10417-617
Deep Learning: Fall 2020

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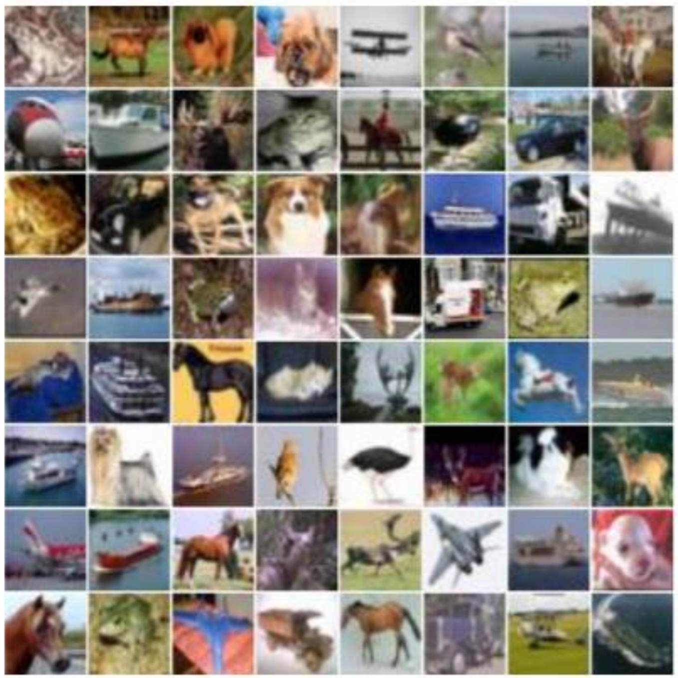
Lecture 16:
Generative adversarial networks, normalizing flows

Some samples generated with VAEs and RBMs



Data

VAE samples

Faces generated using a trained VAE, slides from
http://efrosgans.eecs.berkeley.edu/CVPR18_slides/VAE_GANS_by_Rosca.pdf

Some samples generated with VAEs and RBMs

Faces generated using a trained VAE

The problem

Samples are blurry, though they capture some high-level structure.

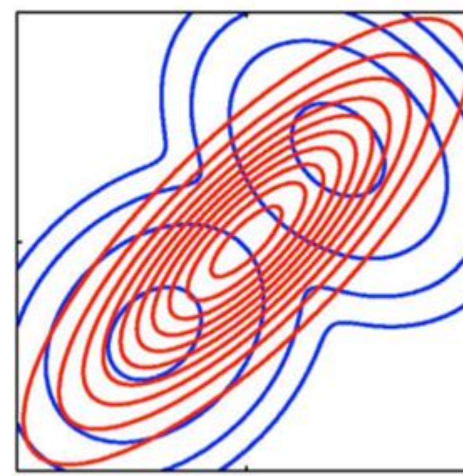
Some hypotheses for what goes wrong:

Strong metric: VAEs try to match the input distribution in KL divergence, which is quite a strong metric.

Poor posteriors: The posteriors in a VAE are Gaussian – very poor modeling power, e.g. cannot model multimodal distributions.

Max-likelihood encourages averaging: finding the max-likelihood q to fit a distribution p is equivalent to minimizing KL(p||q) (by expanding the def. of KL = $E_p \log p \; - \; E_p \log q$).

Recall from when we talked about variational methods: this KL tends to “average” modes.



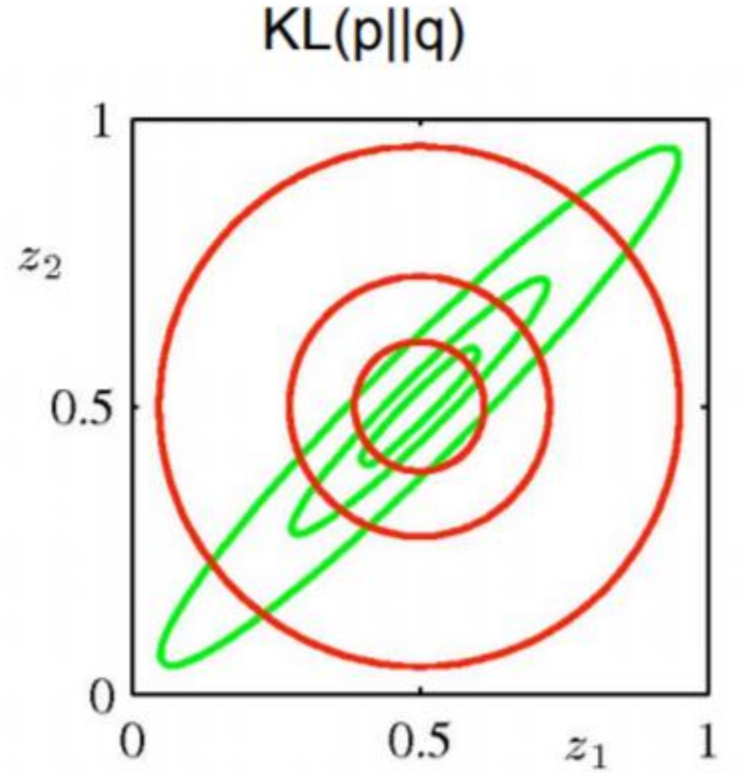
KL(p||q)

Recap: why KL(p||q) averages

$$\mathrm{KL}(p||q) = -\int p(\mathbf{Z}) \ln \frac{q(\mathbf{Z})}{p(\mathbf{Z})} \mathrm{d}\mathbf{Z}.$$

There is a large positive contribution to the KL divergence from regions of Z space in which:
- q(Z) is near zero,
- unless p(Z) is also close to zero.

Minimizing KL(p||q) leads to distributions q(Z) that are nonzero in regions where p(Z) is nonzero.



The idea behind GANs

Matching a distribution on images is hard because we don't have good measures of "**distance**" between images.
(Intuitively, two images could be very different in pixel space, while "**semantically**" being the same image.)

Why don't we simultaneously train a "distance" metric as we are training the model?

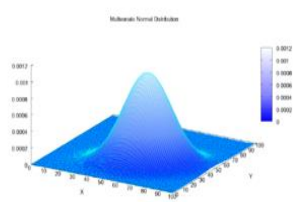
As a result, we will no longer be fitting the "maximum likelihood" model, but instead trying to learn some distribution close to the distribution of the input images in a learned metric.

This is (one of many) models which are "**likelihood-free**": we won't be able to explicitly write a likelihood for the model, but (importantly) we will efficiently be able to draw samples from the model!

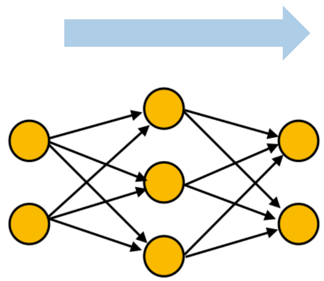
The GAN paradigm (Goodfellow et al. ‘14)

Goal: **Learn** a distribution close to some distribution we have few samples from. (Additionally, we will be able to sample efficiently from distribution.)

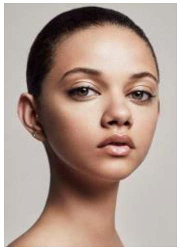
Approach: **Fit** distribution P_g parametrized by **neural network g**

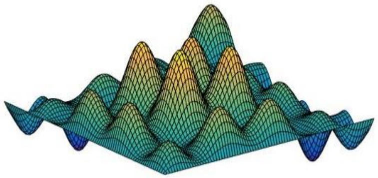


$Z \sim N(0, I_{k \times k})$



Neural network $g(\cdot)$

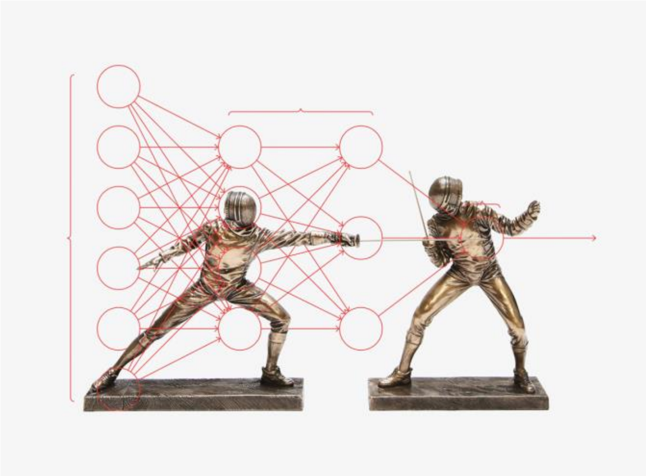




$X = g\,(Z)$

The GAN paradigm (Goodfellow et al. ‘14)

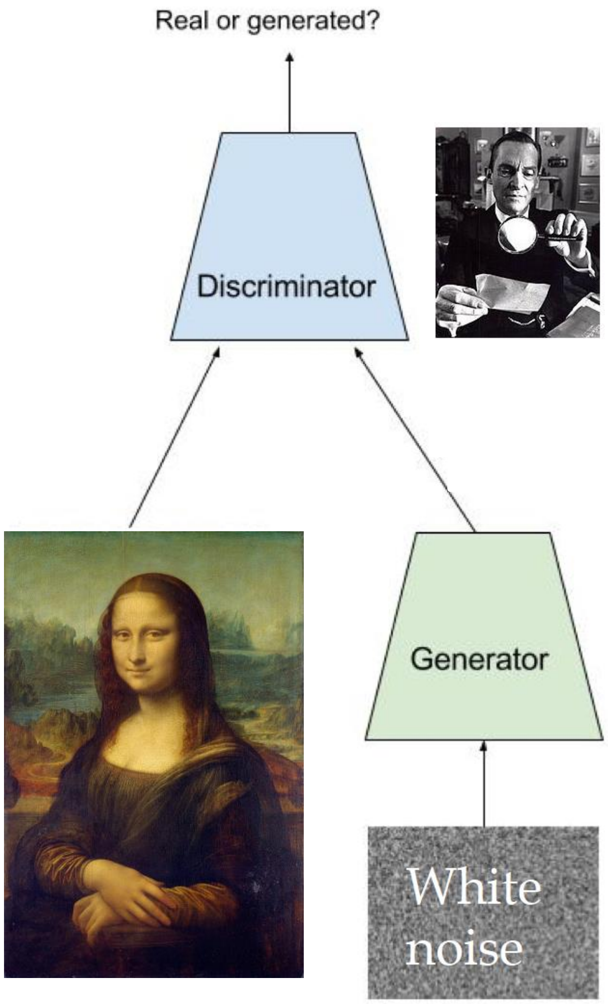
Top 10 Breakthrough Technologies 2018



Photorealistic image/video generation

Extracting complex features

The GAN paradigm (Goodfellow et al. ‘14)



Game theoretic idea:

Generator trained to **fool** discriminator.

Discriminator trained to **beat** generator.

W-GAN formalization (Arjovsky et al. ‘17)

Min-max problem:

- Min-player: generators $g \in G$; Max-player: discriminators f $\in F$.
- Samples from image distr. P_{real}. Unif. distribution over samples: $P_{samples}$
- P_g - generator distribution: $Z \sim N(0, I) \to g(Z)$

Training loss:

$$\min_{g \in G} \max_{f \in F} \left| \mathbb{E}_{P_g}[f] - \mathbb{E}_{P_{\text{samples}}}[f] \right|$$

Difference of expectation of f on **samples vs generated** images

W-GAN formalization (Arjovsky et al. '17)

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Generator g **fools** discriminators F **:**

$$\forall f \in F, \mathbb{E}_{P_g}[f] \approx \mathbb{E}_{P_{\text{samples}}}[f]$$

Equivalently, small training loss!

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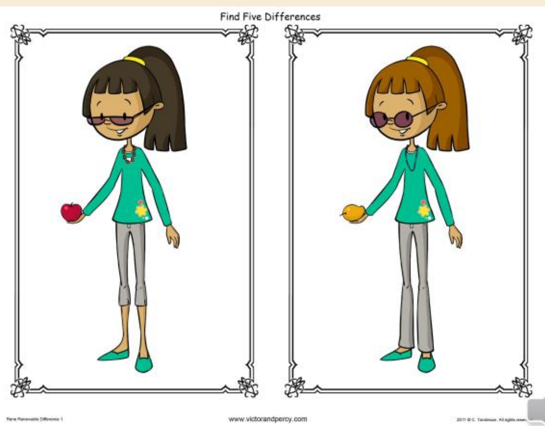
Discriminators F **beat** generators if for all $g \in G$, there is an f $\in F$

$$\mathbb{E}_{P_g}[f] \not\approx \mathbb{E}_{P_{\text{samples}}}[f]$$



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Training loss:

$$\underbrace{\min_{g \in G} \max_{f \in F} \left| \mathbb{E}_{P_g}[f] - \mathbb{E}_{P_{\text{samples}}}[f] \right|}_{d_F(P_{\text{samples}}, P_g)}$$

Discriminators F **beat** generators if for all $g \in G$, there is an f $\in F$

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"Distance" specified by discriminators F .
Captures how well F 's can **distinguish** two distributions

W-GAN formalization (Arjovsky et al. '17)

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$$\mathbb{E}_{P_g}[f] \not\approx \mathbb{E}_{P_{\text{samples}}}[f]$$

$$\textbf{Training loss} = \min_{g \in G} d_F(P_g, P_{\text{samples}})$$

Examples of distances d_F

$$\underbrace{\max_{f \in F} \left| \mathbb{E}_{P_g}[f] - \mathbb{E}_{P_{\text{samples}}}[f] \right|}_{d_F(P_{\text{samples}}, P_g)}$$

Absolute value can be removed (-f is Lip if f is Lip)

$F = \{f : |f|_\infty \leq 1\}$: **Total variation distance**

Measures differences of bounded functions

$F = \{f : \mathrm{Lip}(f) \leq 1\}$: **$W_1$ (Wasserstein, earthmover) distance**

Measures differences of 1-Lipschitz functions

Examples of distances d_F

$$\underbrace{\max_{f \in F} \left| \mathbb{E}_{P_g}[f] - \mathbb{E}_{P_{\text{samples}}}[f] \right|}_{d_F(P_{\text{samples}}, P_g)}$$

If distance d_F is a **metric**: $d_F(p,q) \geq 0$ and $d_F(p,q) = 0$ only if $p = q$

Hence, if we learn a distribution P_g, s.t. $d_F\left(P_g, P_{real}\right) = 0$, and$P_{real}$ is the true data distribution, we have $P_g = P_{real}$.

In the limit of infinite samples,$P_{real} = P_{\text{samples}}$, so if training error is 0, we have learned a distribution $P_g = P_{real}$

Variants

Monotone function $\boldsymbol{\phi}$

$$\underbrace{\max_{f\in F} \mathbb{E}_{P_g}[\boldsymbol{\phi}(f)] - \mathbb{E}_{P_{\text{samples}}}[\boldsymbol{\phi}(1-f)]}_{d_F(P_{\text{samples}},\, P_g)}$$

Maximize log-probability of correct answer

$\boldsymbol{\phi} = \mathbf{log}$: DC-GAN

$$\max_{f\in F} \mathbb{E}_{P_g}[\log(f)] - \mathbb{E}_{P_{\text{samples}}}[\log(1-f)]$$

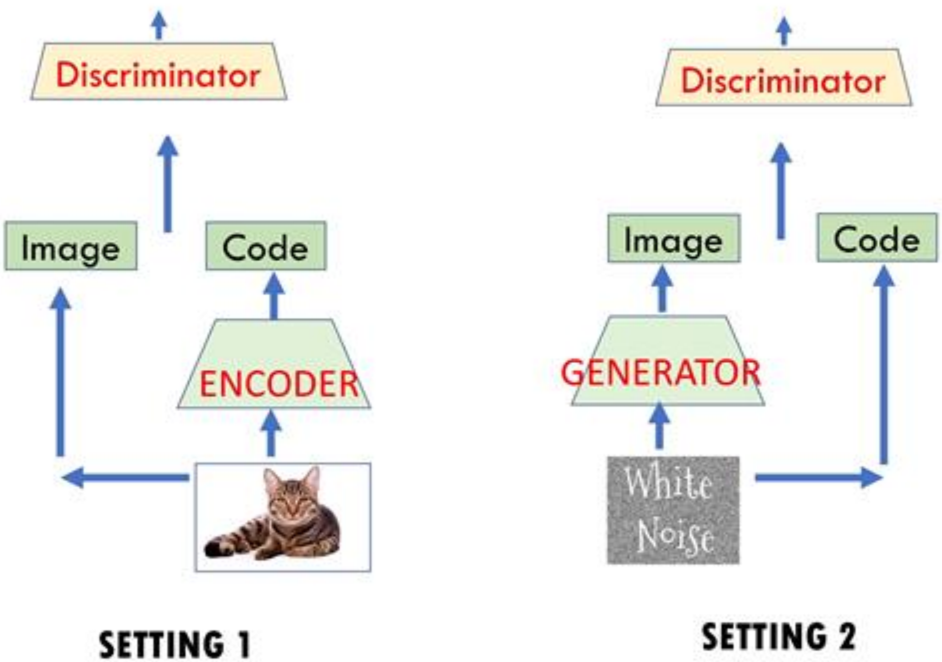
If F contains all function $f: \mathbb{R}^d \to [0,1]$, the above objective converges to

$$\min_{g\in G} \underbrace{KL\left(P_g \middle|\middle| (P_{real}+P_g)/2\right) + KL\left((P_{real}+P_g)/2 \middle|\middle| P_g\right)} - 2\ln 2$$

Jensen-Shannon divergence

Variants

If we also want to train an **encoder E**: that is, a network that tries to output the z, s.t. x was generated from z, there is a way to adapt the adversarial setup:



Discriminator tries to distinguish b/w:

Setting 1: samples are (x, E(x))

Setting 2: samples are (z, G(z))

Dumoulin et al, Donahue et al '16:

In the limit of infinite samples, infinite capacity generators, the distributions of Setting 1 and 2 match.

What affects our choice of F?

Statistical considerations: very powerful discriminators (e.g. large neural networks) will require a lot of samples. Weak discriminators will specify a very weak metric: very "different" distributions will look very "similar" to metric.

Our understanding here is better.

Algorithmic considerations: if discriminators are very powerful, gradient information for generator is too weak and can vanish. If they are too weak – metric is weak.

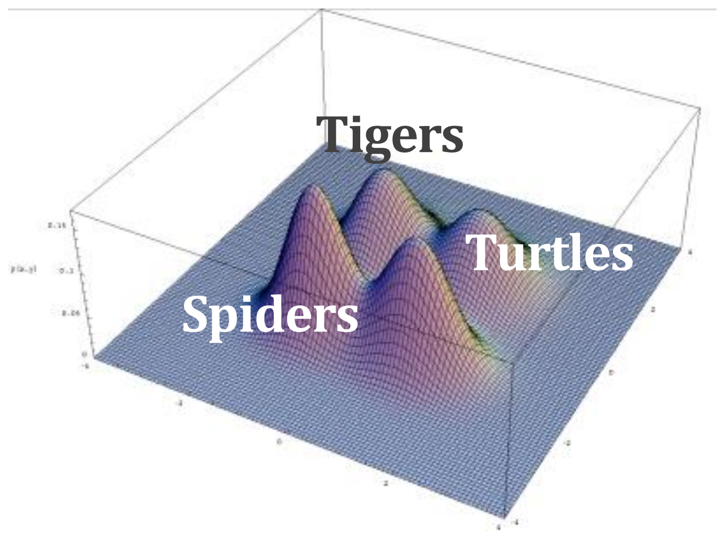
Our understanding of training dynamics is *very* poor.

Statistical questions

<u>Tension</u>: strength of discriminators?

Small (weak) discriminators $\Rightarrow$ mode collapse:

Neural net discriminators with **≤ m parameters** **fooled** by generator w/ support size ≈ **m**.
[Arora et al'17, Arora-Risteski-Zhang **ICLR'18**]



Real-life distributions have large support!

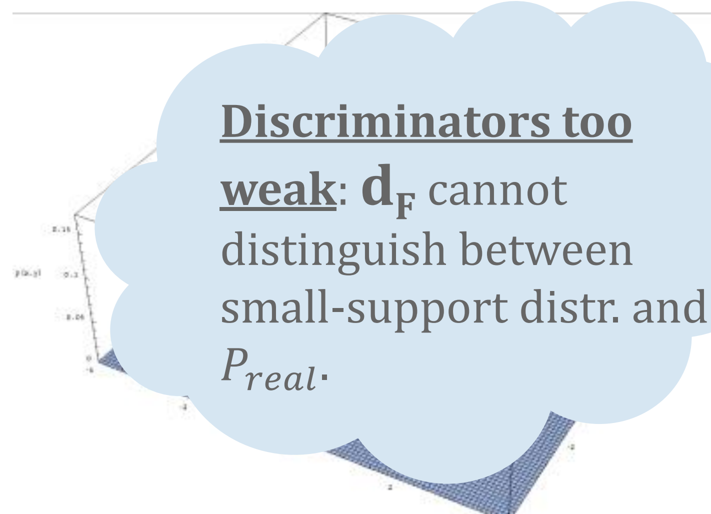
Tension: strength of discriminators?

Small (weak) discriminators ⇒ mode collapse.

Happens for any P_{real}

Neural net discriminators with **≤ m parameters fooled** by generator w/ support size **≈ m**.
[Arora et al'17, Arora-Risteski-Zhang **ICLR'18**]

Not memorization!
More training samples
don't help.



Discriminators too weak: $\mathbf{d_F}$ cannot distinguish between small-support distr. and P_{real}.

Real-life distributions have large support!

Tension: strength of discriminators

Small discriminators ⇒ mode collapse:

Generator w/ support size $\approx m$ **fools**
neural net discriminators with **≤ m parameters.**
[Arora et al'17, Arora-Risteski-Zhang 'ICLR18]

Large discriminators ⇒ poor generalization:

Loss with small # samples differs a lot from loss with infinite # samples.

$$d_F(P_{samples}, P_g) \not\approx d_F\left(P_{real}, P_g\right)$$

Algorithmic questions

How to train a GAN

"**Best response dynamics**": fix generator, find best discriminator; then fix discriminator, find best generator. Repeat.

Better in practice: take one gradient step for generator, do a few gradient steps for discriminator. Repeat.

Going with intuition of Wasserstein distance: we'd like the discriminators to be somewhat Lipschitz – clipping weights is a good idea.

How to train a GAN

How many discriminator gradient steps to take for each generator gradient step

Algorithm 1 WGAN, our proposed algorithm. All experiments in the paper used the default values $\alpha = 0.00005$, $c = 0.01$, $m = 64$, $n_{\text{critic}} = 5$.

Require: : α, the learning rate. c, the clipping parameter. m, the batch size. n_{critic}, the number of iterations of the critic per generator iteration.

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

while θ has not converged **do**

  for $t = 0, ..., n_{\text{critic}}$ **do**

    Sample $\{x^{(i)}\}_{i=1}^m \sim \mathbb{P}_r$ a batch from the real data.

    Sample $\{z^{(i)}\}_{i=1}^m \sim p(z)$ a batch of prior samples.

    $g_w \leftarrow \nabla_w \left[\frac{1}{m}\sum_{i=1}^m f_w(x^{(i)}) - \frac{1}{m}\sum_{i=1}^m f_w(g_\theta(z^{(i)}))\right]$

    $w \leftarrow w + \alpha \cdot \text{RMSProp}(w, g_w)$

    $w \leftarrow \text{clip}(w, -c, c)$

  end for

  Sample $\{z^{(i)}\}_{i=1}^m \sim p(z)$ a batch of prior samples.

  $g_\theta \leftarrow -\nabla_\theta \frac{1}{m}\sum_{i=1}^m f_w(g_\theta(z^{(i)}))$

  $\theta \leftarrow \theta - \alpha \cdot \text{RMSProp}(\theta, g_\theta)$

end while

Empirical estimates of expectations to calculate discriminator gradient

Clip

Generator gradient

Figure from Arjovsky, Chintala, Bottou '17

Common training problems

Unstable training: the problem is a min-max problem (also called saddle point problem) – typically optimization is much less stable than pure minimization.

Particularly common instantiation: **cycling**

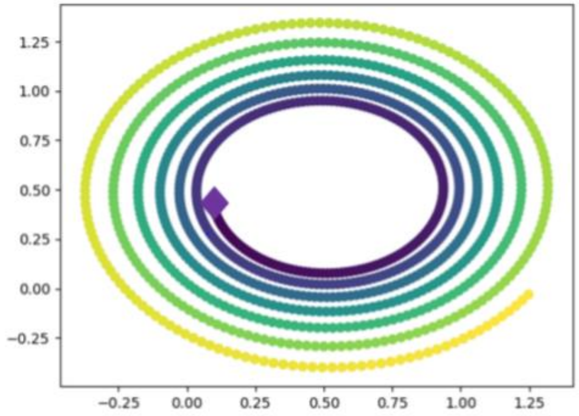


Figure 5: f(x,y)=(x-1/2)(y-1/2). x and y are initialized at the purple diamond. Alternating between gradient ascent/ descent on x and y leads to divergent behavior, spiraling away from the optimum, but the average of the parameters is close to the optimal solution

Figure from https://people.csail.mit.edu/madry/6.883/files/lecture_8.pdf

Common training problems

Unstable training: the problem is a min-max problem (also called saddle point problem) – typically optimization is much less stable than pure minimization.

Vanishing gradient: if the discriminator is too good, the generator gradients have a propensity to be small. (This is concerning, as to be taking gradients of the Wasserstein/JS/… objective, the discriminator needs to be optimal.)

Less of a problem with more modern GANs than with DC-GAN.

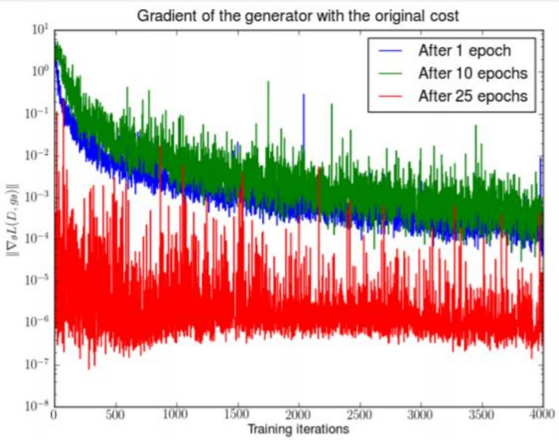


Figure 2: First, we trained a DCGAN for 1, 10 and 25 epochs. Then, with the generator fixed we train a discriminator from scratch and measure the gradients with the original cost function. We see the gradient norms decay quickly, in the best case 5 orders of magnitude after 4000 discriminator iterations. Note the logarithmic scale.

Figure from Arjovsky & Bottou '17

Common training problems

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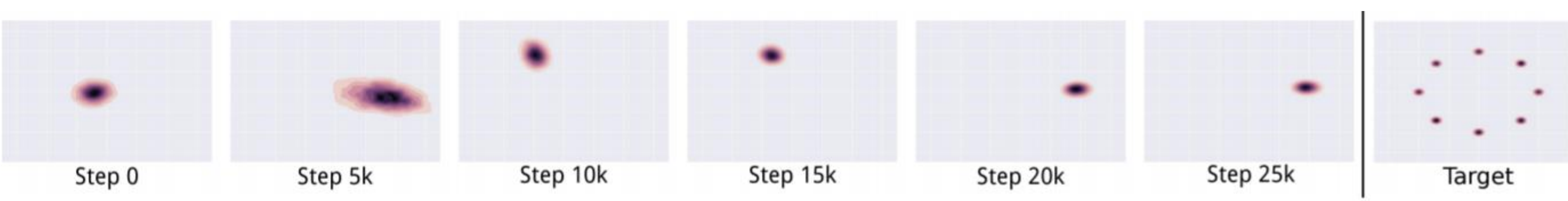
Less of a problem with more modern GANs than with DC-GAN.

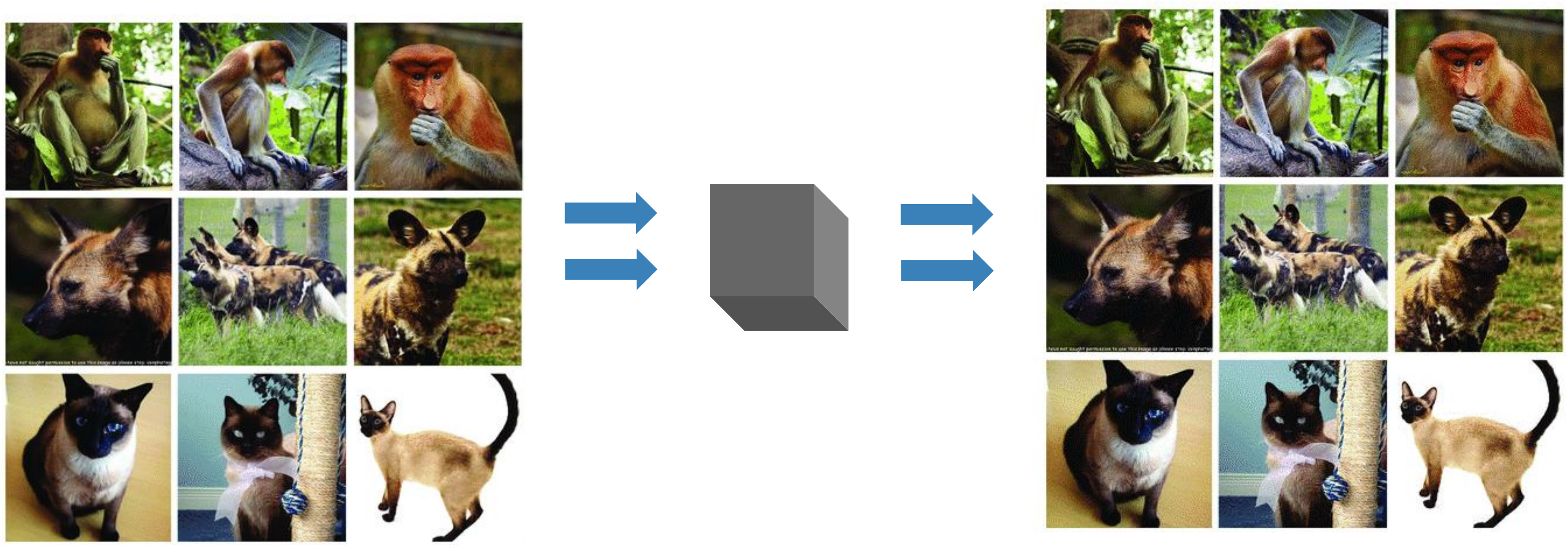
Mode collapse: the training only recovers some of the modes of the underlying distribution. **(NOT** clear if this is a statistical or algorithmic problem.)



Evaluating GANs

How do we evaluate GANs

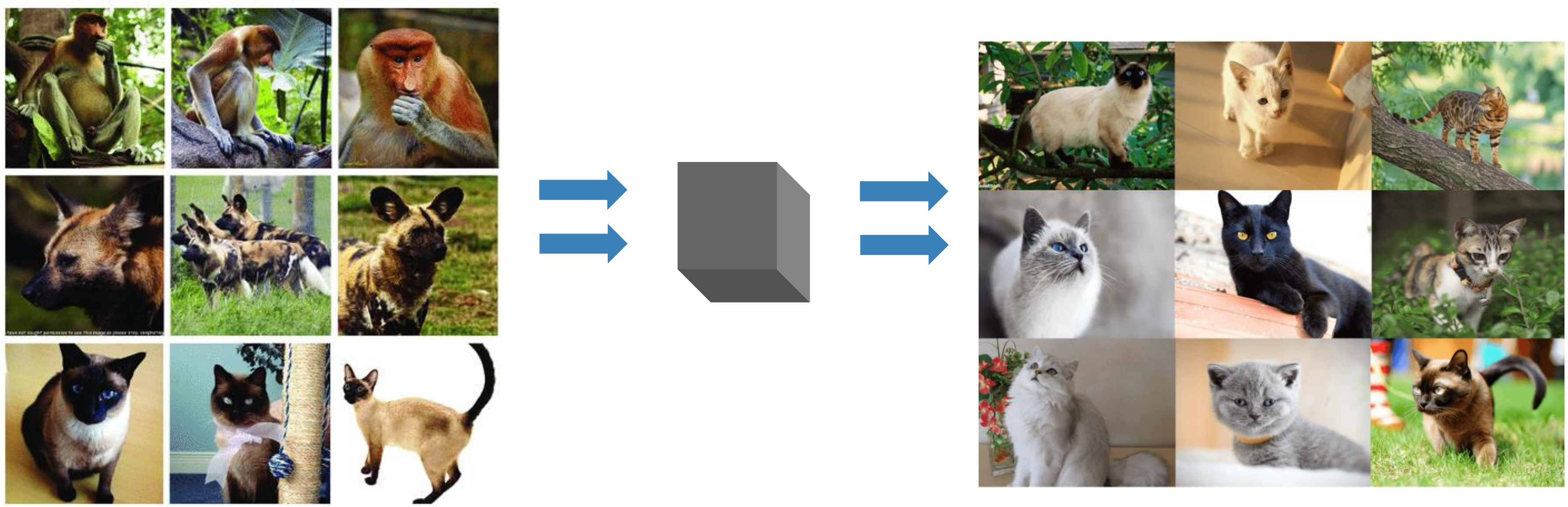
Wins beauty contest, but does the GAN **<u>really</u>** learn distribution?



No, just **<u>memorizing</u>** training samples.

How do we evaluate GANs

Wins beauty contest, but does the GAN **really** learn distribution?



No, **mode collapse:** missing regions (modes) of input distribution.

How do we evaluate GANs

Since we cannot evaluate the likelihood of the input data under a generator, evaluation is hard.

(Disproportionately) frequently, the evaluation is done by visually comparing samples – this cannot exclude issues like memorization, mode collapse, etc.

Can we test for some common ***failure modes****?*

Diagnosing small support size: bday paradox

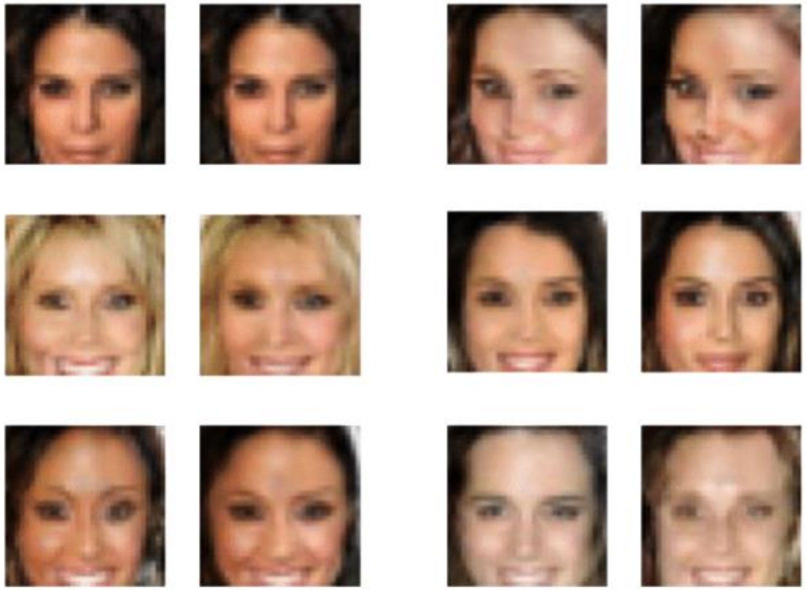
Birthday Paradox:
If there are **23** people in a group, **>** ½ chance that two of them share a birthday.

General version: Suppose a distribution is uniform over N images. Then Pr[sample of size $\sqrt{N}$ has a duplicate image] > ½.

Birthday paradox test [Arora-Risteski-Zhang '18**] :** If a sample of size **s** has **duplicate** images with prob. > ½, then distribution essentially* has only **s^2 distinct images**.

Implementation: Draw sample of size **s**; heuristically flag possible near-duplicates. Use human in the loop to verify duplicates.

Diagnosing small support size: bday paradox



CelebA (faces): 200k training images

DC-GAN [Radford et al.'15]:
Support size ≈ 250K

BiGAN [Donohue et al.'17] and **ALI [Dumoulin et al.'17]:**
Support size ≈ 1M

A lot of **followup** and **parallel** work about diagnosing mode collapse.

Interpolation

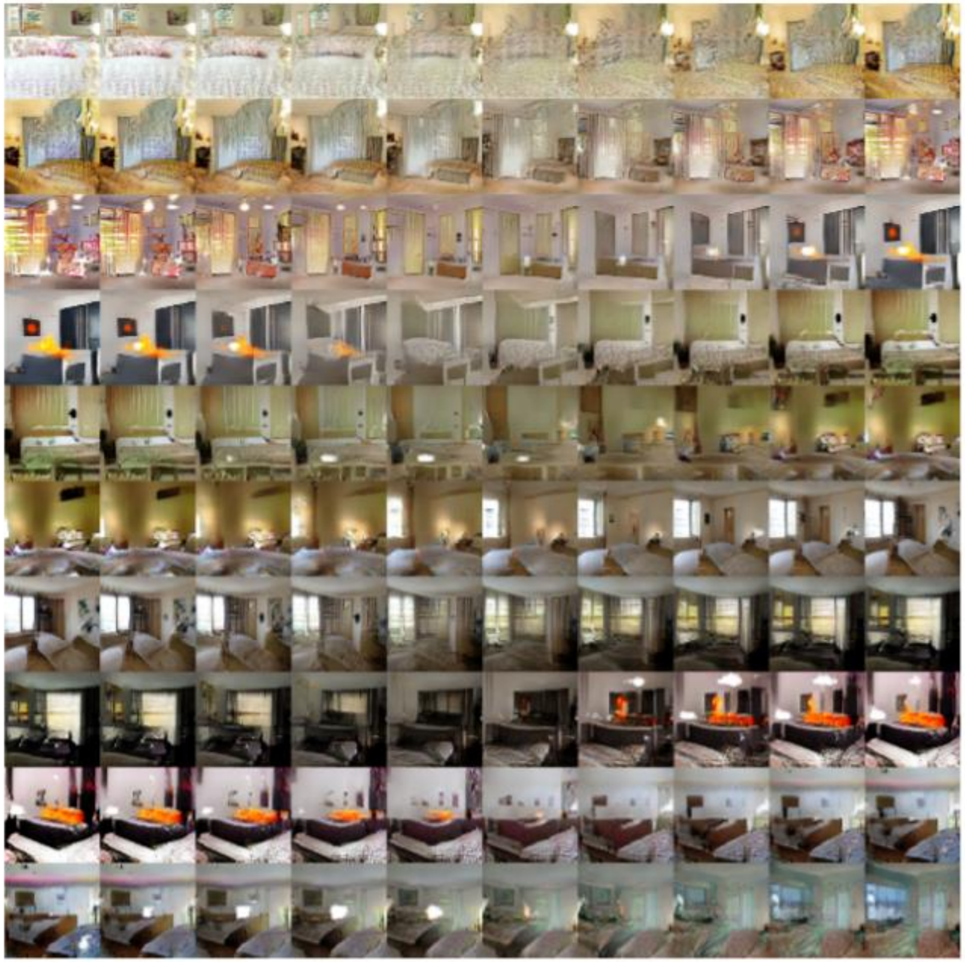


Figure 4: Top rows: Interpolation between a series of 9 random points in Z show that the space learned has smooth transitions, with every image in the space plausibly looking like a bedroom. In the 6th row, you see a room without a window slowly transforming into a room with a giant window. In the 10th row, you see what appears to be a TV slowly being transformed into a window.

If linearly interpolating in latent space gives rise to meaningful images (without sharp transitions), unlikely GAN is just memorizing.

Figure from
Radford, Metz, Chintala '16.

Inception score

Suppose we use trained network – the *Inception* architecture as a **labeler** for images. Inception gives probability over labels y for sample x: p(y|x).

Desirable features of generator: the Inception classifier should be "sure" about the label for most images (p(y|x) should have *low entropy*), and the classes it generates should be diverse (p(y) = $\mathbb{E}_{x\sim P_g} p(y|x)$ should have *high entropy*)

Thus, we want $H\big(p(y|x)\big)$ to be **low**, $H(p(y))$ is **high**.

Consider the expression: $\mathbb{E}_{x\sim P_g} KL(p(y|x)||p(y))$

$$= \mathbb{E}_{x\sim P_g} \mathbb{E}_{y\sim p(y|x)} \log p(y|x) - \log p(y)$$

$$= -\mathbb{E}_{x\sim P_g} H\big(p(y|x)\big) + H\big(p(y)\big)$$

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Consider the expression: $\mathbb{E}_{x\sim P_g} KL(p(y|x)||p(y))$

Inception score: $\exp(\mathbb{E}_{x\sim P_g} KL\big(p(y|x)\big|\big|p(y)\big)\big)$

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Many follow ups, e.g. Frechet inception distance, modified inception score, …

Check for **many** other metrics:

Borji '18: 24 quantitative, 5 qualitative measures

The pros and cons of GANs

Pros

Photorealism: photorealistic images, even w/ **relatively small models.**

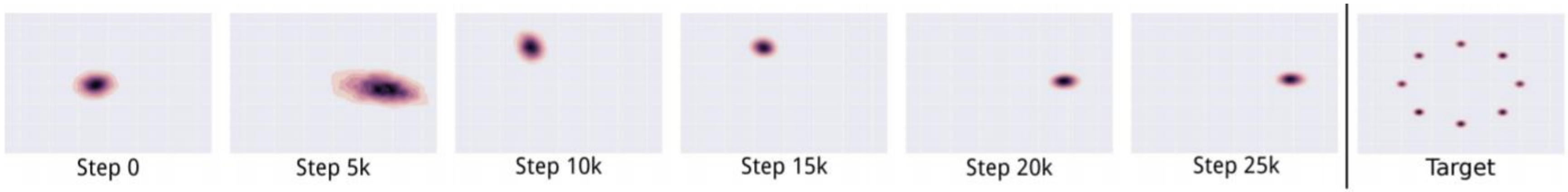
Efficient sampling: easy to draw samples from model (unlike e.g. energy models).

Cons

Unstable training: min-max problem – typically optimization much less stable than pure minimization.

Mode collapse: training only recovers some of the "modes" of the underlying distribution.

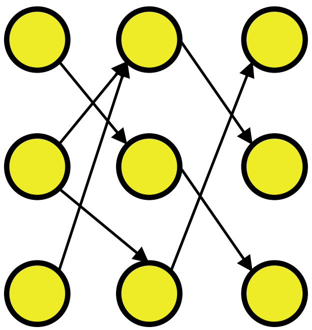
Evaluation: no likelihood, so hard to evaluate fit.



Middle ground:
“Invertible GANs/Normalizing Flows”

Can we “marry” likelihood models w/ GANs?

Suppose generator g: $\mathbb{R}^{d} \to \mathbb{R}^{d}$ were **invertible**.



Recall from the prev. lecture: if we denote by $\phi(z)$ the density of z under the standard Gaussian, by the change of variables formula:

$$P_g(x) = \phi(g^{-1}(x))\left|\det\left(J_x\left(g^{-1}(x)\right)\right)\right|$$

Hence, we can write down the likelihood in terms of the parameters of g^{-1} under this model!

Middle ground: “Invertible GANs/Normalizing Flows”

$$P_g(x) = \phi(g^{-1}(x))\left|\det\left(J_x\left(g^{-1}(x)\right)\right)\right|$$

Hence, denoting $g^{-1} = f_\theta$, for some family of parametric functions $\{f_\theta, \theta \in \Theta\}$, the max-likelihood estimator solves

$$\max_\theta \sum_{i=1}^{N} \log \phi(f_\theta(x_i)) + \log\left|\det\left(J_x\left(f_\theta(x_i)\right)\right)\right|$$

If we can evaluate and differentiate the above objective efficiently, we can do gradient-based likelihood fitting.

Choosing invertible transforms

Note that since the change-of-variables formula composes, so if $f_\theta = f_1 \circ f_2 \circ \cdots f_L$, we have

Value of k-th layer

$$\log p_\theta(x) = \sum_{i=1}^{N} \log \phi(f_\theta(x_i)) + \sum_{k=1}^{L} \log |\det(J_x(f_k\,(h_k(x_i)))|$$

So, if we can design a “simple” family of invertible transforms, we can just keep composing it.

Try 1: *General linear maps.*

<u>Poor representational power</u>: composition of linear maps is linear. If x = Az, and z is sampled from a Gaussian – x is Gaussian too.

<u>Inefficient:</u> Evaluating determinant of a d x d matrix takes O(d^3) time – infeasible.

Choosing invertible transforms

Try 2: *Elementwise (possibly non-linear) maps*.

Suppose that $f_\theta(x) = \left(f_\theta(x_1), f_\theta(x_2), \dots, f_\theta(x_d)\right)$

Efficient evaluation: Determinant is diagonal (since $\frac{\partial f_\theta(x_i)}{\partial x_j} = 0$, for $i \neq j$), so $\det(J_x\left(f_\theta(x)\right) = \Pi_i \frac{\partial f_\theta(x_i)}{\partial x_i}$.

Poor representational power: Transforms don't "combine" coordinates.

But, even if a matrix is triangular, Jacobian is just the product of the diagonals!!

Choosing invertible transforms

Try 3: *NICE/RealNVP (Non-linear Independent Component Estimation)*

Divide the coordinates of x into two sub-vectors with half the coords: $x_{1:\frac{d}{2}}, x_{\frac{d}{2}+1,d}$

Divide the coordinates of $z \coloneqq f_\theta(x)$ into two sub-vectors, $z_{1:\frac{d}{2}}, z_{\frac{d}{2}+1,d}$ and set:

$$z_{1:\frac{d}{2}} = x_{1:\frac{d}{2}}$$

$$z_{d/2+1,d} = x_{d/2+1,d} \odot \exp\left(s_\theta\left(x_{1:d/2}\right)\right) + t_\theta\left(x_{1:d/2}\right)$$

When is this invertible, and is the Jacobian efficiently calculated?

Choosing invertible transforms

Try 3: *NICE/RealNVP (Non-linear Independent Component Estimation)*

$$z_{1:\frac{d}{2}} = x_{1:\frac{d}{2}}$$

$$z_{\frac{d}{2}+1,d} = x_{\frac{d}{2}+1,d} \odot \exp\left(s_\theta\left(x_{1:d/2}\right)\right) + t_\theta\left(x_{1:d/2}\right)$$

$$J_x\left(f_\theta(x)\right) = \begin{bmatrix} I & 0 \\ \frac{\partial \mathbf{z}_{d/2:d}}{\partial \mathbf{x}_{1:d/2}} & \operatorname{diag}\left(\exp(\boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{x}_{\mathbf{1}:\boldsymbol{d}/\mathbf{2}})\right) \end{bmatrix}$$

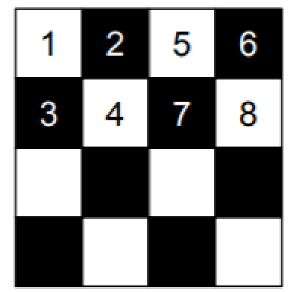
The determinant of a triangular matrix is the product of the diagonals!

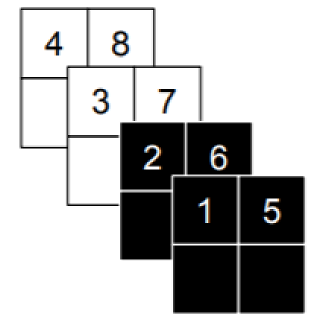
Hence, $\det\ J_x\left(f_\theta(x)\right) = \Pi_i \exp\left(s_\theta\left(x_{1:d/2}\right)\right)_i$

If t_θ, s_θ is say, a neural net, easy to evaluate and take derivatives.

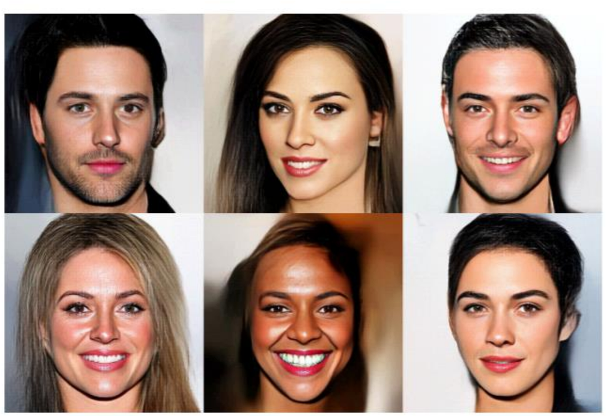
How to choose partitions?

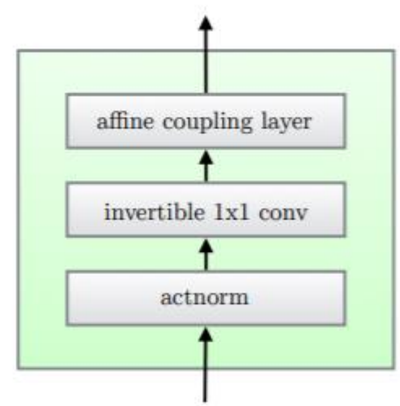
NICE (Dinh et al ‘14), RealNVP (Dinh et al ‘16): The choice of partitions is fixed, checkerboard of channel-wise.





Glow (Kingma et al ‘18): add trained linear transforms between affine coupling layers – i.e. a generalization of a “learned” permutation





Some samples

NICE/RealNVP (Non-linear Independent Component Estimation)

Figure from “*Density estimation using Real NVP*” by *Dinh et al ‘16*

Some samples

Glow

Figure 5: Linear interpolation in latent space between real images

Figure *from (Kingma et al '18)*

The pros and cons of normalizing flows

Pros

Photorealism: photorealistic images.

Efficient sampling: easy to draw samples from model.

Stabl(er) training: likelihood objective

Evaluation: no likelihood, so hard to evaluate fit.

Cons

Extremely large: in practice, good models need to be *extremely* large (Glow: 40 GPUs for ~week)

Model depth: training gets harder as models are typically very deep. (Glow: ~1200 layers in total)