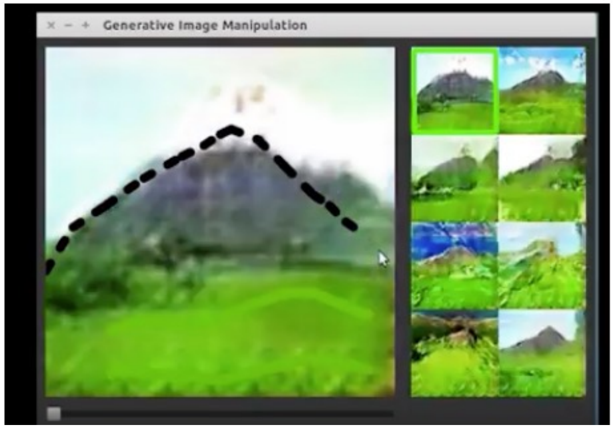
Generative Adversarial Networks (GAN)

ECE57000: Artificial Intelligence

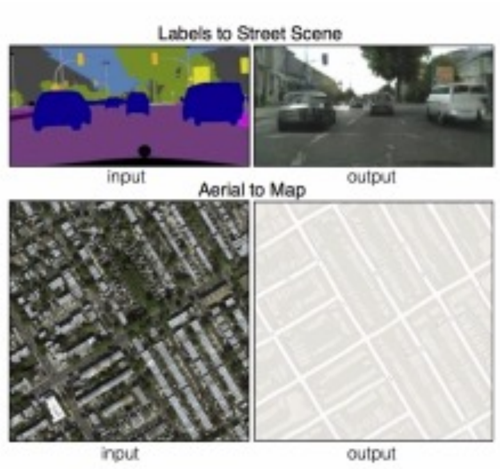
David I. Inouye

Why study generative models?

- Sketching realistic photos



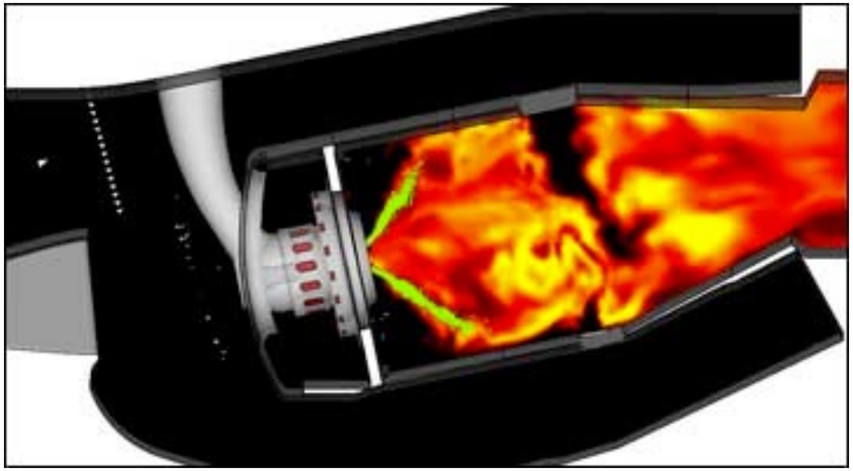
- Style transfer



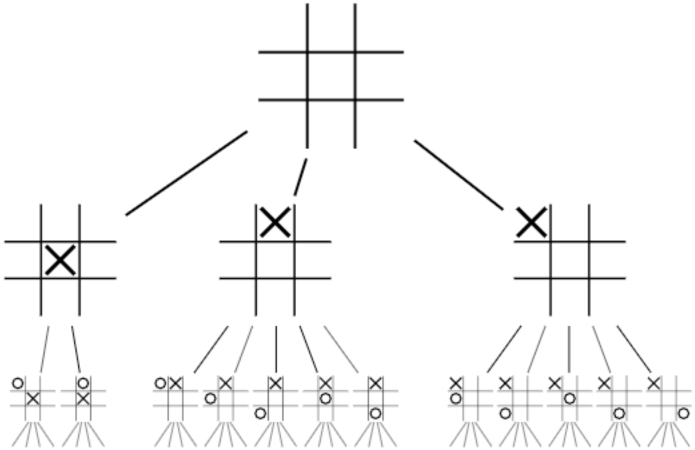
- Super resolution

Much of material from: Goodfellow, 2012 tutorial on GANs.

Why study generative models?



- Emulate complex physics simulations to be faster



- Reinforcement learning - Attempt to model the real world so we can simulate possible futures

Much of material from: Goodfellow, 2012 tutorial on GANs.

Outline of Generative Adversarial Networks (GANs)

Introduction

- Motivation for generative models
- Overview of training generative models

GAN model

- No explicit density
- Only samples available

GAN objective

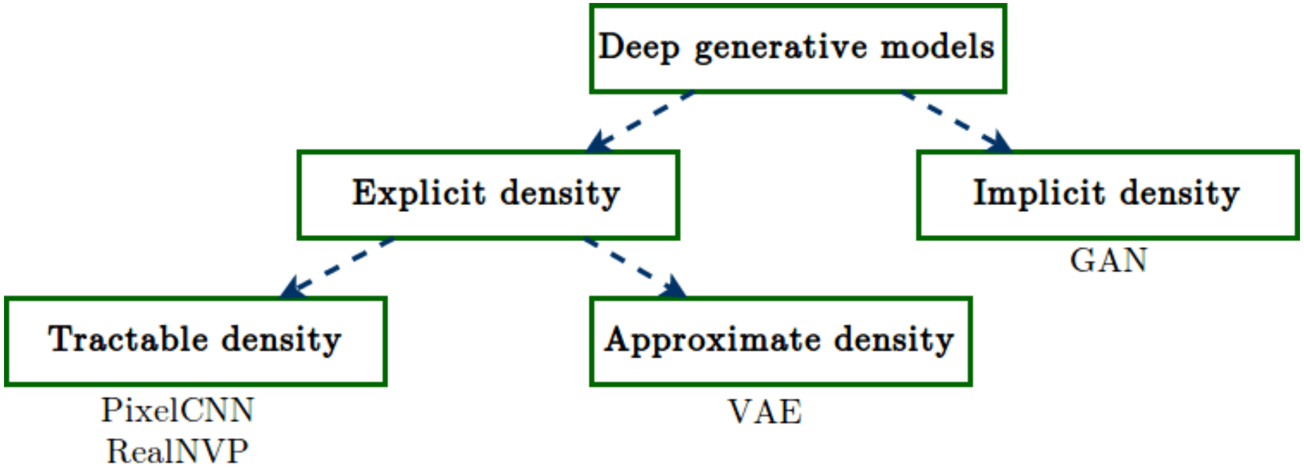
- Intuition as adversarial game
- Mathematics via min-max optimization
- Derivation of theoretical solution as JSD

Practical challenges of GANs

- Gap between theory and practice
- Vanishing gradient issue of JSD
- Failure to converge (min-max optimization)
- Mode collapse
- Evaluation (IS, FID)

How do we learn these generative models?

- Primary classical approach is MLE
  - Density function is explicit parameterized by θ
  - Examples: Gaussian, Mixture of Gaussians
- Problem: Classic methods struggle to model very high dimensional spaces like images
  - Remember a 256x256x3 image is roughly 200k dimensions


Deep generative models

Explicit density

Implicit density

GAN

Tractable density

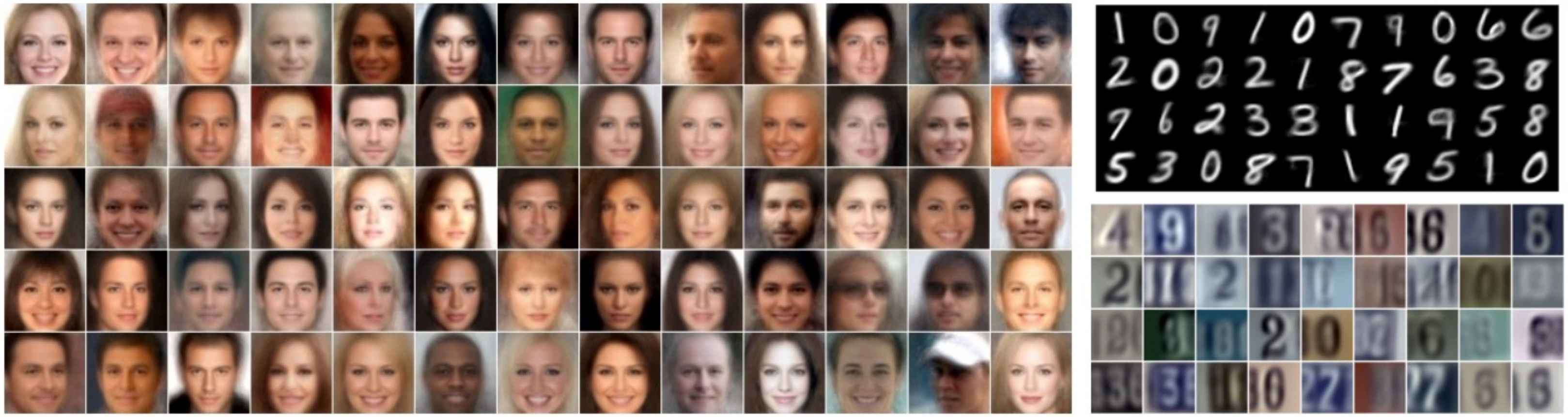
PixelCNN
RealNVP

Approximate density

VAE

Maybe not a problem: GMMs compared to GANs http://papers.nips.cc/paper/7826-on-gans-and-gmms.pdf

- Which one is based on GANs?

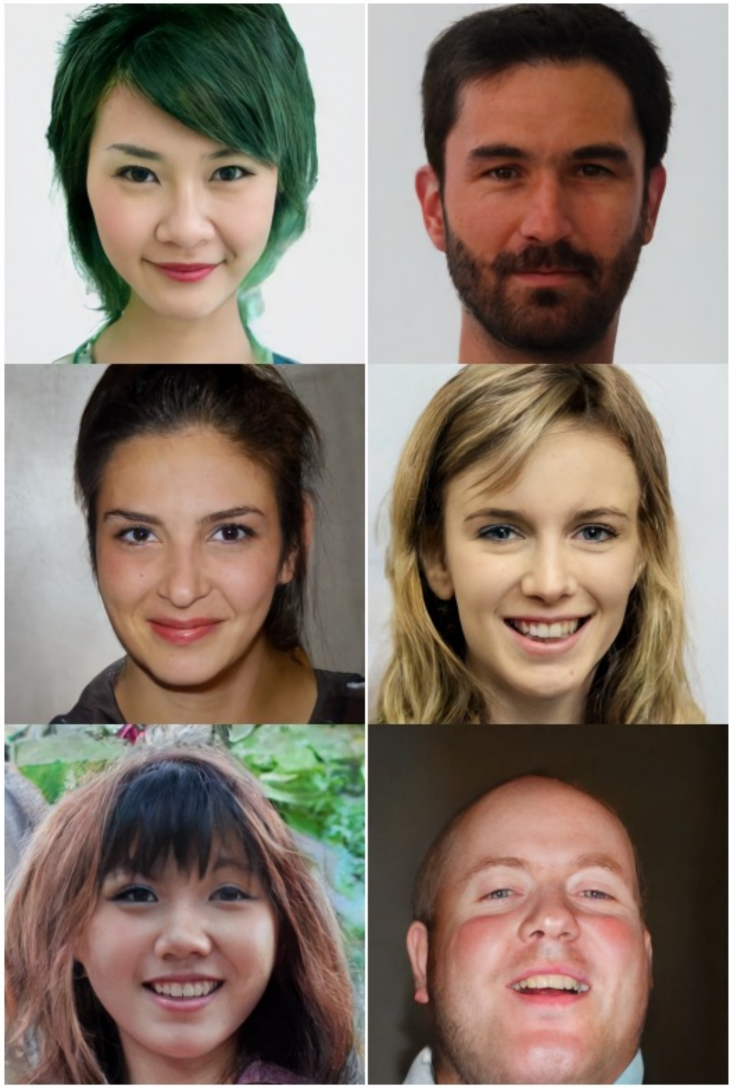


VAEs are one way to create a generative model for images though images are blurry

https://github.com/WojciechMormul/vae

Maybe not a drawback… VQ-VAE-2 at *NeurIPS 2019*

Generated high-quality images (probably don't ask how long it takes to train this though…)



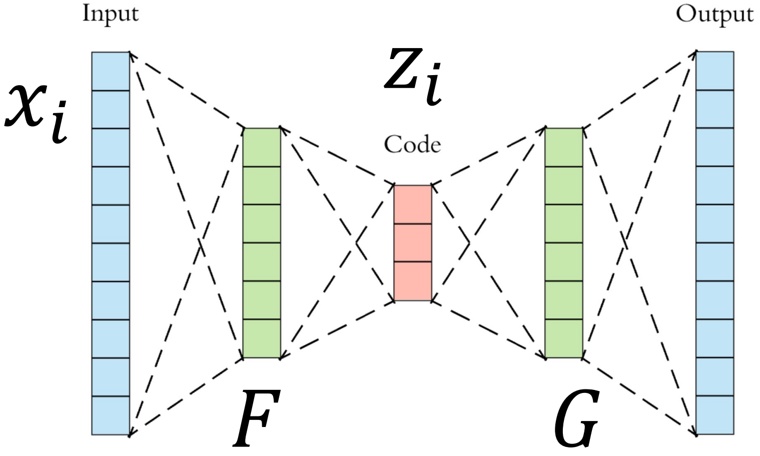
Razavi, A., van den Oord, A., & Vinyals, O. (2019). Generating diverse high-fidelity images with vq-vae-2. In *Advances in Neural Information Processing Systems* (pp. 14866-14876).

Newer (not necessarily better) approach: Train generative model <u>**without explicit density**</u>

- GMMs and VAEs had **explicit** density function
  (i.e., mathematical formula for density $p(x;\theta)$)
- In GANs, we just try learn a sample **generator**
  - **Implicit** density ($p(x)$ exists but cannot be written down)
- Sample generation is simple
  - $z \sim p_z$, e.g., $z \sim \mathcal{N}(0, I) \in \mathbb{R}^{100}$
  - $G_\theta(z) = \hat{x} \sim \hat{p}_g(x)$
  - Where G is a deep neural network

Unlike VAEs, GANs do not (usually) have inference networks

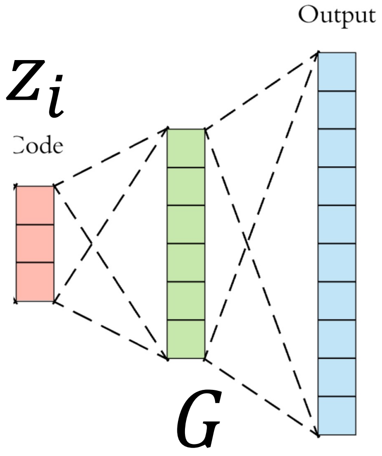
VAE



$\tilde{x}_i \sim p(x_i | G(z_i))$

$L(x_i, \tilde{x}_i)$

GAN



$\tilde{x}_i = G(z_i)$

$L(x_i, \tilde{x}_i)?$

No pair of original and reconstructed
How to train?

Key training challenge: Comparing two distributions known <u>only through samples</u>

- In GANs, we cannot produce pairs of original and reconstructed samples as in VAEs
- But have samples from original data and generated distributions

$$D_{\mathrm{data}} = \{x_i\}_{i=1}^{n}, \qquad x_i \sim p_{\mathrm{data}}(x)$$
$$D_{\mathrm{g}} = \{x_i\}_{i=1}^{\infty}, \qquad x_i \sim p_{\mathrm{g}}(x|G)$$

- How do we compare two distributions only through samples?
  - Fundamental, bigger than generative models

GAN objective:
Could we use KL divergence as in MLE training?

- We can approximate the KL term up to A constant

$$KL\left(p_{data}(x), p_g(x)\right) = \mathbb{E}_{p_{data}}\left[\log \frac{p_{data}(x)}{p_g(x)}\right]$$

$$= \mathbb{E}_{p_{data}}[-\log p_g(x)] + \mathbb{E}_{p_{data}}[\log p_{data}(x)]$$

$$\approx \widehat{\mathbb{E}}_{p_{data}}[-\log p_g(x)] + constant$$

$$= \sum_i -\log p_g(x_i) + constant$$

$$= \sum_i -\log p_g(x_i) + constant$$

Because GANs do not have an explicit density, we cannot compute this KL divergence.

GAN objective mathematics: Competitive game between two players

- Abstract formulation as minimax game

$$\min_G \max_D \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\left[\log\left(1 - D\big(G(z)\big)\right)\right]$$

  - D is a probabilistic binary classifier, i.e., output is probability between 0 and 1
  - G must output an object that is the same shape as the input x
- Minimax/adversarial : “Minimize the ***worst case*** (max) loss”
- What does this adversarial objective mean?

GAN objective: GANs introduce the idea of <u>adversarial training</u> for estimating the distance between two distributions

- GANs approximate the Jensen-Shannon Divergence (JSD) closely related to KL divergence
- GANs optimize both the JSD approximation and the generative model simultaneously
  - A different type of two network setup
- Broadly applicable for comparing distributions only through samples

GAN objective intuition: Competitive game between two players

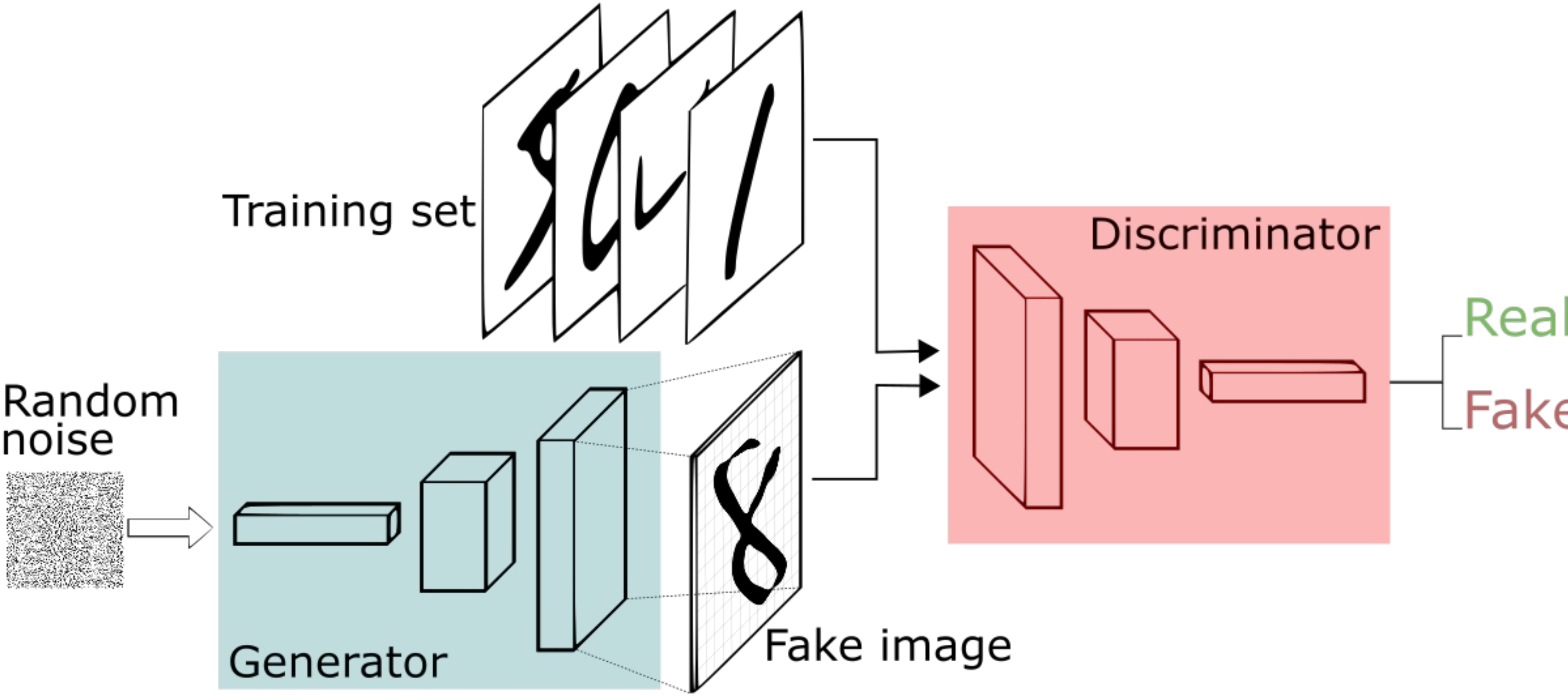
- Intuition: Competitive game between two players
  - Counterfeiter is trying to avoid getting caught
  - Police is trying to catch counterfeiter

$$\min_G \max_D \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\left[\log\left(1 - D\big(G(z)\big)\right)\right]$$

- Analogy with GANs
  - Counterfeiter = Generator denoted G
  - Police = Discriminator denoted D

GAN objective in practice: Train two deep networks simultaneously

$$\min_G \max_D \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\left[\log\left(1 - D\left(G(z)\right)\right)\right]$$



https://www.freecodecamp.org/news/an-intuitive-introduction-to-generative-adversarial-networks-gans-7a2264a81394/

GAN objective mathematics: Competitive game between two players

- Minimax: “Minimize the ***worst case*** (max) loss”
  - Counterfeiter goal: “Minimize chance of getting caught assuming the best possible police.”

- Abstract formulation as minimax game

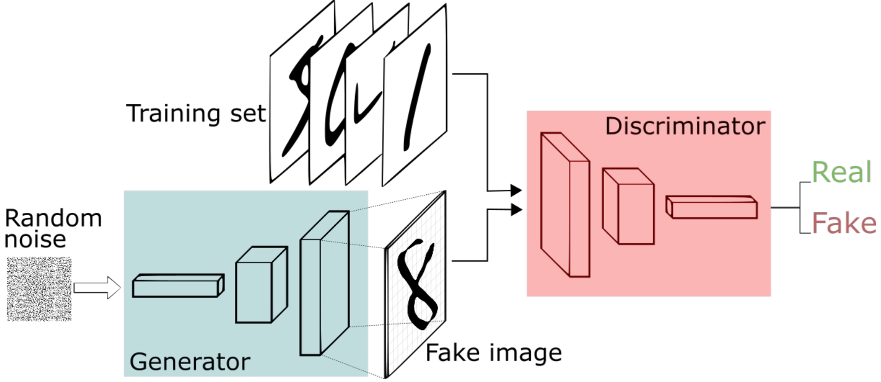
$$\min_G \max_D \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\left[\log\left(1 - D\big(G(z)\big)\right)\right]$$

- The value function is

$$\mathrm{V(D,G)} = \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\left[\log\left(1 - D\big(G(z)\big)\right)\right]$$

- Key feature: Almost no restrictions on the networks D and G

The discriminator seeks to be optimal classifier



- Let’s look at the inner maximization problem

$$D^* = \arg\max_D \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\left[\log\left(1 - D\left(G(z)\right)\right)\right]$$

- **Given a fixed G**, the optimal discriminator is the optimal Bayesian classifier

$$D^*(\tilde{x}) = p^*(\tilde{y} = 1|\tilde{x}) = \frac{p_{data}(\tilde{x})}{p_{data}(\tilde{x}) + \hat{p}_g(\tilde{x})}$$

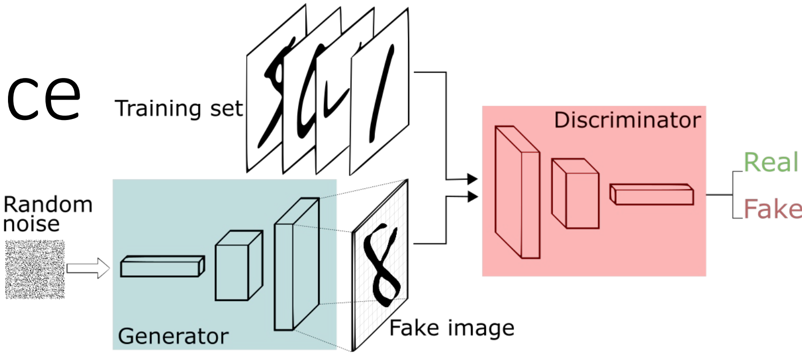
Derivation for the optimal discriminator

- **Given a fixed $\boldsymbol{G}$**, the optimal discriminator is the optimal classifier between images
- $C(G) = \max_D \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\left[\log\left(1 - D\left(G(z)\right)\right)\right]$
- $= \max_D \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{x\sim \hat{p}_g}\left[\log\left(1 - D(x)\right)\right]$

Opposite of reparametrization trick! ☺

- $= \max_D \int p_{\text{data}}(x) \log D(x)\, dx + \int \hat{p}_g(x) \log\left(1 - D(x)\right) dx$
- $= \max_D \int p_{\text{data}}(x) \log D(x) + \hat{p}_g(x) \log\left(1 - D(x)\right) dx$
- $= \max_D \int a_x \log y_x + b_x \log(1 - y_x)\, dx$
- Max of $a \log y + b \log(1 - y)$ is $y^* = \frac{a}{a+b}$.
  - (Hint: Take derivative and set to 0)
- Therefore, $D^*(x) = \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + \hat{p}_g(x)}$

The generator seeks to produce data that is like real data



- **Given that the inner maximization is perfect**, the inner minimization is equivalent to Jensen Shannon Divergence **for the given G**:

$$\begin{aligned} C(G) &= \max_D V(D,G) \\ &= 2\, JSD\left(p_{data}, \hat{p}_g\right) + constant \end{aligned}$$

- **Jensen Shannon Divergence** is a symmetric version of KL divergence

$$\begin{aligned} &JSD\big(p(x), q(x)\big) \\ &= \frac{1}{2} KL\left(p(x), \frac{1}{2}\big(p(x)+q(x)\big)\right) + \frac{1}{2} KL\left(q(x), \frac{1}{2}\big(p(x)+q(x)\big)\right) \\ &= \frac{1}{2} KL(p(x), m(x)) + \frac{1}{2} KL(q(x), m(x)) \end{aligned}$$

- JSD also has the property of KL:

$$JSD\left(p_{data}, \hat{p}_g\right) \geq 0 \text{ and } = 0 \text{ if and only if } p_{data} = \hat{p}_g$$

- Thus, the optimal generator G^* will generate samples that perfectly mimic the true distribution:

$$\arg\min_G C(G) = \arg\min_G JSD\left(p_{data}, \hat{p}_g\right)$$

Derivation of inner maximization being equivalent to JSD

- $C(G) = \max_{D} \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\left[\log\left(1 - D\left(G(z)\right)\right)\right]$
- $= \max_{D} \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{x\sim \hat{p}_g}\left[\log\left(1 - D(x)\right)\right]$
- $= \mathbb{E}_{x\sim p_{\text{data}}}[\log D^*(x)] + \mathbb{E}_{x\sim \hat{p}_g}\left[\log\left(1 - D^*(x)\right)\right]$
- $= \mathbb{E}_{\tilde{x}\sim p_{\text{data}}}\left[\log \frac{p_{\text{data}}(\tilde{x})}{p_{\text{data}}(\tilde{x}) + \hat{p}_g(\tilde{x})}\right] + \mathbb{E}_{\tilde{x}\sim \hat{p}_g}\left[\log\left(1 - \frac{p_{\text{data}}(\tilde{x})}{p_{\text{data}}(\tilde{x}) + \hat{p}_g(\tilde{x})}\right)\right]$
- $= \mathbb{E}_{\tilde{x}\sim p_{\text{data}}}\left[\log \frac{p_{\text{data}}(\tilde{x})}{p_{\text{data}}(\tilde{x}) + \hat{p}_g(\tilde{x})}\right] + \mathbb{E}_{\tilde{x}\sim \hat{p}_g}\left[\log\left(\frac{\hat{p}_g(\tilde{x})}{p_{\text{data}}(\tilde{x}) + \hat{p}_g(\tilde{x})}\right)\right]$
- $= \mathbb{E}_{\tilde{x}\sim p_{\text{data}}}\left[\log \frac{\frac{1}{2} p_{\text{data}}(\tilde{x})}{\frac{1}{2}\left(p_{\text{data}}(\tilde{x}) + \hat{p}_g(\tilde{x})\right)}\right] + \mathbb{E}_{\tilde{x}\sim \hat{p}_g}\left[\log\left(\frac{\frac{1}{2}\hat{p}_g(\tilde{x})}{\frac{1}{2}\left(p_{\text{data}}(\tilde{x}) + \hat{p}_g(\tilde{x})\right)}\right)\right]$
- $= \mathbb{E}_{\tilde{x}\sim p_{\text{data}}}\left[\log \frac{p_{\text{data}}(\tilde{x})}{\frac{1}{2}\left(p_{\text{data}}(\tilde{x}) + \hat{p}_g(\tilde{x})\right)}\right] + \mathbb{E}_{\tilde{x}\sim \hat{p}_g}\left[\log\left(\frac{\hat{p}_g(\tilde{x})}{\frac{1}{2}\left(p_{\text{data}}(\tilde{x}) + \hat{p}_g(\tilde{x})\right)}\right)\right] - \log 4$
- $= 2\, JSD\left(p_{\text{data}}, \hat{p}_g\right) - \log 4$

https://papers.nips.cc/paper/5423-generative-adversarial-nets.pdf

Recap of GAN objective: Inner maximization is equivalent to JSD but *only at the current* G

- Overall GAN adversarial (min-max) problem:

$$\min_G \max_D \mathbb{E}_{x\sim p_{\mathrm{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\Big[\log\Big(1 - D\big(G(z)\big)\Big)\Big]$$

- Optimal solution to inner maximization problem

$$D^*(x) = \frac{p_{\mathrm{data}}(x)}{p_{\mathrm{data}}(x) + \hat{p}_g(x)}$$

- Using this solution, the inner problem is equivalent to JSD:

$$C(G) := \max_D V(D,G) = V(D^*,G) = 2\,JSD\big(p_{\mathrm{data}}, \hat{p}_g\big) - \log 4$$

- In theory, we can then update our G via

$$\nabla_{\mathrm{G}}\mathrm{C}(\mathrm{G}) = \nabla_G JSD\big(p_{\mathrm{data}}, \hat{p}_g\big) = \nabla_G V(D^*, G)$$

- However, after updating G, *the max must be solved again* (at least for this theory to hold).

Practical challenges in training GANs

- Gap between theory and practice
- Vanishing gradient issue of JSD
- Failure to converge (min-max optimization)
- Mode collapse
- Evaluation (IS, FID)

What if inner maximization is not perfect?

- Suppose the true maximum is not attained

$$\hat{C}(G) \\ = \widehat{\max_D} \mathbb{E}_{x\sim p_{\text{data}}}[\log D(x)] + \mathbb{E}_{z\sim p_z}\left[\log\left(1 - D\big(G(z)\big)\right)\right]$$

- Then, $\hat{C}(G)$ becomes a **lower bound** on JSD

$$\hat{C}(G) < C(G) = JSD\left(p_{data}(x), p_{g(x)}\right)$$

- However, the outer optimization is a **minimization**

$$\min_G \max_D V(D, G) \approx \min_G \hat{C}(G)$$

- Ideally, we would want an **upper bound** like in VAEs
- This can lead to significant training instability

Great! But wait… This theoretical analysis depends on critical assumptions

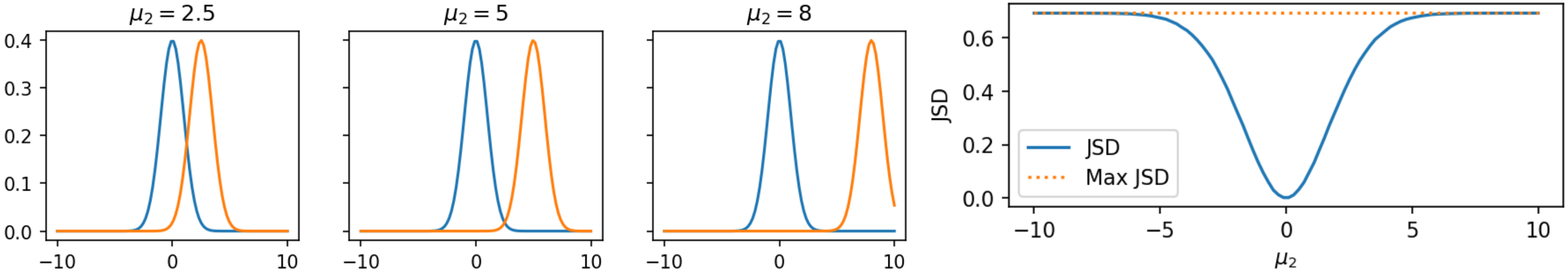
1. Assumptions on possible D and G
    1. Theory – All possible D and G
    2. Reality – Only functions defined by a neural network
2. Assumptions on optimality
    1. Theory – Both optimizations are solved perfectly
    2. Reality – The inner maximization is only solved approximately, and this interacts with outer minimization
3. Assumption on expectations
    1. Theory – Expectations over true distribution
    2. Reality – Empirical expectations over finite sample; for images, much of the high-dimensional space does not have samples

- **GANs can be very difficult/finicky to train**

Common problems with GANs: <u>Vanishing gradients</u> for generator caused by a discriminator that is “too good”

From: https://developers.google.com/machine-learning/gan/problems

- Vanishing gradient means $\nabla_G V(D, G) \approx 0$.
  - Gradient updates do not improve G
- Theoretically, this is an issue of JSD



- Practically, careful balance during training required:
  - Optimizing D too much leads to vanishing gradient
  - **But** training too little means it is not close to JSD

Arjovsky, M., Chintala, S., & Bottou, L. (2017, July). Wasserstein generative adversarial networks. In International conference on machine learning (pp. 214-223). PMLR.

Common problems with GANs: Vanishing gradients for generator caused by a discriminator that is "too good"

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- Vanishing gradient means $\nabla_G V(D, G) \approx 0$.
  - Gradient updates do not improve G

- Modified minimax loss for generator (original GAN)

$$\min_G \mathbb{E}_{p_g}\left[\log\left(1 - D\big(G(z)\big)\right)\right] \approx \min_G \mathbb{E}_{p_z}\left[-\log D\big(G(z)\big)\right]$$

- Wasserstein GANs

$$V(D, G) = \mathbb{E}_{p_{data}}[D(x)] - \mathbb{E}_{p_z}\left[D\big(G(z)\big)\right]$$

where D is 1-Lipschitz (special smoothness property).

Gulrajani, I., Ahmed, F., Arjovsky, M., Dumoulin, V., & Courville, A. C. (2017). Improved training of wasserstein gans. In *Advances in neural information processing systems* (pp. 5767-5777).

Common problems with GANs: Failure to converge because of minimax and other instabilities

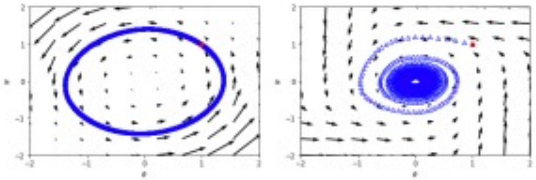
From: https://developers.google.com/machine-learning/gan/problems

- Loss function may oscillate or never converge
- Disjoint support of distributions
  - Optimal JSD is constant value (i.e., no gradient information)
  - Add noise to discriminator inputs (similar to VAEs)
- Regularization of parameter weights

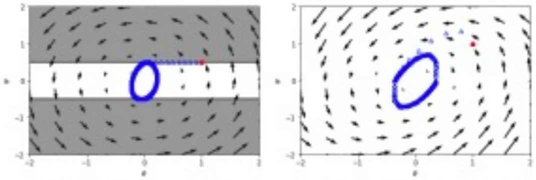
Arjovsky, M., & Bottou, L. (2017). Towards principled methods for training generative adversarial networks. *arXiv preprint arXiv:1701.04862*.

https://machinelearningmastery.com/practical-guide-to-gan-failure-modes/

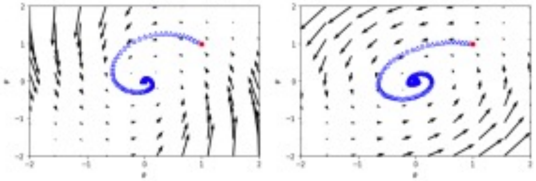
Mescheder, L., Geiger, A., & Nowozin, S. (2018, July). Which training methods for GANs do actually converge?. In International conference on machine learning (pp. 3481-3490). PMLR.



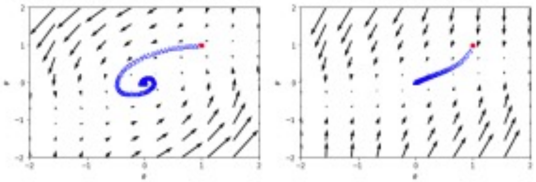
(a) Standard GAN (b) Non-saturating GAN



(c) WGAN ($n_d = 5$) (d) WGAN-GP ($n_d = 5$)



(e) Consensus optimization (f) Instance noise



(g) Gradient penalty (h) Gradient penalty (CR)

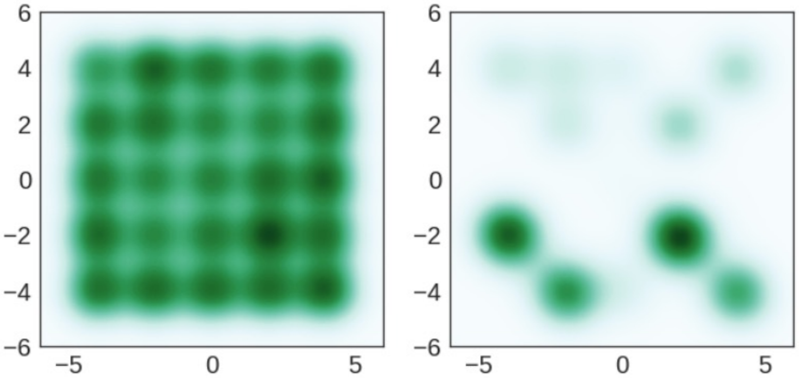
Figure 3. Convergence properties of different GAN training algorithms using alternating gradient descent with recommended number of discriminator updates per generator update ($n_d = 1$ if not noted otherwise). The shaded area in Figure 3c visualizes the set of forbidden values for the discriminator parameter ψ. The starting iterate is marked in red.

Common problems with GANs: Mode collapse hinders diversity of samples

From: https://developers.google.com/machine-learning/gan/problems

- Wasserstein GANs
- Unrolled GANs
  - Trained on multiple discriminators simultaneously

Metz, L., Poole, B., Pfau, D., & Sohl-Dickstein, J. (2016). Unrolled generative adversarial networks. *arXiv preprint arXiv:1611.02163*.



(f) True Data (g) GAN

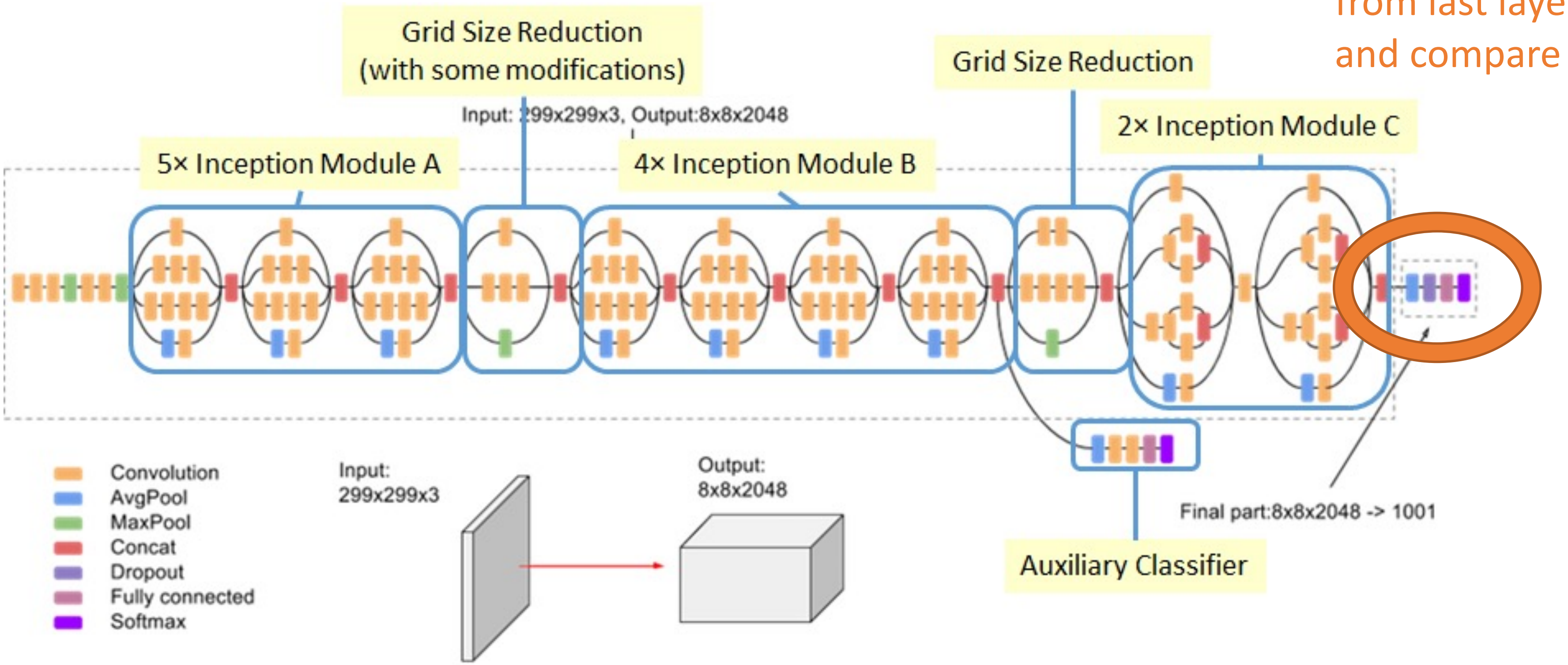
http://papers.nips.cc/paper/6923-veegan-reducing-mode-collapse-in-gans-using-implicit-variational-learning.pdf

https://software.intel.com/en-us/blogs/2017/08/21/mode-collapse-in-gans

Evaluation of GANs is quite challenging

- In explicit density models, we could use test log likelihood to evaluate
- Without a density model, how do we evaluate?
- Visually inspect image samples
  - Qualitative and biased
  - Hard to compare between methods

Common GAN metrics compare latent representations of InceptionV3 network



Extract features from last layers and compare

https://medium.com/@sh.tsang/review-inception-v3-1st-runner-up-image-classification-in-ilsvrc-2015-17915421f77c

Szegedy, C., Vanhoucke, V., Ioffe, S., Shlens, J., & Wojna, Z. (2016). Rethinking the inception architecture for computer vision. In *Proceedings of the IEEE conference on computer vision and pattern recognition (CVPR)* (pp. 2818-2826).

Inception score (IS) considers both clarity of images and diversity of images

- Extract Inception-V3 distribution of predicted labels, $p_{inceptionV3}(y|x_i), \forall x_i$
- Images should have "meaningful objects", i.e., $p(y|x_i)$ has **low entropy**
- The average over all generated images should be diverse, i.e., $p(y) = \frac{1}{n}\sum_i p(y|x_i)$ should have **high entropy**
- Combining these two (higher is better):

$$IS = \exp\left(\mathbb{E}_{p_g}\left[KL\left(p(y|x), p(y)\right)\right]\right)$$

  - Consider if $p(y|x) = p(y)$, i.e., all images give the same distribution over images
  - Either, all images are indistinct (e.g., they don't look like images so predictions are random)
  - Or, all images are the same (e.g., all images are dog)

Salimans, T., Goodfellow, I., Zaremba, W., Cheung, V., Radford, A., & Chen, X. (2016). Improved techniques for training gans. In *Advances in Neural Information Processing Systems* (pp. 2234–2242).

Frechet inception distance (FID) compares latent features from generated and real images

- Problem: Inception score ignores real images
  - Generated images may look nothing like real images

- Extract latent representation at last pooling layer of Inception-V3 network ($d = 2048$)

- Compute empirical mean and covariance for real and generated from latent representation

$$\mu_{data}, \Sigma_{data} \text{ and } \mu_g, \Sigma_g$$

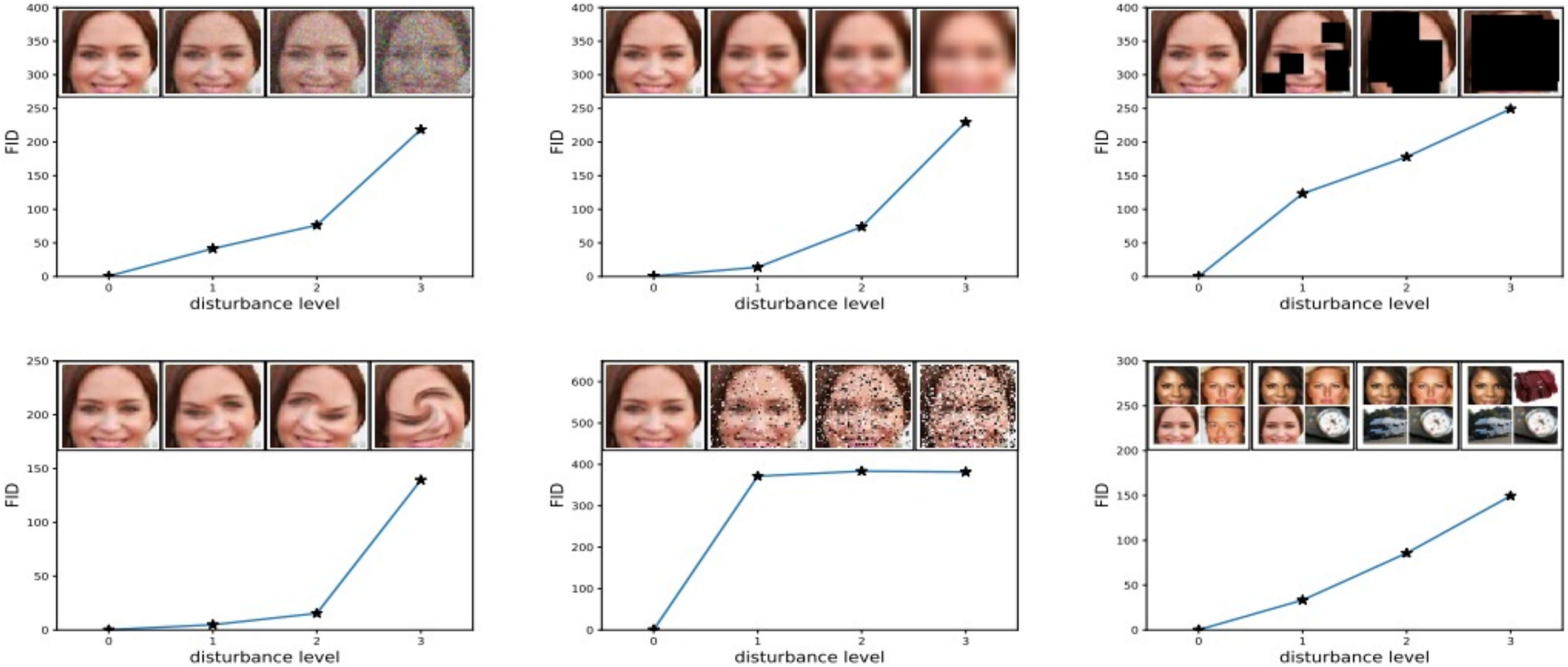
- FID score:

$$FID = \left\| \mu_{data} - \mu_g \right\|_2^2 + \mathrm{Tr}\left(\Sigma_{data} + \Sigma_g - 2\left(\Sigma_{\mathrm{data}} \Sigma_g \right)^{-\frac{1}{2}} \right)$$

  - Considers both mean **and covariance** of latent distribution

Heusel, M., Ramsauer, H., Unterthiner, T., Nessler, B., & Hochreiter, S. (2017). Gans trained by a two time-scale update rule converge to a local nash equilibrium. In *Advances in neural information processing systems* (pp. 6626-6637).

FID correlates with common distortions and corruptions



Randomly add ImageNet images unlike celebrity dataset

Figure from Heusel, M., Ramsauer, H., Unterthiner, T., Nessler, B., & Hochreiter, S. (2017). Gans trained by a two time-scale update rule converge to a local nash equilibrium. In *Advances in neural information processing systems* (pp. 6626-6637).

GAN Summary: Impressive innovation with strong empirical results but hard to train

- Good empirical results on generating sharp images
- Training is challenging in practice
- Evaluation is challenging and unsolved
- Much open research on this topic

Excellent online visualization and demo of GANs

- https://poloclub.github.io/ganlab/