated.

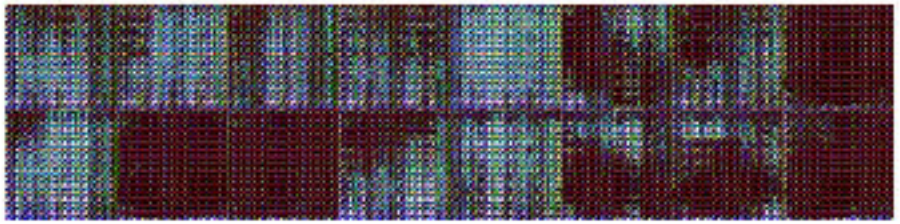
- In their empirical findings, no mode collapse problems
- And training longer resulted in good quality images (motivates that distributions overlap)
- Still some of the most competitive GAN results



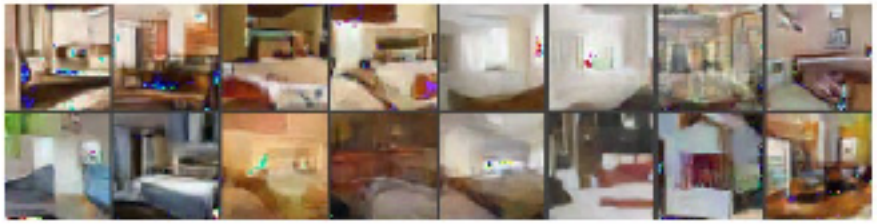
WGAN with DCGAN generator

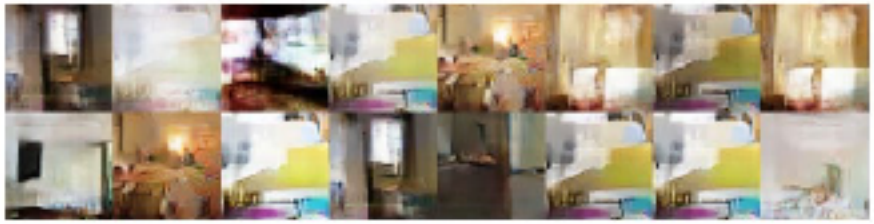


GAN with DCGAN generator



Without batch normalization &
constant number of filters at each layer





Using a MLP as the generator

So we should always use Wasserstein!

- **Actually not really**
- Its really, really,…. really slow
- Clipping (from WGAN paper):

Weight clipping is a clearly terrible way to enforce a Lipschitz constraint. If the clipping parameter is large, then it can take a long time for any weights to reach their limit, thereby making it harder to train the critic till optimality. If the clipping is small, this can easily lead to vanishing gradients when the number of layers is big, or batch normalization is not used (such as in RNNs).

- Others have made improvements by incorporating gradient constraints
- New critic: WGAN with gradient penalty

WGAN-GP

WGAN-GP (Gradient Penalty)

$$\frac{1}{m}\sum_{i=1}^{m} f(g(z^{(i)}))$$

Maximize g,
freeze weights of critic
No change

- Theorem: a function is 1-Lipschitz if and only if its gradient norm is $\|\nabla f(\hat{x})\|_2 \leq 1$, but that is very constraining

Maximize f
freeze generator weights,

incentivize critic gradient norm to be one
Choose large lambda (e.g., 10)

$$\frac{1}{m}\sum_{i=1}^{m} f(x_{real}^{(i)}) - f(g(z^{(i)})) - \lambda \frac{1}{W}\sum_{i=1}^{W} \left(\|\nabla f(\hat{x}^{(i)})\|_2 - 1\right)^2$$

where for ϵ in U[0,1] $\hat{x}^{(i)} = \epsilon \cdot x_{real}^{(i)} + (1-\epsilon)\cdot g(z^{(i)})$

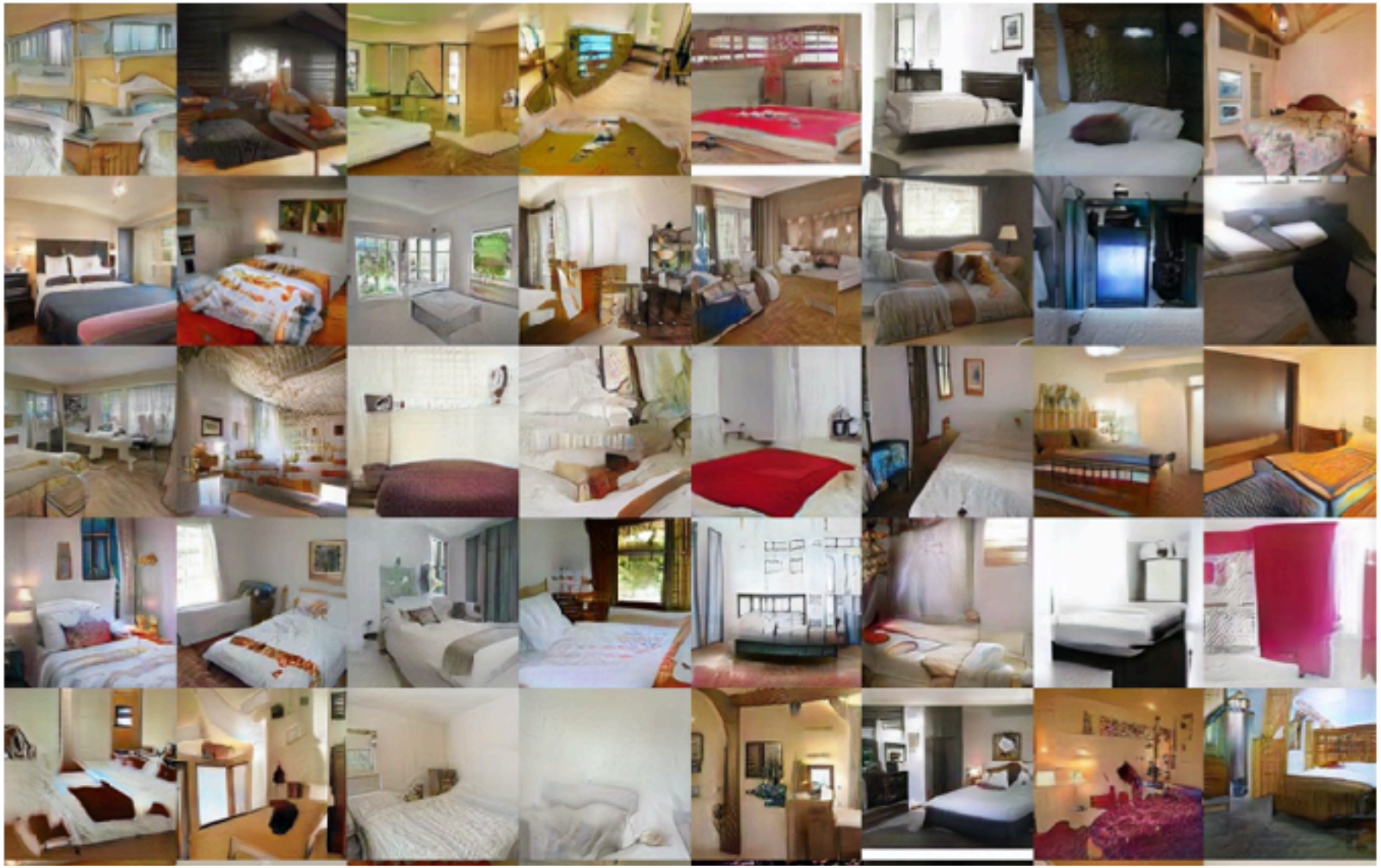
randomly mix together real and fake images, for gradient estimation

WGAN-GP Heuristics

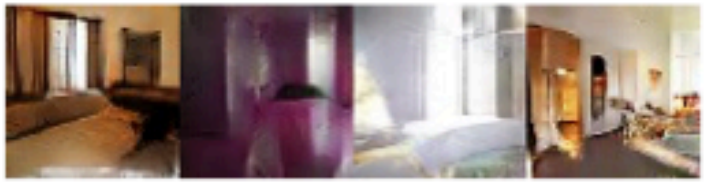
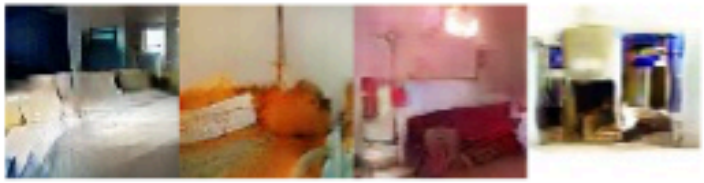
- Choose large penalty coefficient
- Don't use batch normalization (in critic)
  - it forces the gradient norm to be dependent on batches
  - but layer norm seems to be okay
- Enforce gradient norm to be close to one, rather than less than one

Two-sided penalty We encourage the norm of the gradient to go towards 1 (two-sided penalty) instead of just staying below 1 (one-sided penalty). Empirically this seems not to constrain the critic too much, likely because the optimal WGAN critic anyway has gradients with norm 1 almost everywhere under $\mathbb{P}_r$ and $\mathbb{P}_g$ and in large portions of the region in between (see subsection 2.3). In our early observations we found this to perform slightly better, but we don't investigate this fully. We describe experiments on the one-sided penalty in the appendix.

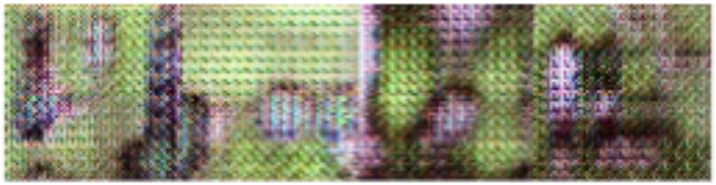
WGAN-GP Results



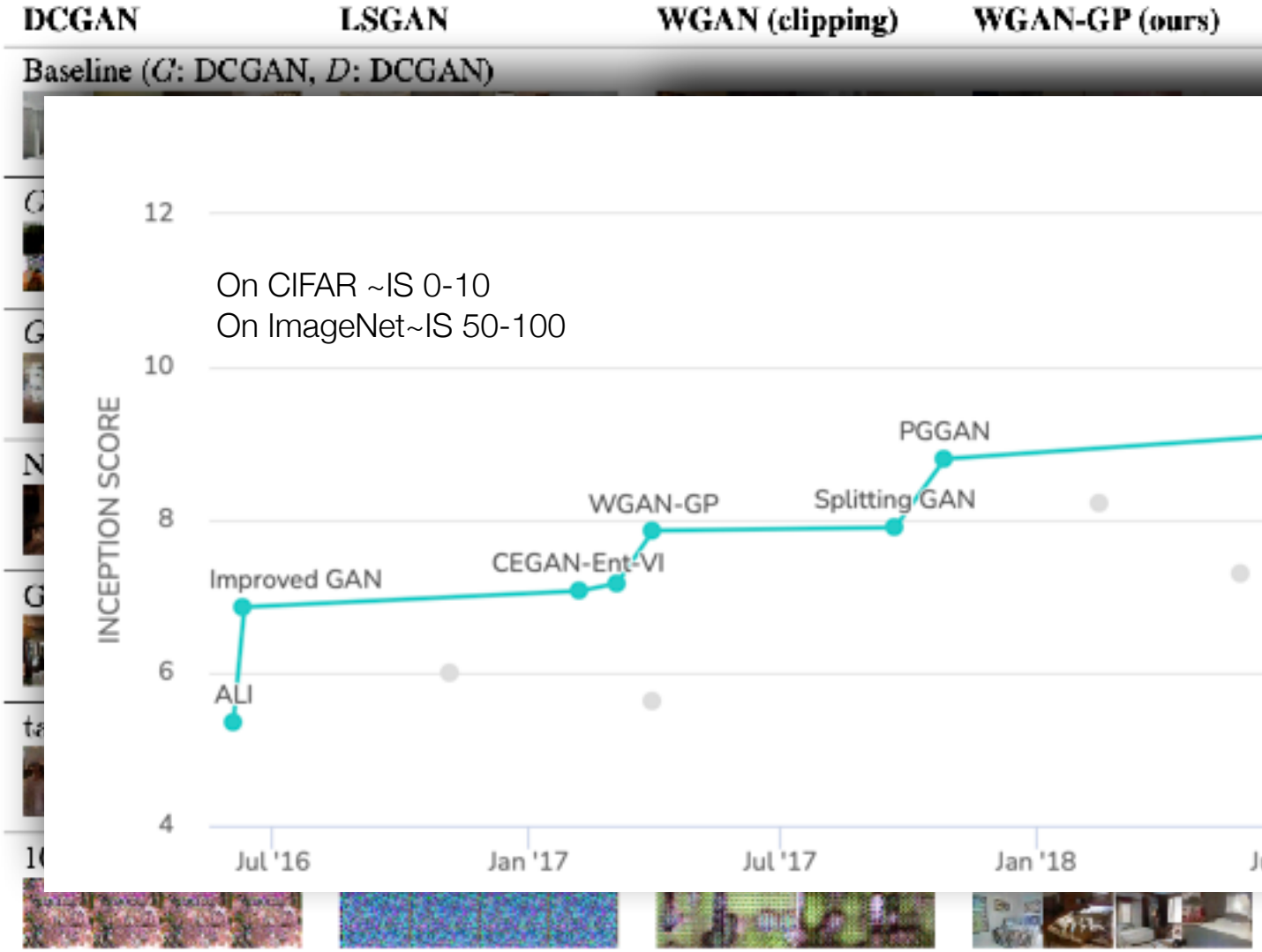
WGAN-GP Comparative Results

WGAN (clipping)	WGAN-GP (ours)
Baseline: G: DCGAN	Crit: DCGAN
	
G: DCGAN no BN	Crit: DCGAN
	
G: MLP	Crit: DCGAN
	

WGAN-GP Comparative Results

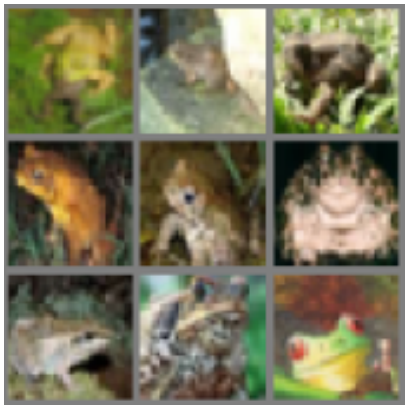
WGAN (clipping)	WGAN-GP (ours)
G/Crit: Tanh Non-linearities	
	
G/Crit: 101 Layer ResNet	
	

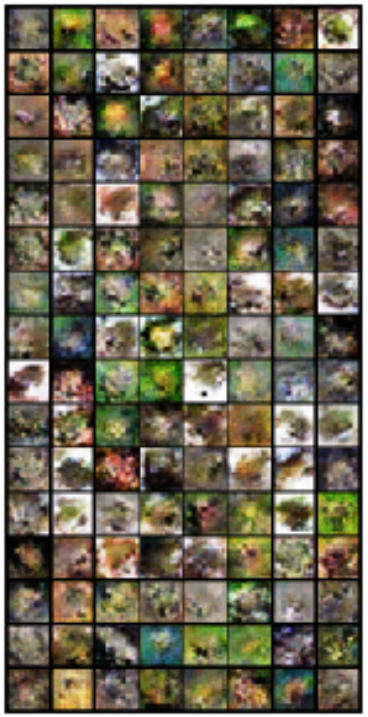
WGAN-GP Comparative Results



WGAN-GP

Main Repository:
07c GANsWithTorch.ipynb





Other Examples

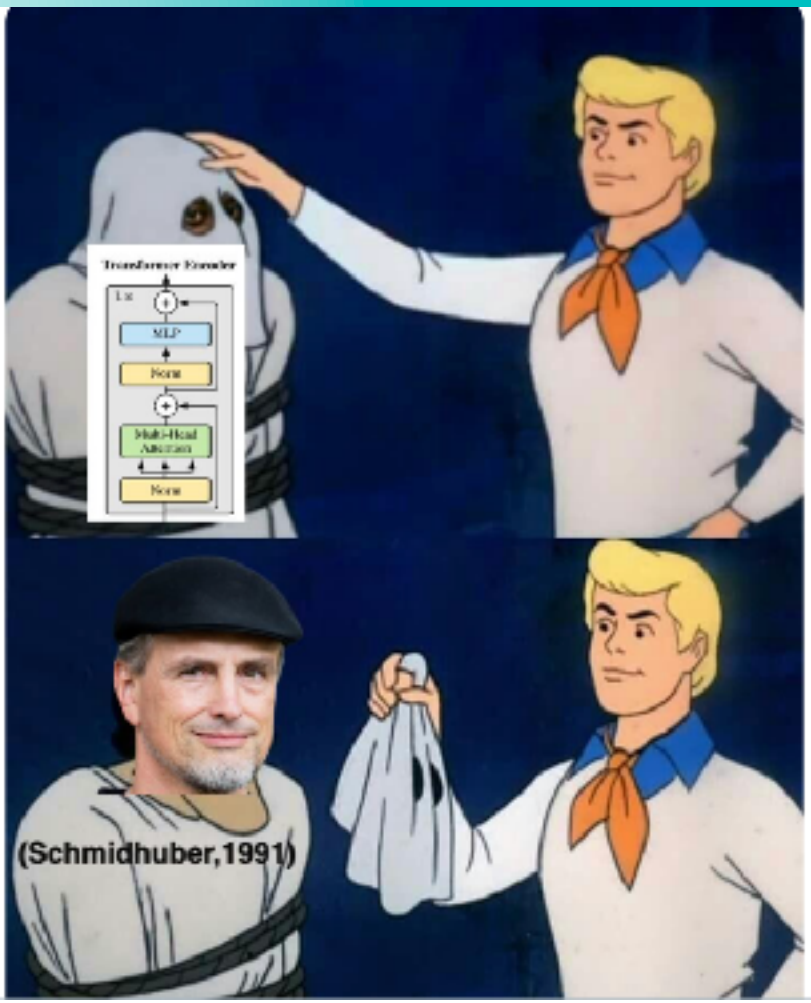
Keras Example: https://github.com/keras-team/keras-contrib/blob/master/examples/improved_wgan.py DCGAN

Demo by Keras Contrib Community

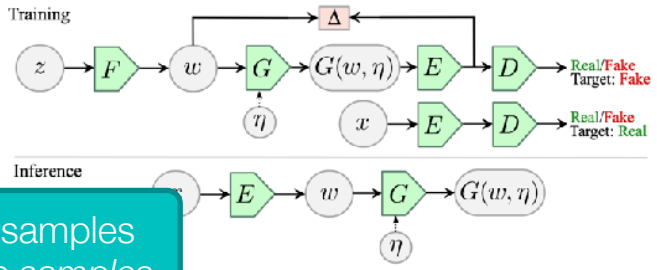
Other Example: https://github.com/eriklindernoren/PyTorch-GAN/blob/master/implementations/wgan_gp/wgan_gp.py MLP-GAN

Demo by Erik Linder-Norén

Aside: Back to ALAEs



Adversarial Latent Auto-Encoders, ALAE



Algorithm 1 ALAE Training

1: $\theta_F, \theta_G, \theta_E, \theta_D \leftarrow$ Initialize network parameters
2: **while** not converged **do**
3: St
4: x
5: $z \leftarrow$ Samples from prior $\mathcal{N}(0, I)$
6: $L^{E,D}_{adv} \leftarrow \text{softplus}(D \circ E \circ G \circ F(z)) + \text{softplus}(-D \circ E(x)) + \frac{\gamma}{2} \mathrm{E}_{p_{\mathcal{D}}(x)} \left[\|\nabla D \circ E(x)\|^2 \right]$
7: $\theta_E, \theta_D \leftarrow \text{ADAM}(\nabla_{\theta_D, \theta_E} L^{E,D}_{adv}, \theta_D, \theta_E, \alpha, \beta_1, \beta_2)$
8: Step II. Update F, and G
9: $z \leftarrow$ Samples from prior $\mathcal{N}(0, I)$
10: $L^{F,G}_{adv} \leftarrow \text{softplus}(-D \circ E \circ G \circ F(z))$
11: $\theta_F, \theta_G \leftarrow \text{ADAM}(\nabla_{\theta_F, \theta_G} L^{F,G}_{adv}, \theta_F, \theta_G, \alpha, \beta_1, \beta_2)$
12: Step III. Update E, and G
13: $z \leftarrow$ Samples from prior $\mathcal{N}(0, I)$
14: $L^{E,G}_{error} \leftarrow \|F(z) - E \circ G \circ F(z)\|_2^2$
15: $\theta_E, \theta_G \leftarrow \text{ADAM}(\nabla_{\theta_E, \theta_G} L^{E,G}_{error}, \theta_E, \theta_G, \alpha, \beta_1, \beta_2)$
16: **end while**

Based On Nash Equilibrium

E,D: Detect fake samples
minimize D for fake samples

E,D: Detect real samples
minimize -D for real samples

E,D: Gradient Penalty
Keep Gradient Magnitude Small
Now we know why!!

F,G: Try to fool discriminator,
minimize -D for fake samples

E,G: Keep latent spaces similar

Pidhorskyi, Stanislav, Donald A. Adjeroh, and Gianfranco Doretto. "Adversarial latent autoencoders." In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp. 14104-14113. 2020.