Generative Adversarial Networks

Machine Learning and Data Mining, 2025

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Generative modelling

Problem setup

Training data – a set of objects, e.g.:

- Photos of animals / people faces / rooms / whatever
- Text
- Audio of speech / music / whatever
- Signals from a high energy physics experiment detector

Goal: build a model to sample similar data

Set of objects:

$$\{x_i \mid i = 1, \dots N\}$$

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I.e. $\{x_i\}$ are i.i.d. sampled from $p(x)$

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Goal: build a model to sample similar data

- Learn the **population distribution** to **sample more objects** from it
  - (may be done implicitly, i.e. when we can't evaluate the probability density, yet can sample from it)

Set of objects:

$\{x_i \mid i = 1, \dots N\}$

Population PDF:

$p(x)$

I.e. $\{x_i\}$ are i.i.d. sampled from $p(x)$

Learn $q(x) \sim p(x)$ to sample x' from $q(x)$

Possible applications

To name a few:

Creative professions, e.g.

- Generating textures for 3D modelling, audio samples for music etc.
- Style transfer

Data privacy

- Publishing samples without disclosing private information from the original data

Physics and engineering

- Building a deep learning model to reproduce the stochastic output of an accurate but slow simulator algorithm

This X does not exist

This Person Does Not Exist

The site that started it all, with the name that says it all. Created using a style-based generative adversarial network (StyleGAN), this website had the tech community buzzing with excitement and intrigue and inspired many more sites.

Created by Phillip Wang.

This Cat Does Not Exist

These purr-fect GAN-made cats will freshen your feeline-gs and make you wish you could reach through your screen and cuddle them. Once in a while the cats have visual deformities due to imperfections in the model – beware, they can cause nightmares.

Created by Ryan Hoover.

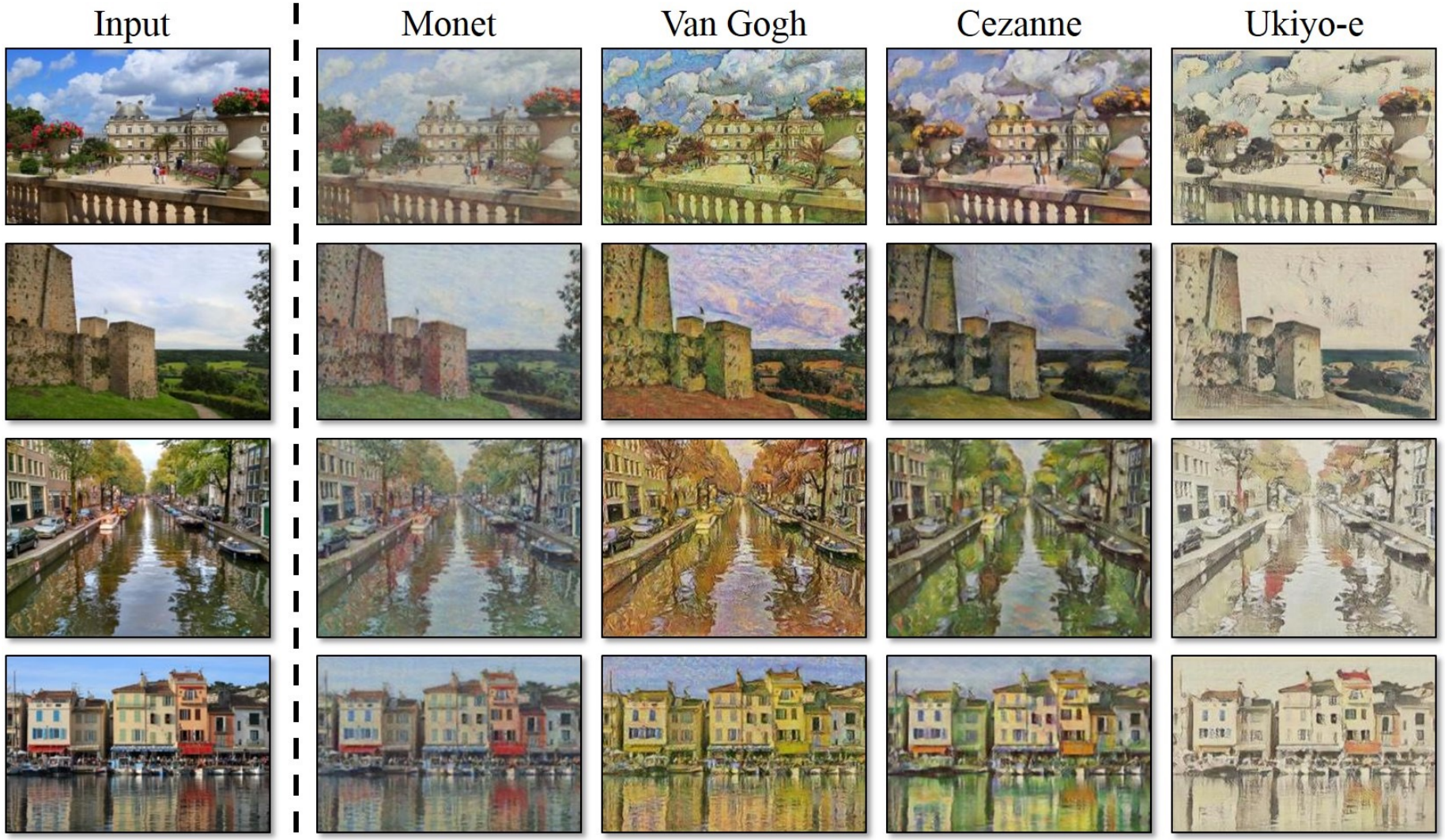
This Rental Does Not Exist

Why bother trying to look for the perfect home when you can create one instead? Just find a listing you like, buy some land, build it, and then enjoy the rest of your life.

Created by Christopher Schmidt.

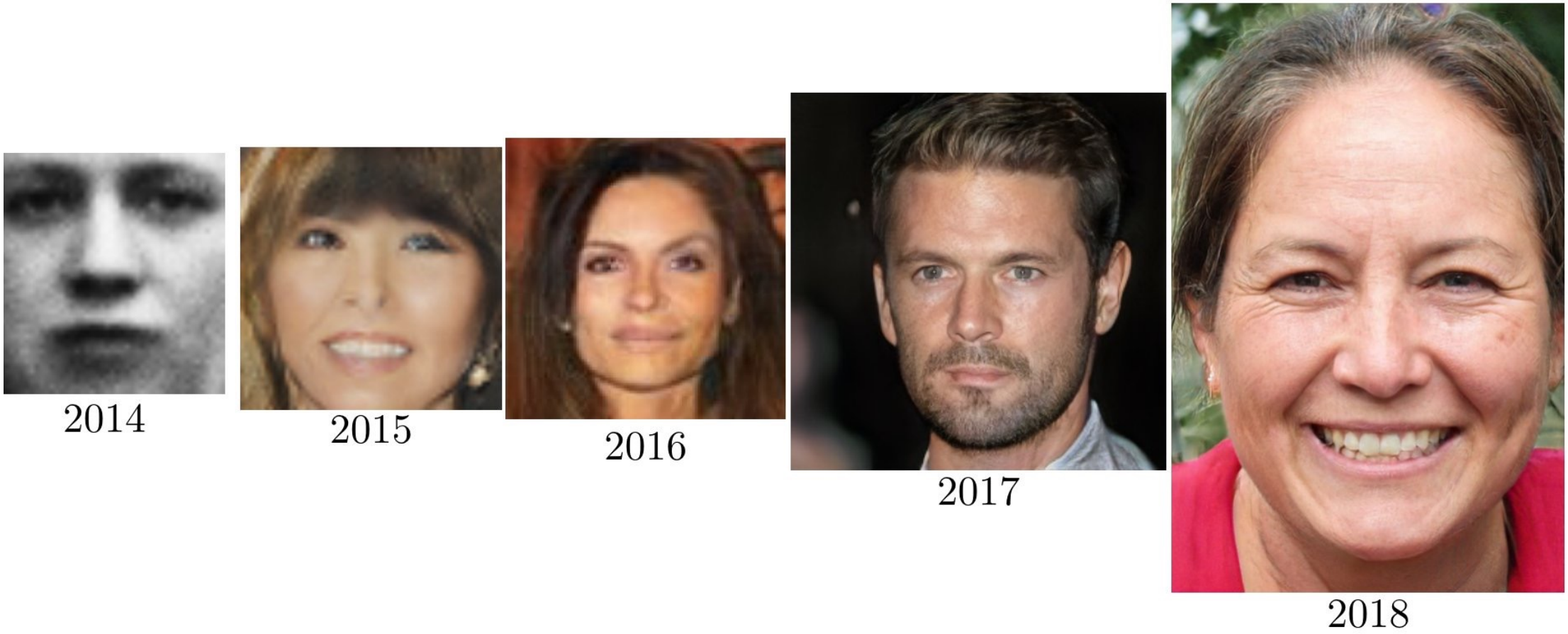
https://thisxdoesnotexist.com/

Style transfer



https://junyanz.github.io/CycleGAN/

Generative models progress



https://twitter.com/goodfellow_ian/status/1084973596236144640

Connection to supervised learning

Supervised learning ↔ Generative modelling

Supervised: learning relation f between features x and targets y:

$$y = f(x)$$

f is typically stochastic:

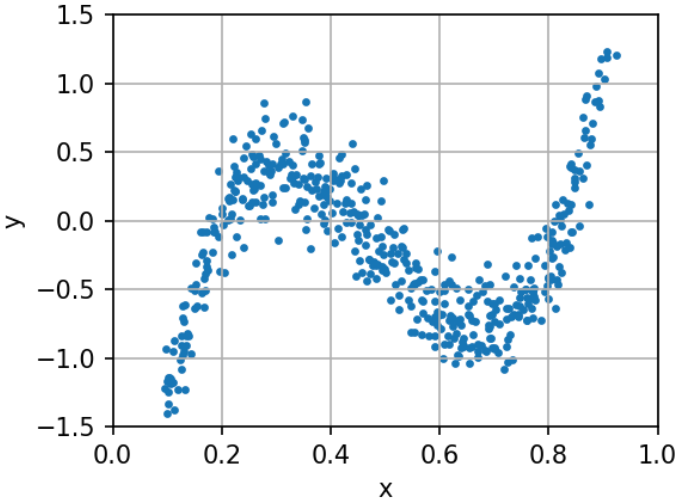
$$y|x \sim p_f(y|x)$$

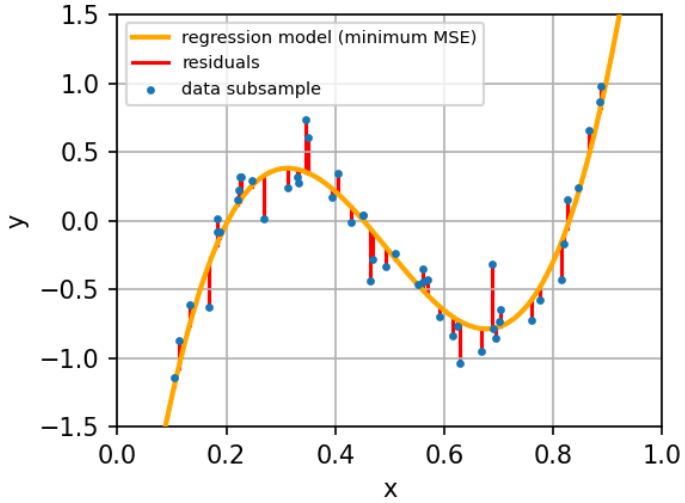
Typically, we model $p_f(y|x)$ in a very simple form like:

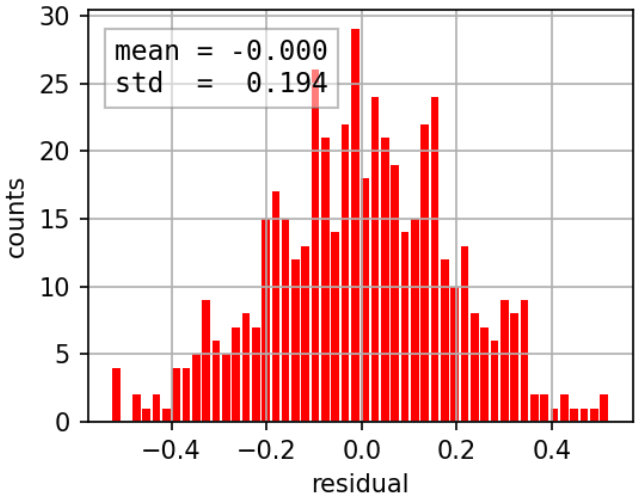
$$p_\theta(y|x) = \mathcal{N}(y|\mu = f_\theta(x), \sigma^2),$$

which leads to optimizing MSE

Generative modelling ≈ learning a generic distribution $p_f(y|x)$







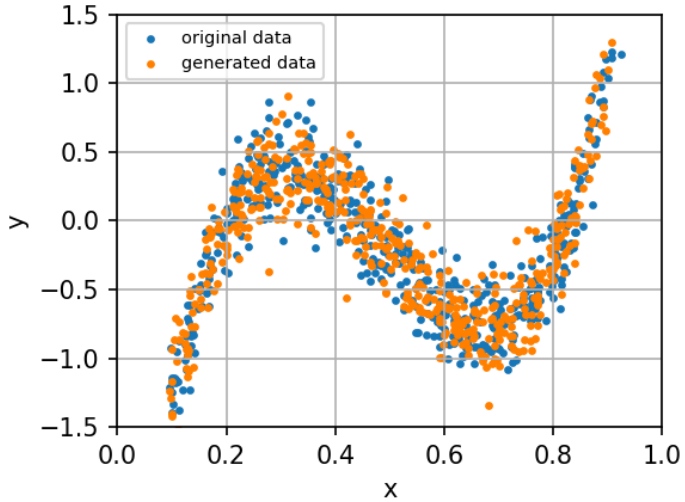
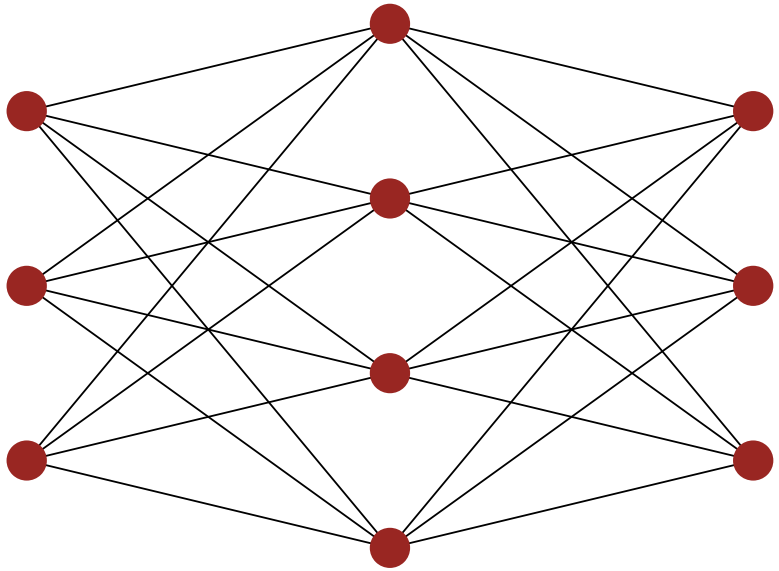


Image reference: https://en.pelican.study/
https://alemira.com/examples/

Generative Adversarial Networks

How can a neural network generate data?



Neural network

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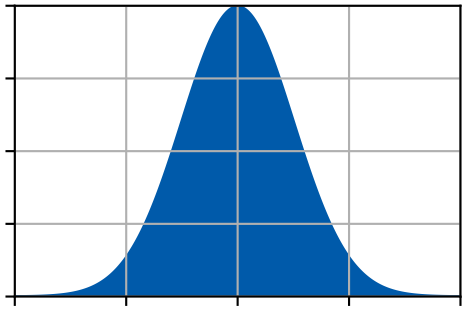
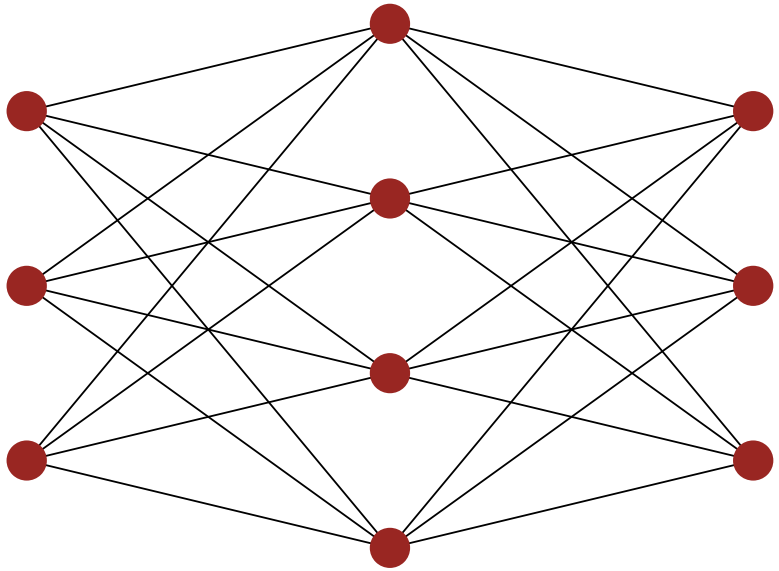


Random noize
e.g. multivariate normal

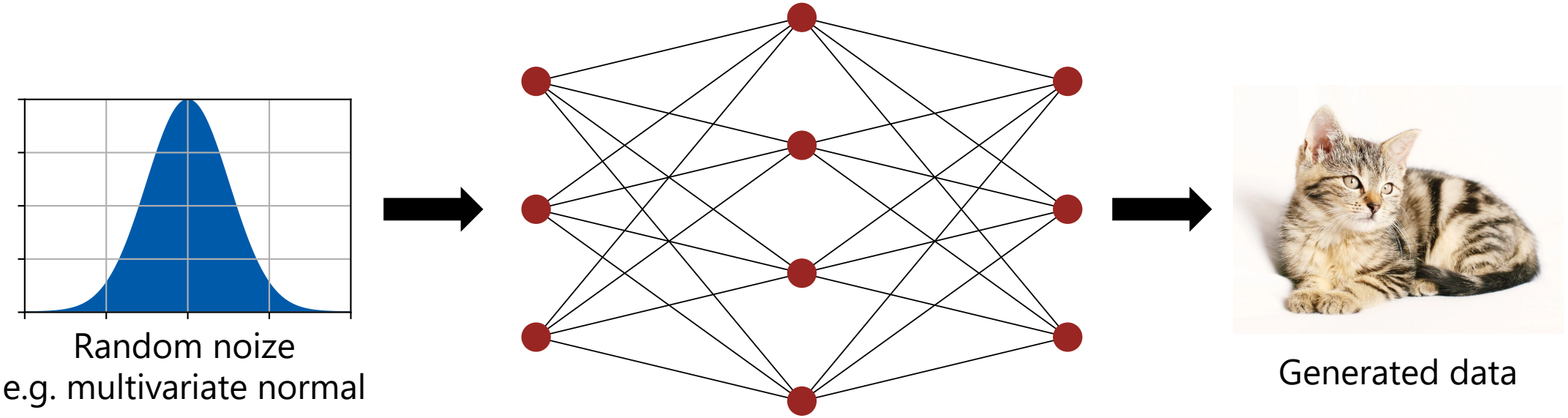


Neural network

Generated data

Cat image attribution: https://pixabay.com/users/chiemsee2016-1892688/

How can a neural network generate data?



This makes the generated object being a **differentiable function** of the network parameters

Cat image attribution: https://pixabay.com/users/chiemsee2016-1892688/

How to train such a generator?

Generated object is a differentiable function of the network parameters

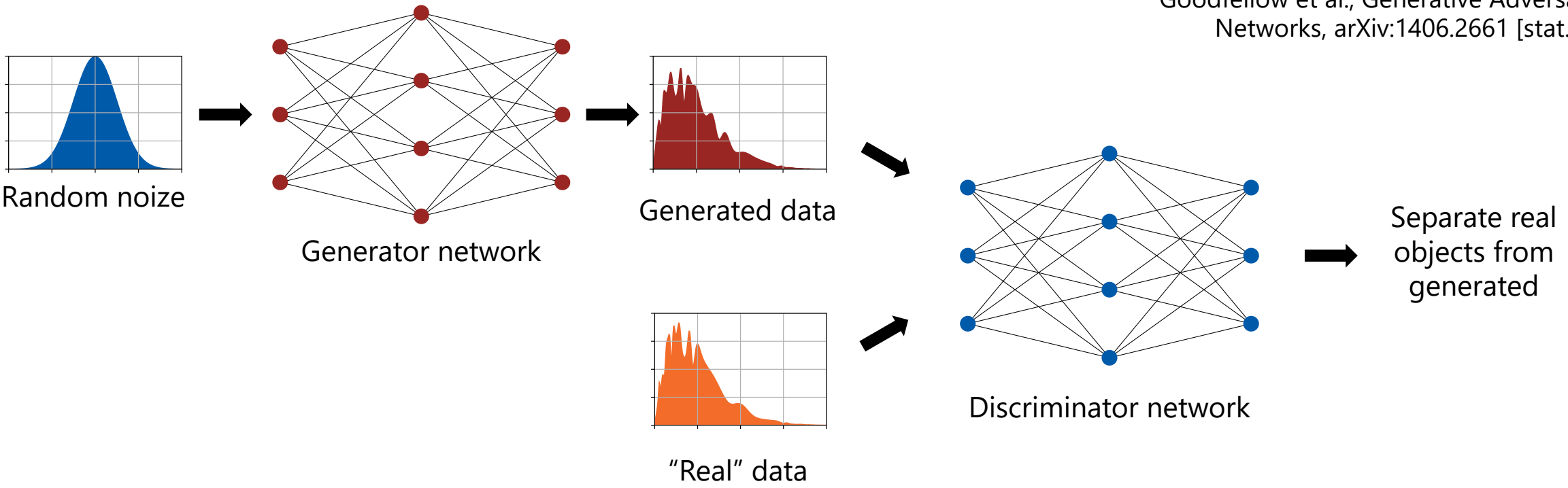
Need a differentiable **measure of similarity** between the sets of generated objects and real ones

- Can optimize with gradient descent

How to find such a measure?

Adversarial approach

Goodfellow et al., Generative Adversarial Networks, arXiv:1406.2661 [stat.ML]



Measure of similarity: how well can another neural network (discriminator) tell the generated objects apart from the real ones

Let’s put it in formulas

Noise samples:

$$z_i \sim p_z(z)$$

where p_z is some simple PDF we can sample from, e.g. $\mathcal{N}(0, \mathbb{I})$.

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returns the probability for x being a real sample rather than a generated one

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Measure of similarity between the generated and real samples:

$$L_G = \max_\phi \left[\mathbb{E}_{x \sim p(x)} \left[\log D_\phi(x) \right] + \mathbb{E}_{z \sim p_z(z)} \left[\log \left(1 - D_\phi \left(G_\theta(z) \right) \right) \right] \right] \rightarrow \min_\theta$$

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Probability the sample was generated

Log-likelihood for discriminator prediction

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where G_θ is the generator network with parameters θ.

May characterize this loss as **adversarial**: two networks compete against each other

Discriminator network (with parameters ϕ):

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Log-likelihood for discriminator prediction

Training the networks

Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used $k = 1$, the least expensive option, in our experiments.

for number of training iterations **do**

  for k steps **do**

  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
  - Update the discriminator by ascending its stochastic gradient:

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

  end for

  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Update the generator by descending its stochastic gradient:

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

end for

The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.

https://arxiv.org/abs/1406.2661

A view on the adversarial loss

Evolution from classical machine learning to deep learning:

- "Let's build a model that automatically finds the best features for us"

Evolution to adversarial loss:

- "Let's build a model that **learns the loss function** for us"

$$L_G = \max_{\phi} \left[\mathbb{E}_{x \sim p(x)} \left[\log D_\phi(x) \right] + \mathbb{E}_{z \sim p_z(z)} \left[\log \left(1 - D_\phi \left(G_\theta(z) \right) \right) \right] \right] \rightarrow \min_{\theta}$$

Generator loss is learned by optimising the discriminator

Problems with GANs

The optimal discriminator solution

If we re-write the loss using $p_{\text{gen},\theta}(x)$ – the distribution of $x' = G_\theta(z)$, and expand the expectations as integrals:

$$L_G = \max_{\phi} \int_x \left[p(x) \log\left(D_\phi(x)\right) + p_{\text{gen},\theta}(x) \log\left(1 - D_\phi(x)\right) \right] dx$$

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it's easy to show that $\max_\phi$ is obtained at $\phi^*(\theta)$ with:

$$D_{\phi^*(\theta)}(x) = \frac{p(x)}{p(x) + p_{\text{gen},\theta}(x)}$$

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So the objective becomes:

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$$= -\log 4 + JSD\left(p \,||\, p_{gen,\theta}\right)$$

Jensen–Shannon divergence

Vanishing gradients

In case p and $p_{\text{gen},\theta}$ have non-overlapping support:

$$L_G = \mathbb{E}_{x\sim p(x)}\left[\log\frac{p(x)}{p(x)+p_{\text{gen},\theta}(x)}\right] + \mathbb{E}_{x\sim p_{\text{gen},\theta}(x)}\left[\log\frac{p_{\text{gen},\theta}(x)}{p(x)+p_{\text{gen},\theta}(x)}\right]$$

$$= \mathbb{E}_{x\sim p(x)}\left[\log\frac{p(x)}{p(x)}\right] + \mathbb{E}_{x\sim p_{\text{gen},\theta}(x)}\left[\log\frac{p_{\text{gen},\theta}(x)}{p_{\text{gen},\theta}(x)}\right] = 0 = const$$

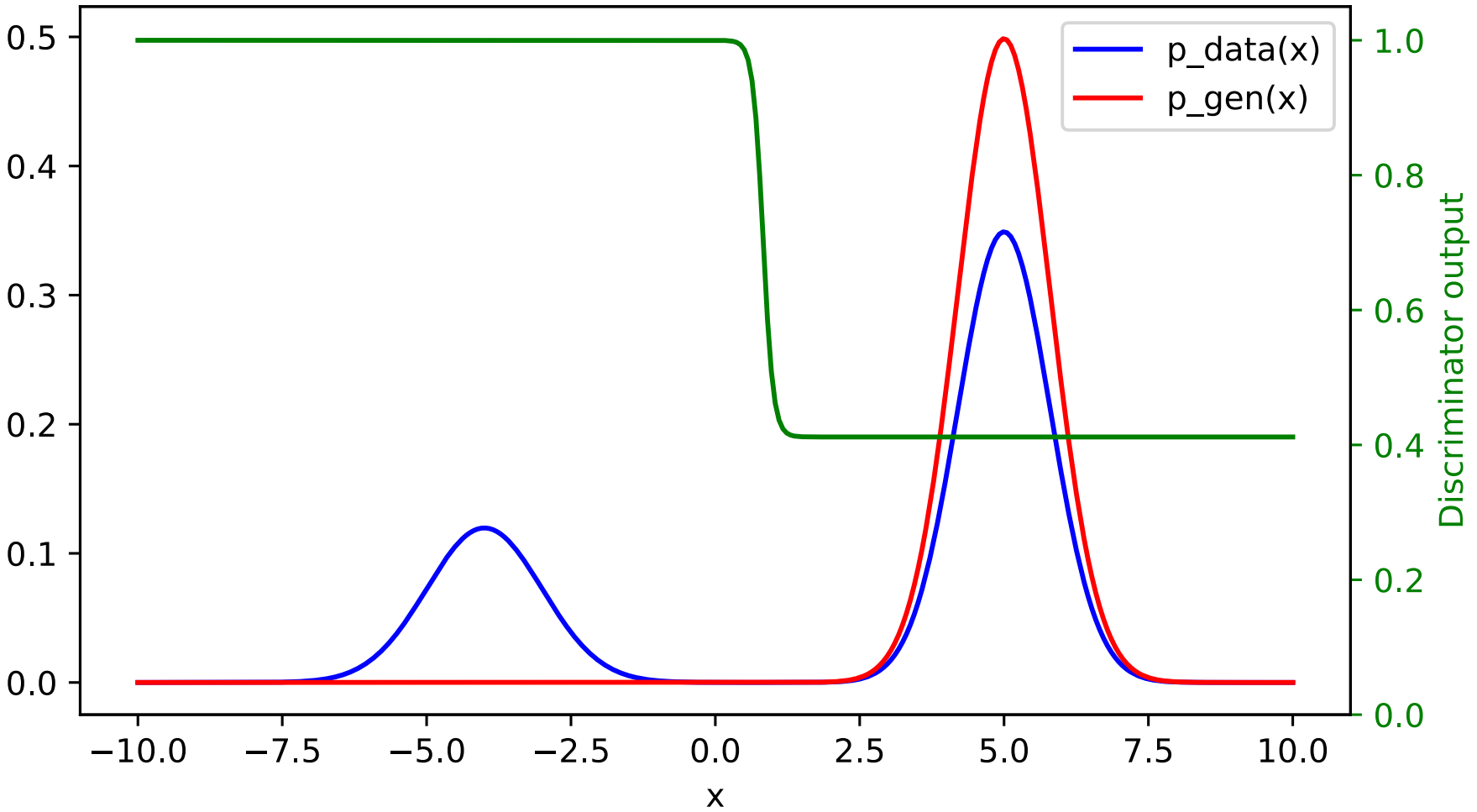
No meaningful gradient, can't learn

Mode collapse

Assume at some point the generator has learned one of the modes

No meaningful gradients to drive the solution towards covering the other modes

```
x = np.linspace(-10, 10, 300)
p_data = 0.7 * normal(x, 5, 0.8) + 0.3 * normal(x, -4, 1)
p_gen  = 1.0 * normal(x, 5, 0.8)
D = p_data / (p_data + p_gen)
```



Wasserstein GAN

Alternative distance measure

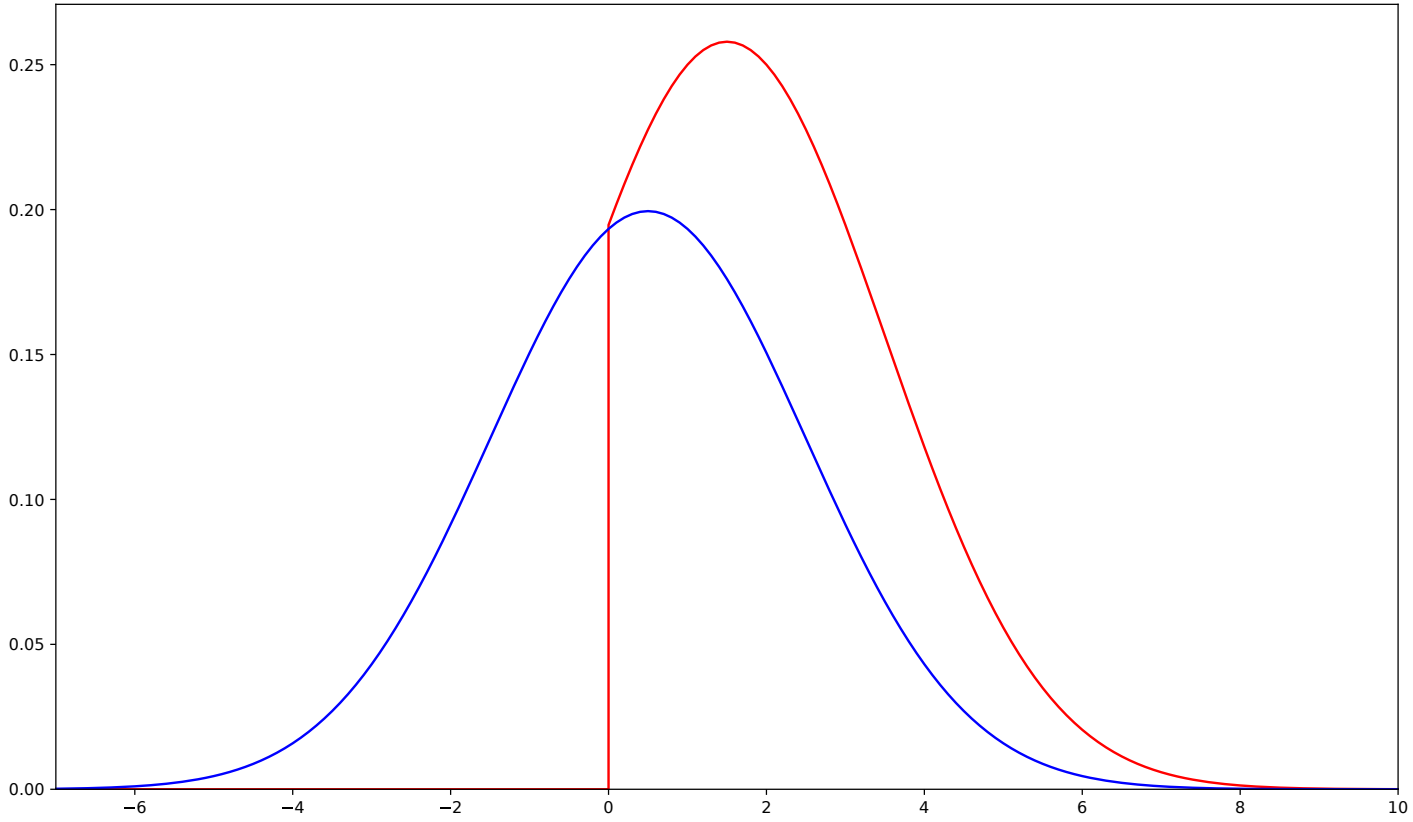
The problems with GANs are mainly due to Jensen–Shannon divergence providing problematic gradients

What if we try to find some other measure of distance between real and generated distributions that doesn't have these problems?

Wasserstein distance

Also called “Earth mover’s distance” (EMD)

Distributions $P(x)$ and $Q(x)$ are viewed as describing the **amounts of “dirt” at point x**

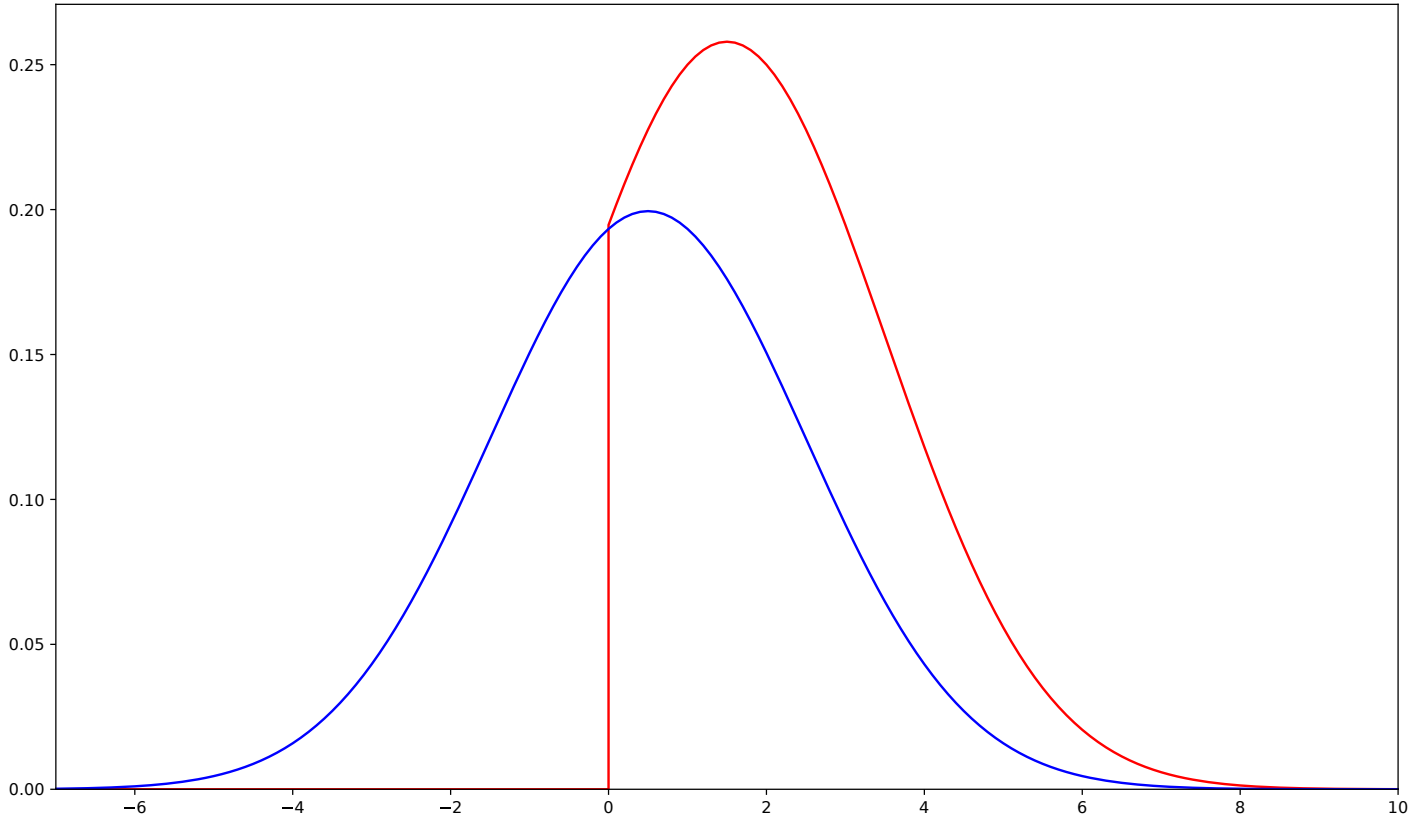


Wasserstein distance

Also called “Earth mover’s distance” (EMD)

Distributions $P(x)$ and $Q(x)$ are viewed as describing the **amounts of “dirt” at point x**

We want to convert one distribution into the other by **moving around** some amounts of dirt



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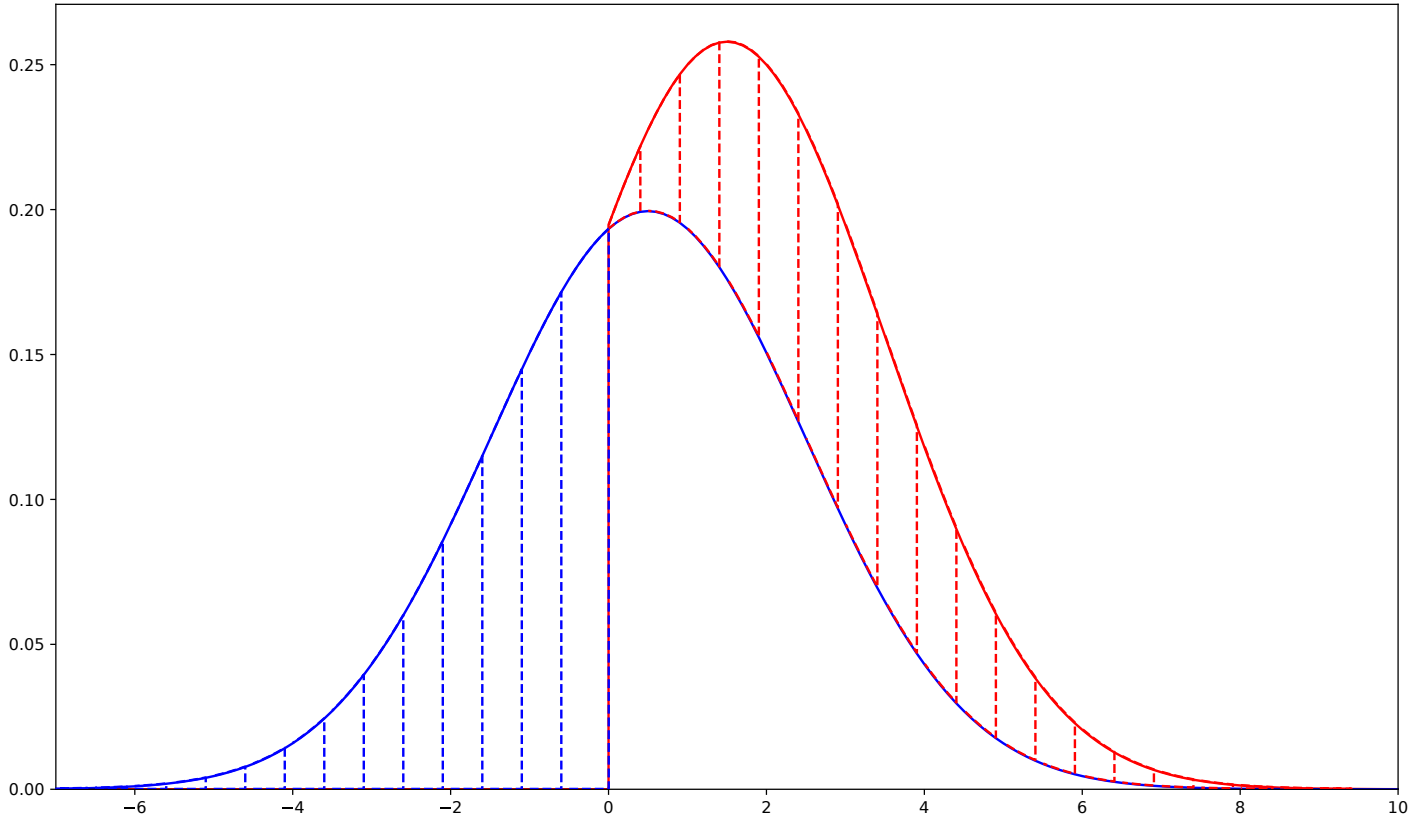

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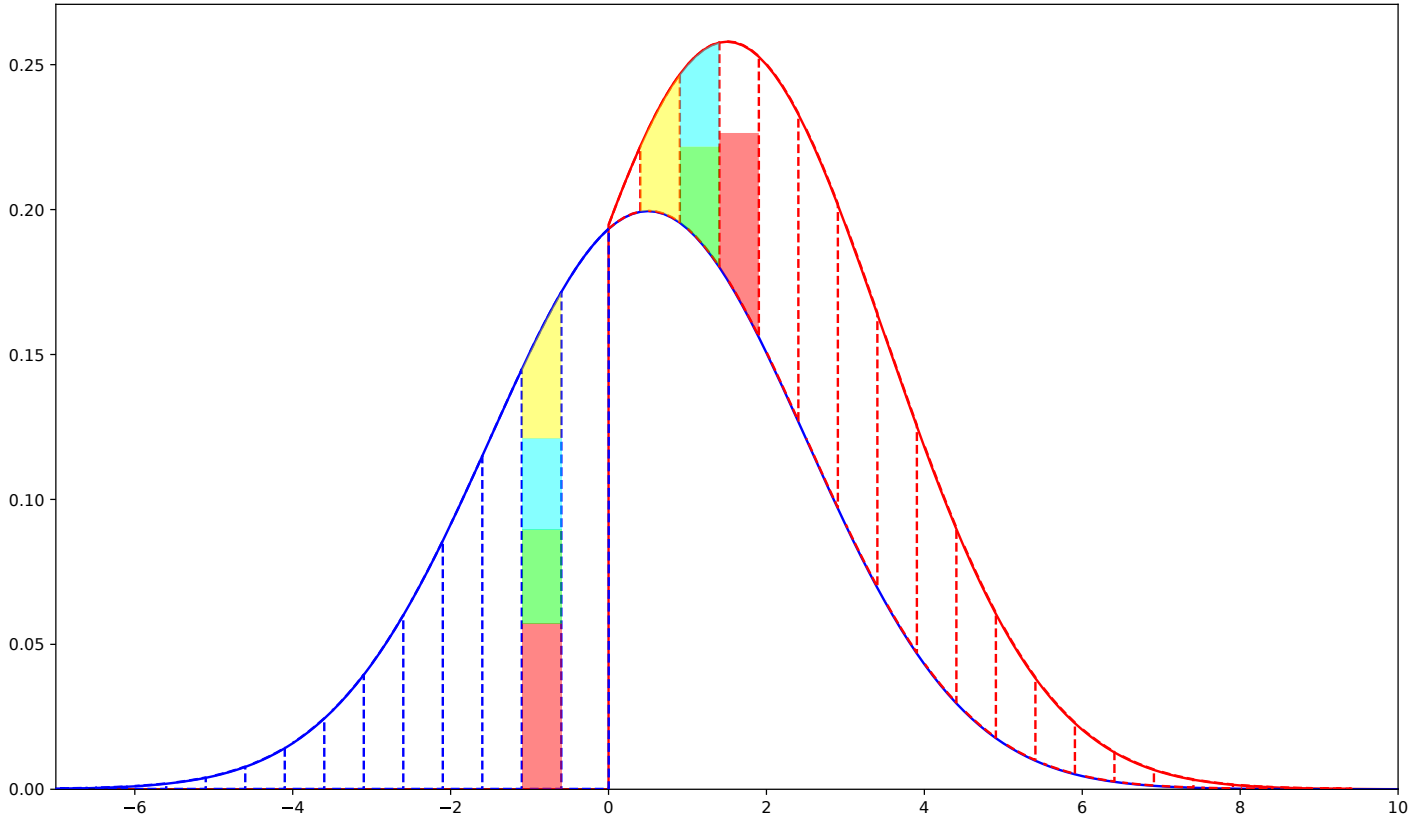

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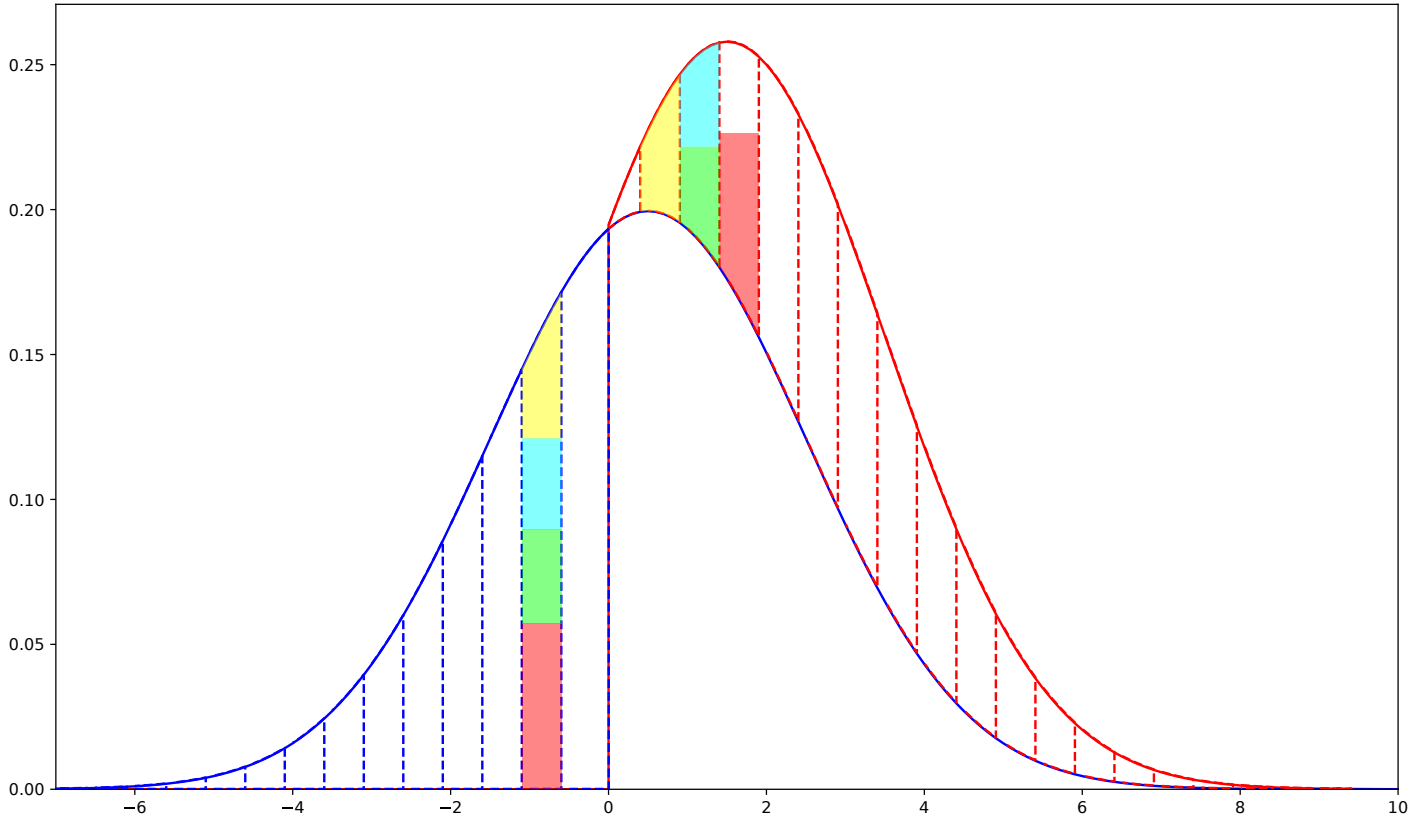

The cost of moving an amount m from x_1 to x_2 is $m \times \|x_2 - x_1\|$

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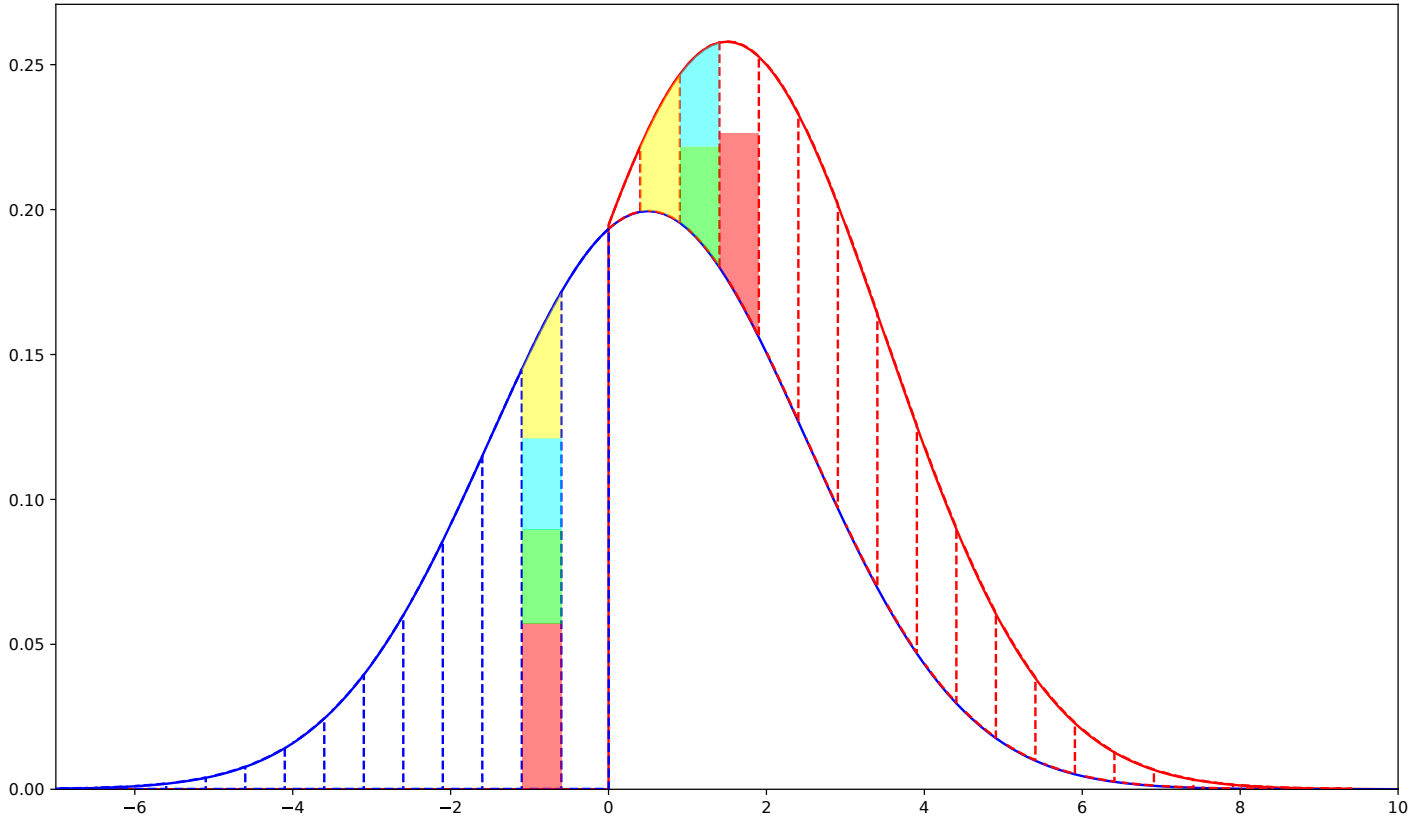

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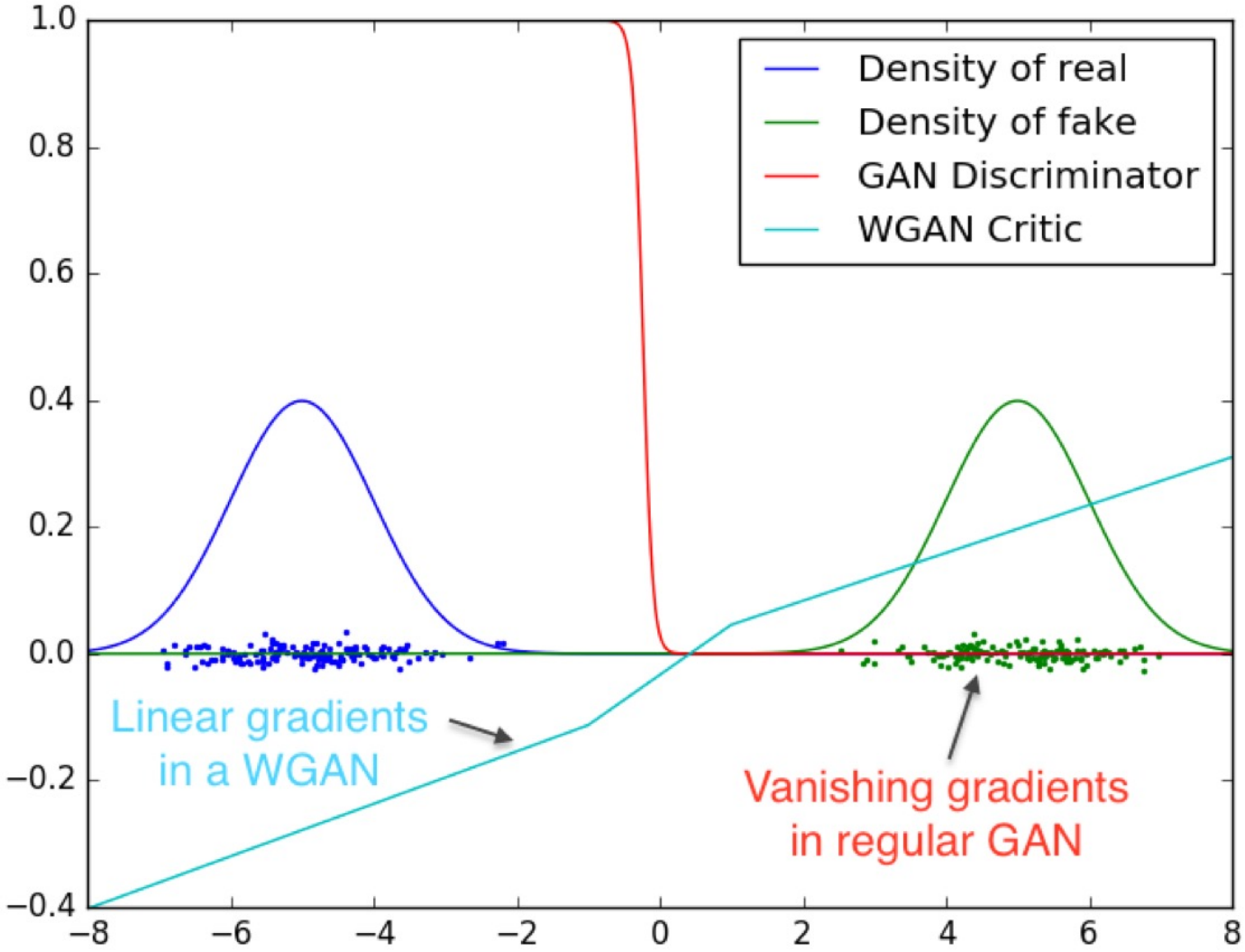
$\mathrm{EMD}(P, Q)$ = **minimum total cost** of converting P into Q

Why is it better?



https://arxiv.org/abs/1701.07875

Formal definition

Say, we have a moving plan $\gamma(x_1, x_2) \geq 0$:

$\gamma(x_1, x_2)dx_1dx_2$ – how much dirt we're moving from $[x_1, x_1 + dx_1]$ to $[x_2, x_2 + dx_2]$

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Then, the cost of moving from $[x_1, x_1 + dx_1]$ to $[x_2, x_2 + dx_2]$ is:

$$\|x_2 - x_1\| \cdot \gamma(x_1, x_2)dx_1dx_2$$

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and the total cost is:

$$C = \int_{x_1, x_2} \|x_2 - x_1\| \cdot \gamma(x_1, x_2)dx_1dx_2$$

Formal definition

Say, we have a moving plan $\gamma(x_1, x_2) \geq 0$:

$\gamma(x_1, x_2)dx_1dx_2$ – how much dirt we're moving from $[x_1, x_1 + dx_1]$ to $[x_2, x_2 + dx_2]$

Then, the cost of moving from $[x_1, x_1 + dx_1]$ to $[x_2, x_2 + dx_2]$ is:

$$\|x_2 - x_1\| \cdot \gamma(x_1, x_2)dx_1dx_2$$

and the total cost is:

$$C = \int_{x_1, x_2} \|x_2 - x_1\| \cdot \gamma(x_1, x_2)dx_1dx_2 = \mathbb{E}_{x_1, x_2 \sim \gamma(x_1, x_2)}\|x_2 - x_1\|$$

Interpreting γ as a PDF

Formal definition

Say, we have a moving plan $\gamma(x_1, x_2) \geq 0$:

$\gamma(x_1, x_2)dx_1dx_2$ – how much dirt we're moving from $[x_1, x_1 + dx_1]$ to $[x_2, x_2 + dx_2]$

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$$C = \int_{x_1, x_2} \|x_2 - x_1\| \cdot \gamma(x_1, x_2)dx_1dx_2 = \mathbb{E}_{x_1, x_2 \sim \gamma(x_1, x_2)}\|x_2 - x_1\|$$

Interpreting γ as a PDF

Since we want to convert P to Q, the plan has to satisfy:

$$\int_{x_1} \gamma(x_1, x_2)dx_1 = Q(x_2), \qquad \int_{x_2} \gamma(x_1, x_2)dx_2 = P(x_1)$$

Formal definition

Let π be the set of all plans that convert P to Q, i.e.:

$$\pi = \left\{ \gamma: \quad \gamma \geq 0, \qquad \int_{x_1} \gamma(x_1, x_2) dx_1 = Q(x_2), \qquad \int_{x_2} \gamma(x_1, x_2) dx_2 = P(x_1) \right\}$$

Then, the Wasserstein distance between P and Q is:

$$\mathrm{EMD}(P, Q) = \inf_{\gamma \in \pi} \mathbb{E}_{x_1, x_2 \sim \gamma} \|x_2 - x_1\|$$

Formal definition

Let π be the set of all plans that convert P to Q, i.e.:

$$\pi = \left\{ \gamma: \quad \gamma \geq 0, \qquad \int_{x_1} \gamma(x_1, x_2) dx_1 = Q(x_2), \qquad \int_{x_2} \gamma(x_1, x_2) dx_2 = P(x_1) \right\}$$

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Optimization over all transport plans – not too friendly

Formal definition

Let π be the set of all plans that convert P to Q, i.e.:

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Then, the Wasserstein distance between P and Q is:

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Optimization over all transport plans – not too friendly

Dual form (Kantorovich-Rubinstein duality):

$$\mathrm{EMD}(P, Q) = \sup_{\|f\|_L \leq 1} \left[\mathbb{E}_{x \sim P} f(x) - \mathbb{E}_{x \sim Q} f(x) \right]$$

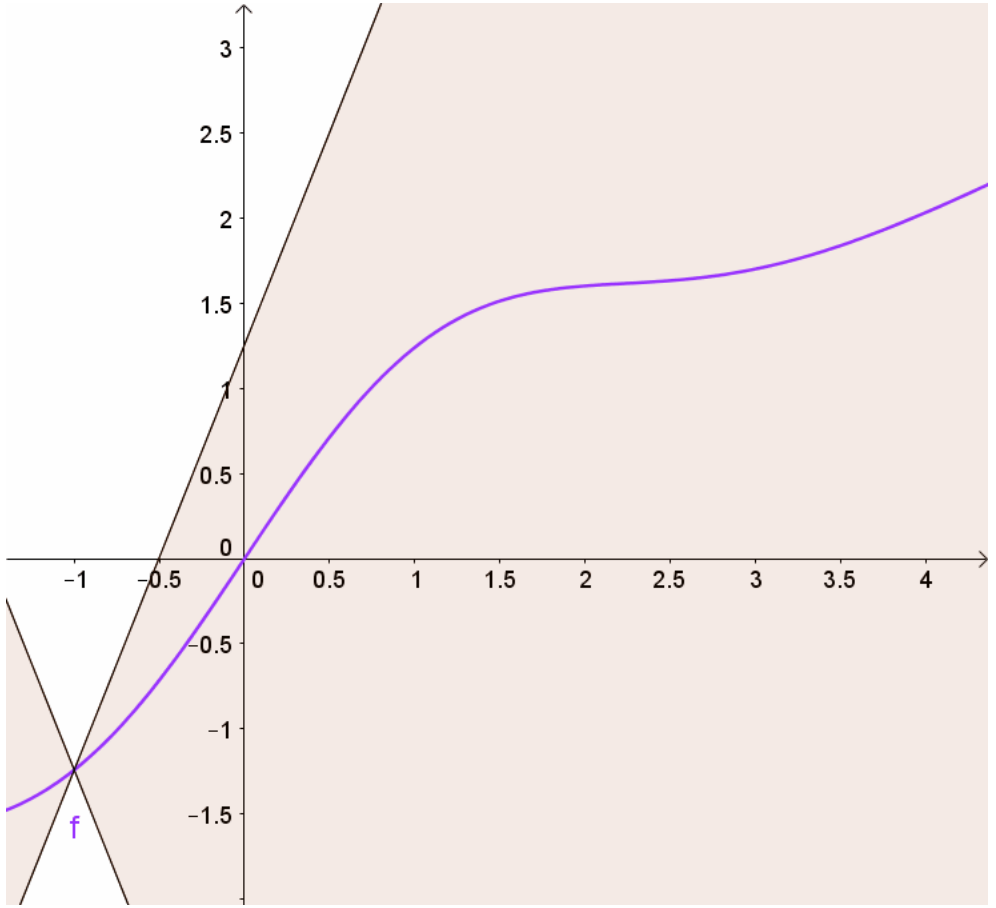
Optimization over Lipschitz-1 continuous functions acting in $\mathcal{X} \to \mathbb{R}$

Lipschitz continuity

f is Lipschitz-k continuous if

there exists a constant $k \geq 0$, such that for all x_1 and x_2:

$$|f(x_1) - f(x_2)| \leq \mathrm{k} \cdot \|x_1 - x_2\|$$



img from https://en.wikipedia.org/wiki/Lipschitz_continuity

[intuition behind the dual form]

disclaimer: not a strict mathematical derivation

$$\mathrm{EMD}(P,Q) = \inf_{\gamma \in \pi} \mathbb{E}_{x_1,x_2 \sim \gamma} ||x_1 - x_2||$$

Let's add the following term to this expression:

$$+ \inf_{\gamma} \sup_{f} \mathbb{E}_{x_1,x_2 \sim \gamma} \left[\mathbb{E}_{s \sim P} f(s) - \mathbb{E}_{t \sim Q} f(t) - (f(x_1) - f(x_2)) \right]$$

$f(x)$ — real-valued function

These cancel out when $\gamma \in \pi$
otherwise supremum over $f(x)$ goes to $+\infty$

Therefore, we can remove the $\gamma \in \pi$ condition from the whole expression:

$$= \inf_{\gamma} \sup_{f} \mathbb{E}_{x_1,x_2 \sim \gamma} \left[||x_1 - x_2|| + \mathbb{E}_{s \sim P} f(s) - \mathbb{E}_{t \sim Q} f(t) - (f(x_1) - f(x_2)) \right]$$

Infimum and supremum operations can be swapped under certain conditions
(satisfied here — see https://vincentherrmann.github.io/blog/wasserstein/ for more detailed info)

[intuition behind the dual form]

disclaimer: not a strict mathematical derivation

$$= \sup_f \inf_\gamma \left[\mathbb{E}_{s\sim P} f(s) - \mathbb{E}_{t\sim Q} f(t) + \mathbb{E}_{x_1,x_2\sim\gamma} \left[||x_1 - x_2|| - (f(x_1) - f(x_2)) \right] \right]$$

Consider the following case: $|f(a) - f(b)| \leq ||a - b||, \quad \forall a,\ b$
We'll denote it as: $||f||_L \leq 1$

For such case this term is 0

Otherwise the whole expression is -∞

Therefore we can finally rewrite the whole thing as:

$$\mathrm{EMD}(P, Q) = \sup_{||f||_L \leq 1} \left[\mathbb{E}_{x\sim P} f(x) - \mathbb{E}_{x\sim Q} f(x) \right]$$

WGAN

$$\mathrm{EMD}(P,Q) = \sup_{\|f\|_L \leq 1} \left[\mathbb{E}_{x\sim P} f(x) - \mathbb{E}_{x\sim Q} f(x)\right]$$

The function can be expressed as a neural net – discriminator ('critic' in the original paper)

https://arxiv.org/abs/1701.07875

WGAN

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The expectations can be estimated as sample mean

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Lipschitz-1 continuity can be replaced with Lipschitz-k continuity

- In such case we'll estimate $k \times \mathrm{EMD}(P,Q)$

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We wouldn't know what k is, but it doesn't matter: all we want is to **minimize** the EMD!

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WGAN

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The function can be expressed as a neural net – discriminator ('critic' in the original paper)

Lipschitz-1 continuity can be replaced with Lipschitz-k continuity

- In such case we'll estimate $k\times$ $\mathrm{EMD}(P,Q)$
- Can be achieved by clipping the weights of the critic: $w \to \mathrm{clip}(w,-c,c)$ with some constant c

The expectations can be estimated as sample mean

We wouldn't know what k is, but it doesn't matter: all we want is to **minimize** the EMD!

https://arxiv.org/abs/1701.07875

WGAN

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

WGAN-GP

Weight clipping makes the critic less expressive and the training harder to converge

Optimal f should satisfy $\|\nabla f\| = 1$ almost everywhere under P and Q

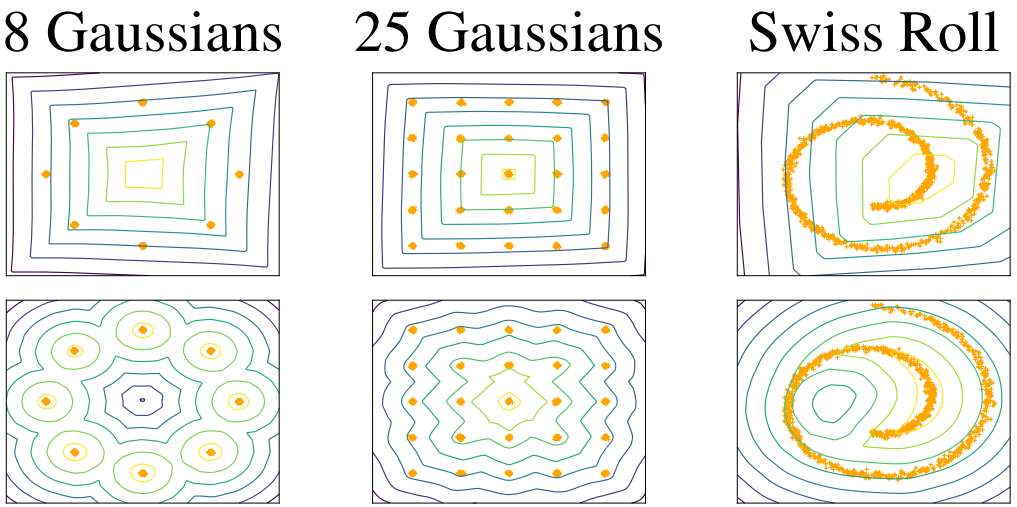
Also: $\|f\|_L \leq 1 \iff \|\nabla f\| \leq 1$

Can replace weight clipping with a gradient penalty term:

$$\text{GP} = \lambda \mathbb{E}_{\tilde{x} \sim \mathbb{P}_{\tilde{x}}}[(\|\nabla_{\tilde{x}} f(\tilde{x})\| - 1)^2]$$

or alternatively ('one-sided' penalty):

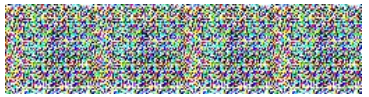
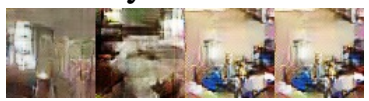
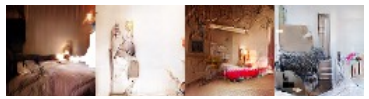
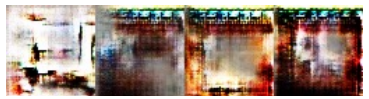
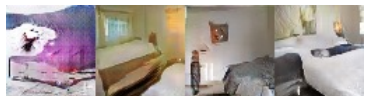
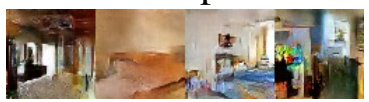
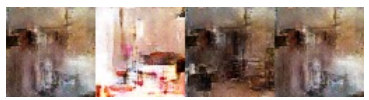
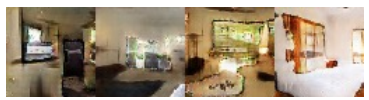
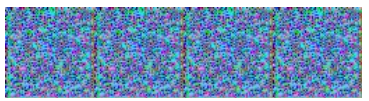
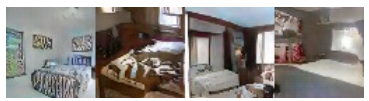
$$\text{GP} = \lambda \mathbb{E}_{\tilde{x} \sim \mathbb{P}_{\tilde{x}}}[\max(0, \|\nabla_{\tilde{x}} f(\tilde{x})\| - 1)^2]$$



$$\mathbb{P}_{\tilde{x}}: \begin{bmatrix} \tilde{x} = \alpha x_1 + (1-\alpha) x_2 \\ \alpha \sim \text{Uniform}(0,1) \\ x_1 \sim P \\ x_2 \sim Q \end{bmatrix}$$

https://arxiv.org/abs/1704.00028

WGAN-GP

DCGAN	LSGAN	WGAN (clipping)	WGAN-GP (ours)
Baseline (G: DCGAN, D: DCGAN)				
G: No BN and a constant number of filters, D: DCGAN				
G: 4-layer 512-dim ReLU MLP, D: DCGAN				
No normalization in either G or D				
Gated multiplicative nonlinearities everywhere in G and D				
tanh nonlinearities everywhere in G and D				
101-layer ResNet G and D				

This technique allowed for very deep networks to be used for GANs

https://arxiv.org/abs/1704.00028

Some notable architectures

Conditional distributions

It's often necessary to learn not just $P(x)$, but $P(x|a)$

- E.g. generate the face of a person with a given hair color

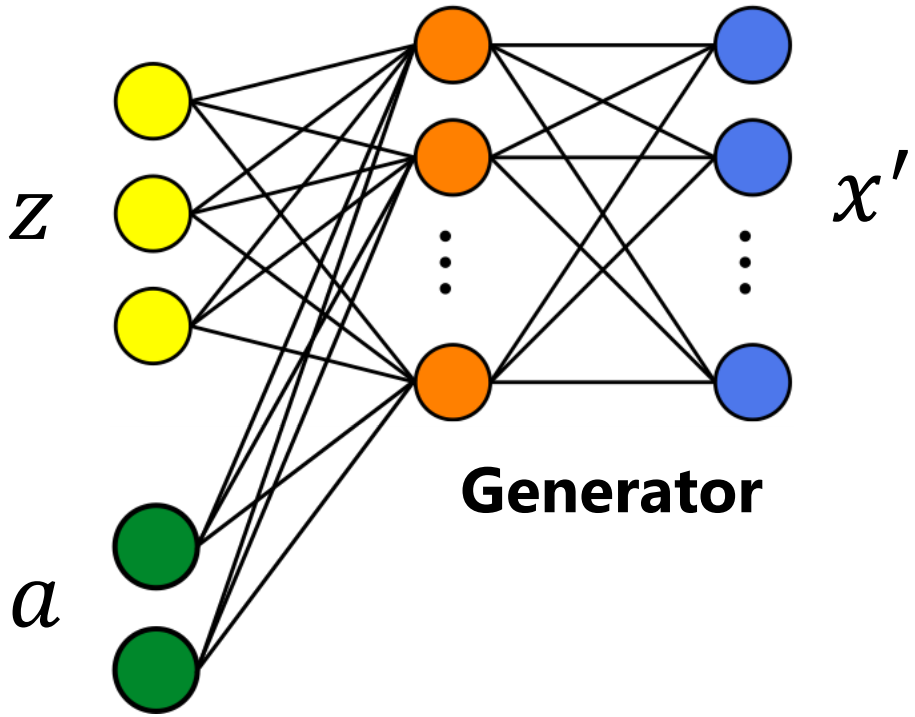
This can be achieved by:

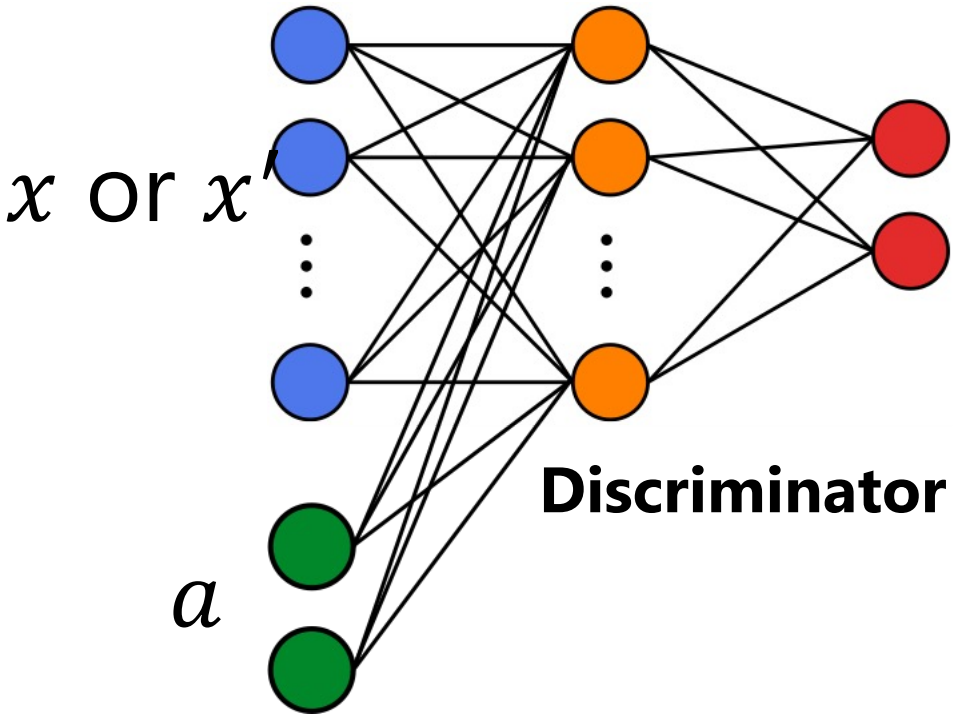
$$x'_j = G_\theta(z_j) \quad \rightarrow \quad x'_j = G_\theta(z_j, a_j)$$
$$D_\phi = D_\phi(x_i) \quad \rightarrow \quad D_\phi = D_\phi(x_i, a_i)$$

I.e. we need to provide this information to the generator and discriminator

Conditional distributions

Simple for fully-connected architectures





pix2pix

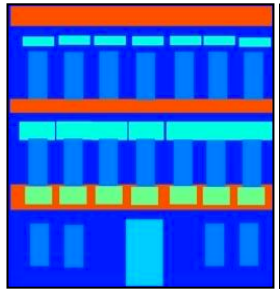
Labels to Street Scene


input output

Aerial to Map


input output

Labels to Facade

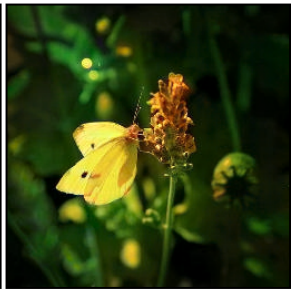



input output

Day to Night


input output

BW to Color

input output

Edges to Photo


input output

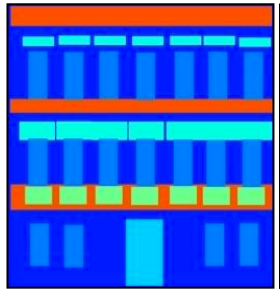
https://arxiv.org/abs/1611.07004

pix2pix

Labels to Street Scene


input output

Labels to Facade




input output

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Aerial to Map


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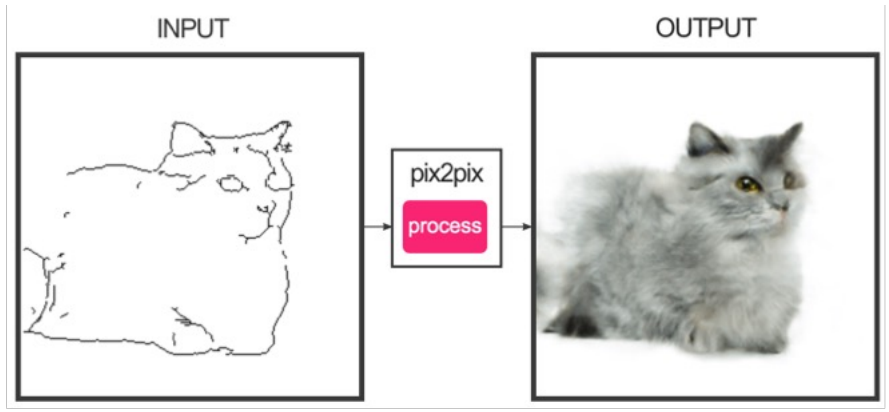


https://arxiv.org/abs/1611.07004

images generated at https://affinelayer.com/pixsrv/

pix2pix

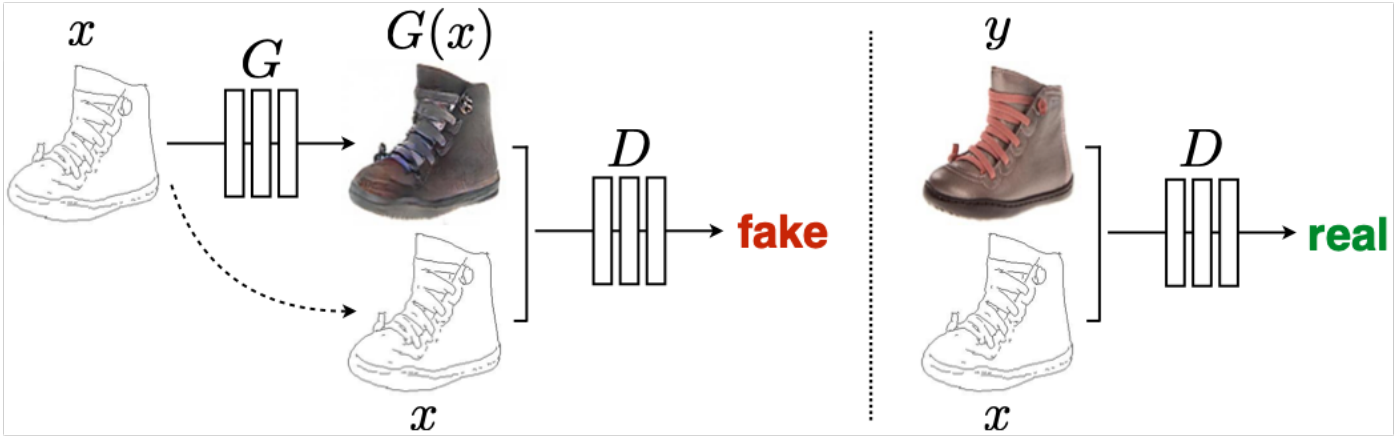
https://arxiv.org/abs/1611.07004

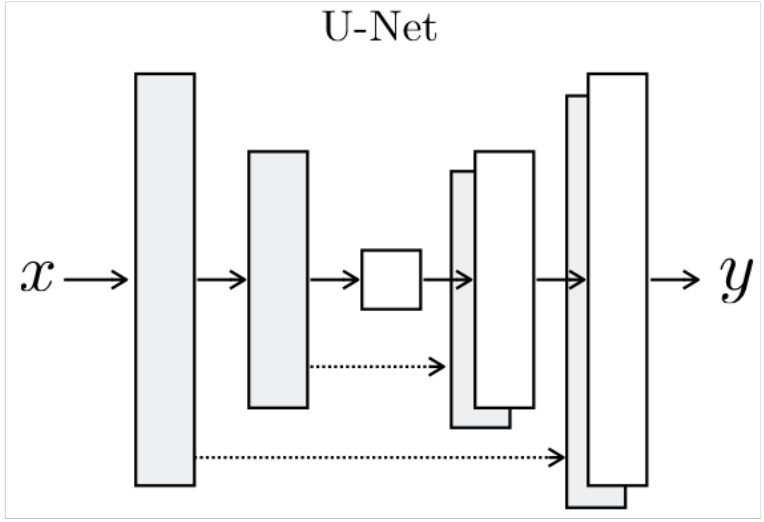
$$\mathcal{L}_{L1}(G) = \mathbb{E}_{x,y,z}[\|y - G(x,z)\|_1].$$

Our final objective is

$$G^* = \arg\min_G \max_D \mathcal{L}_{cGAN}(G,D) + \lambda \mathcal{L}_{L1}(G).$$

L1 loss term to capture low-frequency information





'U-Net' generator architecture

- Discriminator doesn't need to classify the entire image
- Instead it 'convolutionally' scans smaller patches of the image and averages the result

pix2pix

https://arxiv.org/abs/1611.07004

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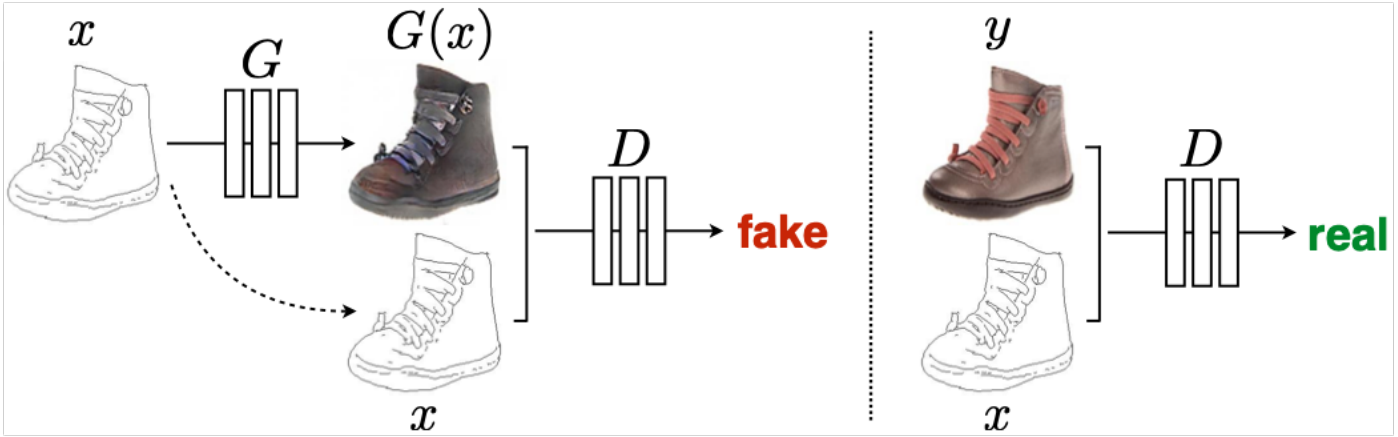
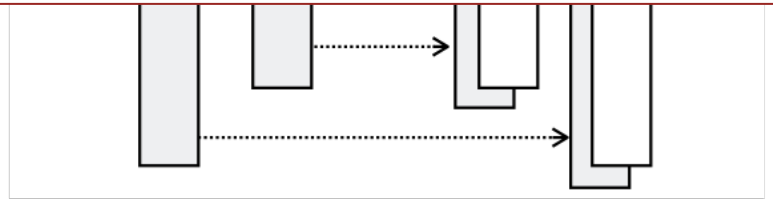


U-Net

No noise input to the generator:
«The generator simply **learned to ignore the noise** …
Instead we provide noise only in the form of **dropout, applied at both training and test time**»



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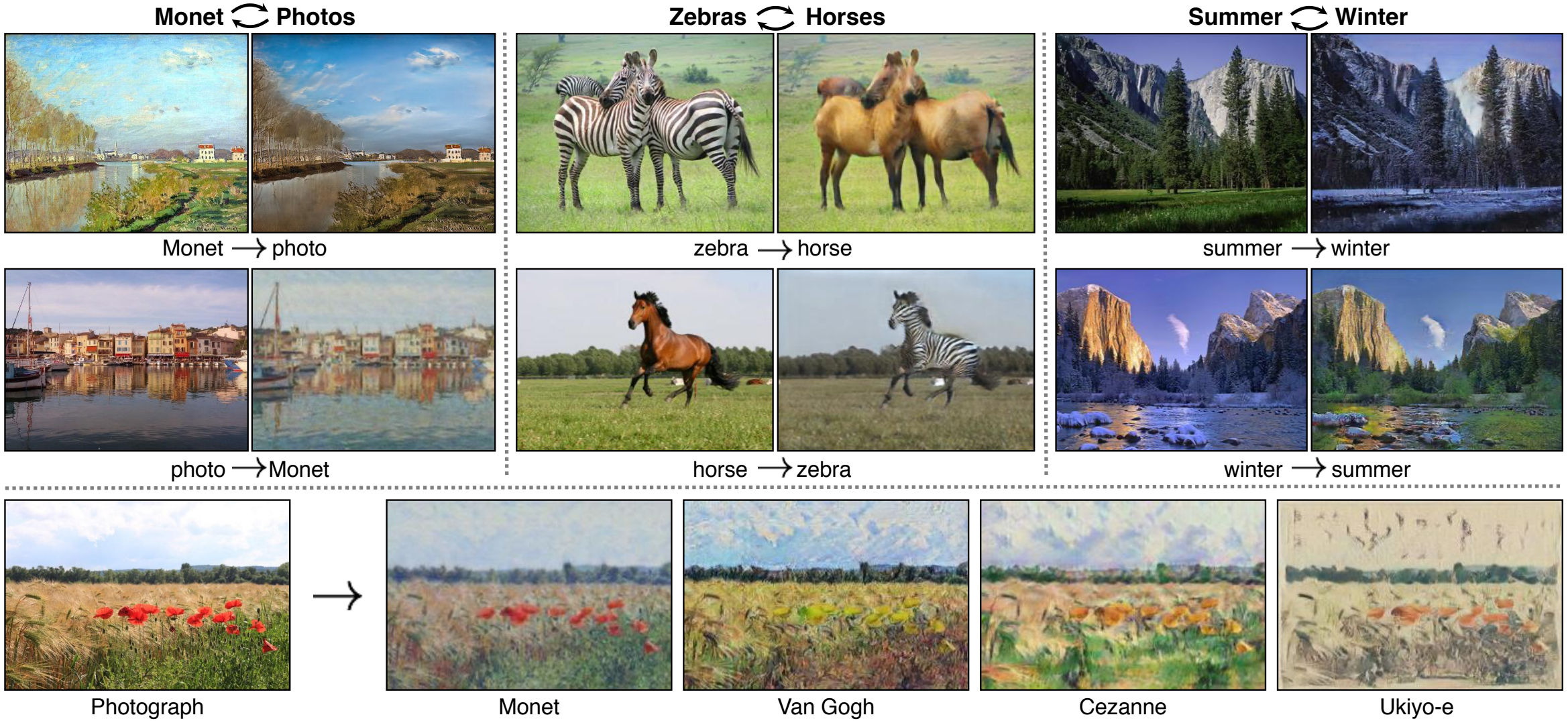
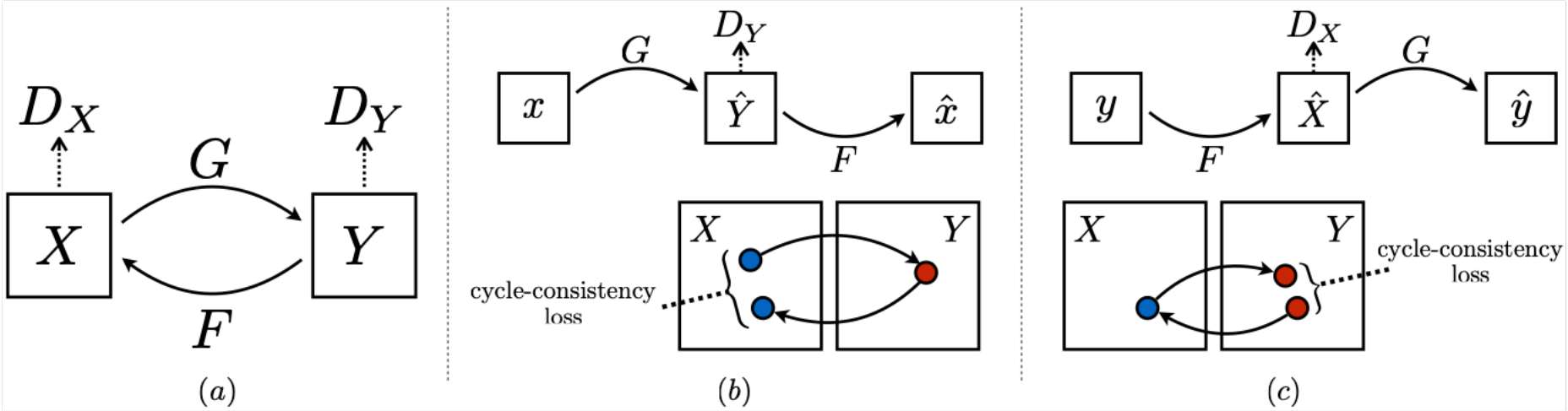
CycleGAN



https://arxiv.org/abs/1703.10593

CycleGAN

https://arxiv.org/abs/1703.10593



$$\mathcal{L}_{\text{GAN}}(G, D_Y, X, Y) = \mathbb{E}_{y \sim p_{\text{data}}(y)}[\log D_Y(y)] + \mathbb{E}_{x \sim p_{\text{data}}(x)}[\log(1 - D_Y(G(x))], \quad (1)$$

$$\mathcal{L}_{\text{cyc}}(G, F) = \mathbb{E}_{x \sim p_{\text{data}}(x)}[\|F(G(x)) - x\|_1] + \mathbb{E}_{y \sim p_{\text{data}}(y)}[\|G(F(y)) - y\|_1]. \quad (2)$$

$$\mathcal{L}(G, F, D_X, D_Y) = \mathcal{L}_{\text{GAN}}(G, D_Y, X, Y) + \mathcal{L}_{\text{GAN}}(F, D_X, Y, X) + \lambda \mathcal{L}_{\text{cyc}}(G, F), \quad (3)$$

Progressive Growing of GANs

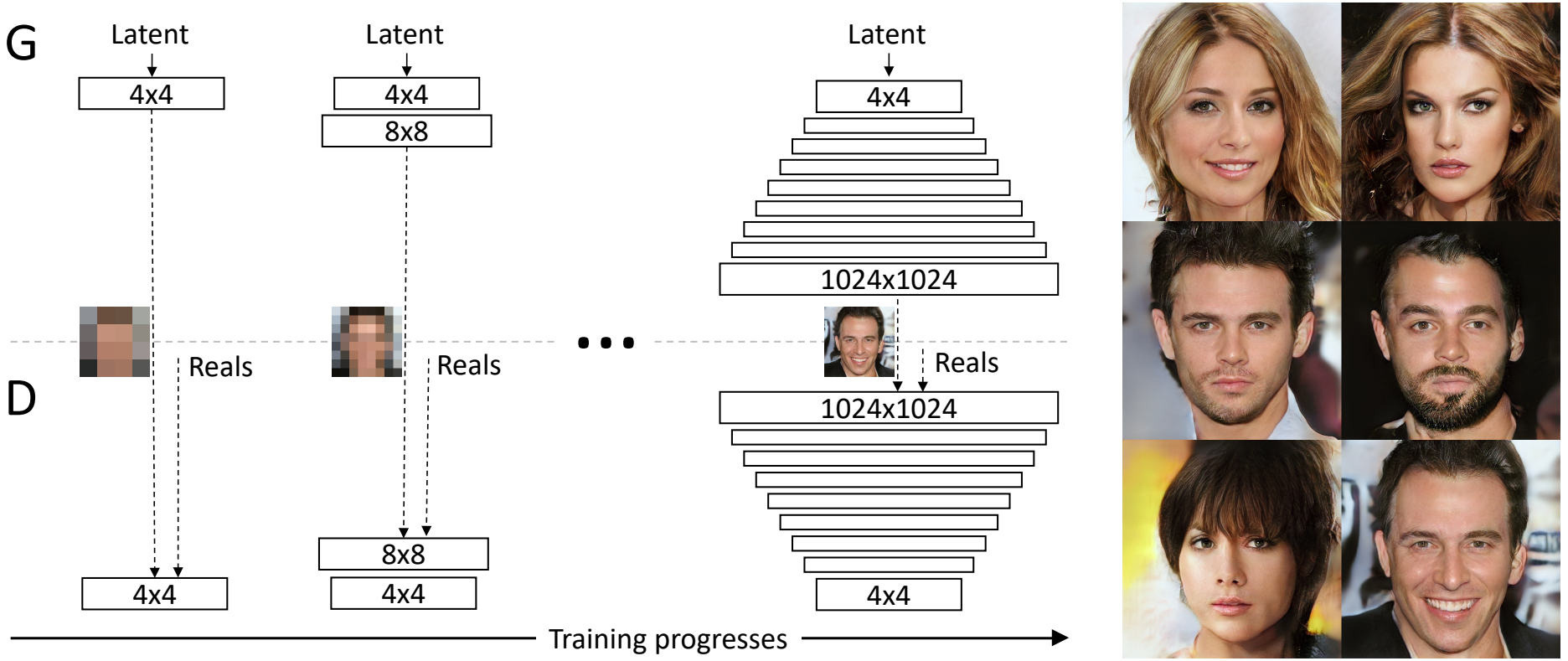


Figure 1: Our training starts with both the generator (G) and discriminator (D) having a low spatial resolution of 4×4 pixels. As the training advances, we incrementally add layers to G and D, thus increasing the spatial resolution of the generated images. All existing layers remain trainable throughout the process. Here $\boxed{N \times N}$ refers to convolutional layers operating on $N \times N$ spatial resolution. This allows stable synthesis in high resolutions and also speeds up training considerably. One the right we show six example images generated using progressive growing at 1024×1024.

https://arxiv.org/abs/1710.10196

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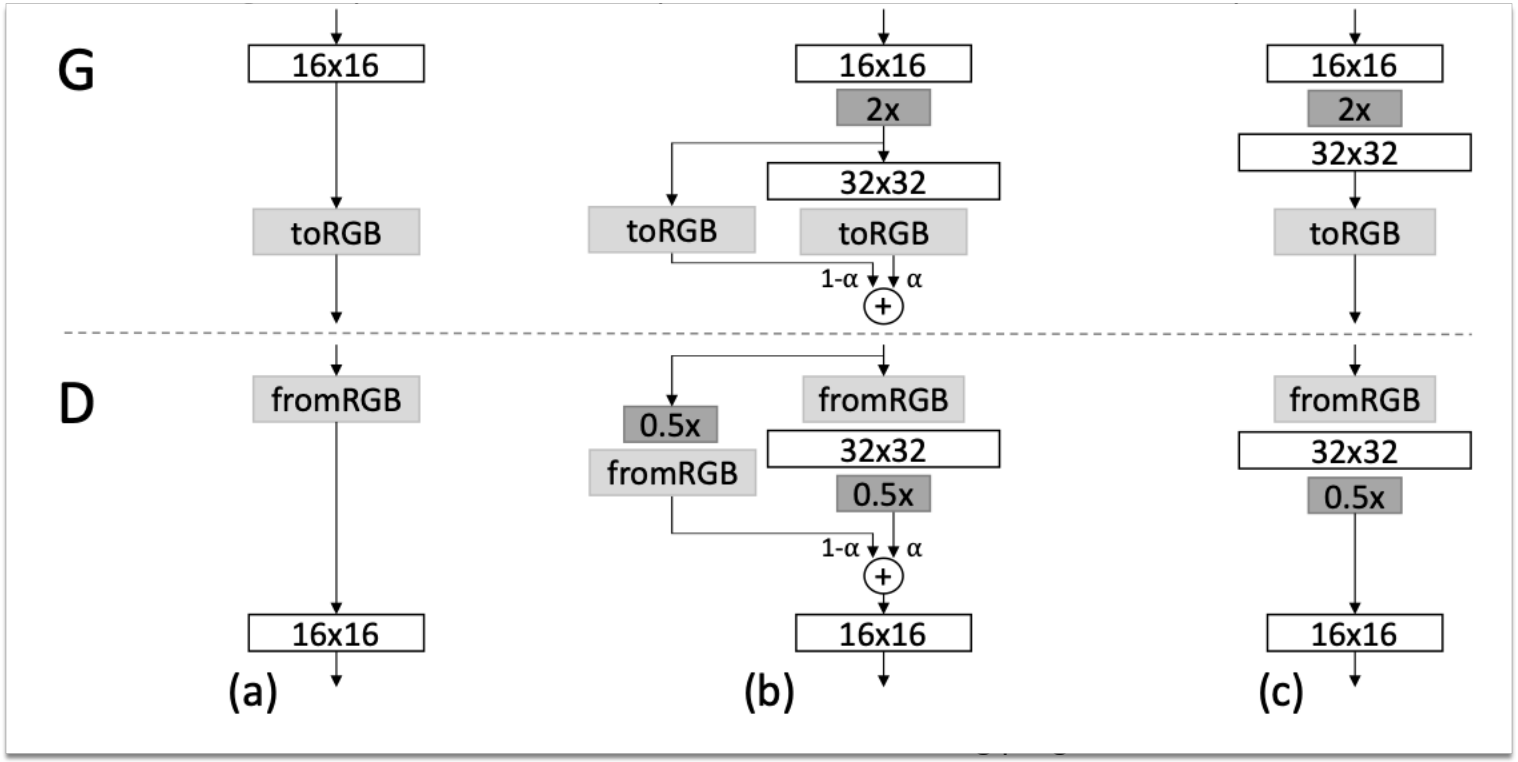

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Evaluating generative models

Evaluating generative models

No single guide to follow

Approaches are very problem-specific

- E.g. perceived visual quality of generated images vs. quality of a generated dental crown model (https://arxiv.org/abs/1804.00064)
- Most solutions are adapted to or invented for a given particular task

We'll mention some approaches

Evaluating generative models

(most obvious thing to do)

By-eye comparison (if your data allows that)

- Compare individual objects or whole distributions (e.g. in projections)
- There might be no need to do any complicated evaluation if the model results simply look bad

Evaluating generative models

(simple things to do)

Compare meaningful physical characteristics (if applicable)

- Means, medians, standard deviations, etc.
- Correlations

Statistical tests (χ^2, Kolmogorov-Smirnov, etc.)

- between individual dimensions or projections

Additional classifier

Train an independent model (e.g. xgboost) to distringuish real and fake samples

Evaluate your GAN by checking the classifier's score (e.g. ROC AUC)

Pros:

- An objective quality measure

Cons:

- Resource consuming
- Requires hyper-parameter tuning
- May get picky to things that are not important

Inception score

Introduced in https://arxiv.org/abs/1606.03498

Apply the Inception model (pre-trained image classifier) to obtain the conditional label distribution $p(y|x)$ for each image x

- this should be low-entropy (the classifier should be certain)

Calculate marginal $p(y) = \int p(y|x = G(z))p(z)dz$

- this should be high-entropy (diversity of samples)

Combining these two requirements:

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

Fréchet inception distance (FID score)

Introduced in https://arxiv.org/abs/1706.08500

One of the drawbacks of IS is that it doesn't care about the true distribution

Instead one can compare distributions of activations at some Inception layer (originally – last pooling layer)

The authors proposed calculating the Fréchet (aka Wasserstein-2) distance

Distance between multivariate Gaussian approximations:

$$\mathrm{FID} = \|\mu_r - \mu_g\|^2 + \mathrm{Tr}\left[\Sigma_r + \Sigma_g - 2\left(\Sigma_r\Sigma_g\right)^{1/2}\right]$$

Precision and Recal distance (PRD)

Definition 1. *For $\alpha, \beta \in (0, 1]$, the probability distribution Q has precision α at recall β w.r.t. P if there exist distributions μ, ν_P and ν_Q such that*

Decomposition with a common part

$$P = \beta\mu + (1 - \beta)\nu_P \quad \text{and} \quad Q = \alpha\mu + (1 - \alpha)\nu_Q. \tag{3}$$

Definition 2. *The set of attainable pairs of precision and recall of a distribution Q w.r.t. a distribution P is denoted by* $\mathrm{PRD}(Q, P)$ *and it consists of all (α, β) satisfying Definition 1 and the pair $(0, 0)$.*

- The authors provide an algorithm to calculate it for discrete distributions
- They convert Inception activations to discrete distribution using *k*-means clustering

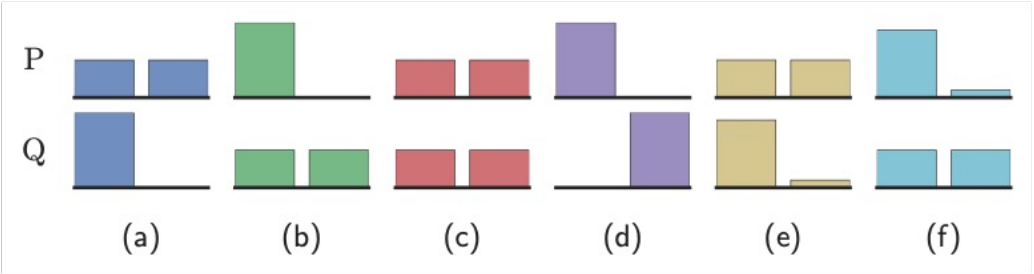

Figure 2: Intuitive examples of P and Q.

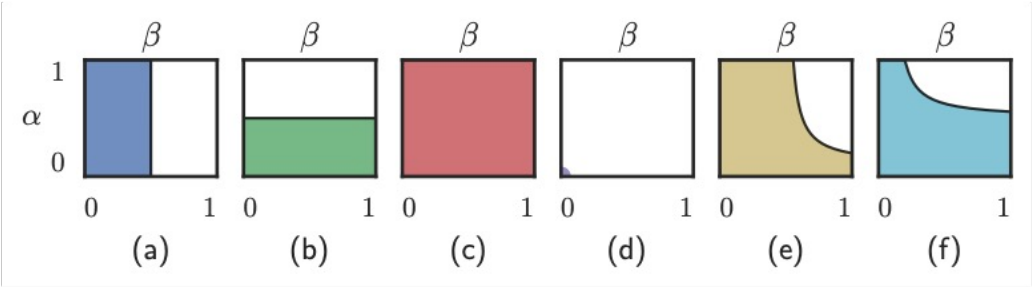

Figure 3: $\mathrm{PRD}(Q, P)$ for the examples above.

https://arxiv.org/abs/1806.00035

More metrics…

An extensive comparison of a large variety of measures:

- https://arxiv.org/abs/1802.03446

	Measure	Description
Quantitative	1. Average Log-likelihood [18, 22]	• Log likelihood of explaining realworld held out/test data using a density estimated from the generated data (*e.g.* using KDE or Parzen window estimation). $L = \frac{1}{N}\sum_i \log P_{model}(\mathbf{x}_i)$
	2. Coverage Metric [33]	• The probability mass of the true data "covered" by the model distribution $C := P_{data}(dP_{model} > t)$ with t such that $P_{model}(dP_{model} > t) = 0.95$
	3. Inception Score (IS) [3]	• KLD between conditional and marginal label distributions over generated data. $\exp\left(\mathbb{E}_{\mathbf{x}}\left[\mathbb{KL}\left(p\left(\mathrm{y} \mid \mathbf{x}\right) \parallel p\left(\mathrm{y}\right)\right)\right]\right)$
	4. Modified Inception Score (m-IS) [34]	• Encourages diversity within images sampled from a particular category. $\exp(\mathbb{E}_{\mathbf{x}_i}[\mathbb{E}_{\mathbf{x}_j}[(\mathbb{KL}(P(y\|\mathbf{x}_i)\|\|P(y\|\mathbf{x}_j))]])$
	5. Mode Score (MS) [35]	• Similar to IS but also takes into account the prior distribution of the labels over real data. $\exp\left(\mathbb{E}_{\mathbf{x}}\left[\mathbb{KL}\left(p\left(y \mid \mathbf{x}\right) \parallel p\left(y^{train}\right)\right)\right] - \mathbb{KL}\left(p\left(y\right) \parallel p\left(y^{train}\right)\right)\right)$
	6. AM Score [36]	• Takes into account the KLD between distributions of training labels vs. predicted labels, as well as the entropy of predictions. $\mathbb{KL}(p(y^{\text{train}}) \parallel p(y)) + \mathbb{E}_{\mathbf{x}}\left[H(y\|\mathbf{x})\right]$
	7. Fréchet Inception Distance (FID) [37]	• Wasserstein-2 distance between multi-variate Gaussians fitted to data embedded into a feature space $FID(r,g) = \|\mu_r - \mu_g\|_2^2 + Tr(\Sigma_r + \Sigma_g - 2(\Sigma_r\Sigma_g)^{\frac{1}{2}})$
	8. Maximum Mean Discrepancy (MMD) [38]	• Measures the dissimilarity between two probability distributions P_r and P_g using samples drawn independently from each distribution. $M_k(P_r, P_g) = \mathbb{E}_{\mathbf{x},\mathbf{x}'\sim P_r}[k(\mathbf{x},\mathbf{x}')] - 2\mathbb{E}_{\mathbf{x}\sim P_r,\boldsymbol{y}\sim P_g}[k(\mathbf{x},\boldsymbol{y})] + \mathbb{E}_{\boldsymbol{y},\boldsymbol{y}'\sim P_g}[k(\boldsymbol{y},\boldsymbol{y}')]$
	9. The Wasserstein Critic [39]	• The critic (*e.g.* an NN) is trained to produce high values at real samples and low values at generated samples $\hat{W}(\mathbf{x}_{test}, \mathbf{x}_g) = \frac{1}{N}\sum_{i=1}^{N}\hat{f}(\mathbf{x}_{test}[i]) - \frac{1}{N}\sum_{i=1}^{N}\hat{f}(\mathbf{x}_g[i])$
	10. Birthday Paradox Test [27]	• Measures the support size of a discrete (continuous) distribution by counting the duplicates (near duplicates)
	11. Classifier Two Sample Test (C2ST) [40]	• Answers whether two samples are drawn from the same distribution (*e.g.* by training a binary classifier)
	12. Classification Performance [1, 15]	• An indirect technique for evaluating the quality of unsupervised representations (*e.g.* feature extraction; FCN score). See also the GAN Quality Index (GQI) [41].
	13. Boundary Distortion [42]	• Measures diversity of generated samples and covariate shift using classification methods.
	14. Number of Statistically-Different Bins (NDB) [43]	• Given two sets of samples from the same distribution, the number of samples that fall into a given bin should be the same up to sampling noise
	15. Image Retrieval Performance [44]	• Measures the distributions of distances to the nearest neighbors of some query images (*i.e.* diversity)
	16. Generative Adversarial Metric (GAM) [31]	• Compares two GANs by having them engaged in a battle against each other by swapping discriminators or generators. $p(\mathbf{x}\|y=1;M_1')/p(\mathbf{x}\|y=1;M_2') = \left(p(y=1\|\mathbf{x};D_1)p(\mathbf{x};G_2)\right)/\left(p(y=1\|\mathbf{x};D_2)p(\mathbf{x};G_1)\right)$
	17. Tournament Win Rate and Skill Rating [45]	• Implements a tournament in which a player is either a discriminator that attempts to distinguish between real and fake data or a generator that attempts to fool the discriminators into accepting fake data as real.
	18. Normalized Relative Discriminative Score (NRDS) [32]	• Compares n GANs based on the idea that if the generated samples are closer to real ones, more epochs would be needed to distinguish them from real samples.
	19. Adversarial Accuracy and Divergence [46]	• Adversarial Accuracy. Computes the classification accuracies achieved by the two classifiers, one trained on real data and another on generated data, on a labeled validation set to approximate $P_g(y\|\mathbf{x})$ and $P_r(y\|\mathbf{x})$. Adversarial Divergence: Computes $\mathbb{KL}(P_g(y\|\mathbf{x}), P_r(y\|\mathbf{x}))$
	20. Geometry Score [47]	• Compares geometrical properties of the underlying data manifold between real and generated data.
	21. Reconstruction Error [48]	• Measures the reconstruction error (*e.g.* L_2 norm) between a test image and its closest generated image by optimizing for z (*i.e.* $min_{\mathbf{z}}\|\|G(\mathbf{z}) - \mathbf{x}^{(test)}\|\|^2$)
	22. Image Quality Measures [49, 50, 51]	• Evaluates the quality of generated images using measures such as SSIM, PSNR, and sharpness difference
	23. Low-level Image Statistics [52, 53]	• Evaluates how similar low-level statistics of generated images are to those of natural scenes in terms of mean power spectrum, distribution of random filter responses, contrast distribution, etc.
	24. Precision, Recall and F_1 score [23]	• These measures are used to quantify the degree of overfitting in GANs, often over toy datasets.
Qualitative	1. Nearest Neighbors	• To detect overfitting, generated samples are shown next to their nearest neighbors in the training set
	2. Rapid Scene Categorization [18]	• In these experiments, participants are asked to distinguish generated samples from real images in a short presentation time (*e.g.* 100 ms); *i.e.* real v.s fake
	3. Preference Judgment [54, 55, 56, 57]	• Participants are asked to rank models in terms of the fidelity of their generated images (*e.g.* pairs, triples)
	4. Mode Drop and Collapse [58, 59]	• Over datasets with known modes (*e.g.* a GMM or a labeled dataset), modes are computed as by measuring the distances of generated data to mode centers
	5. Network Internals [1, 60, 61, 62, 63, 64]	• Regards exploring and illustrating the internal representation and dynamics of models (*e.g.* space continuity) as well as visualizing learned features

Summary

GANs – a rather broad field of ML

- Lots of different architectures, this lecture doesn't pretend to be comprehensive

May say, that in GANs we 'learn' the loss for the generator

Wasserstein GAN is a useful technique that allows really deep networks to be used for data generation

Finding universal quality evaluation method is rather an open question

GANs for fast simulation

K. Matchev, P. Shyamsundar, Uncertainties associated with GAN-generated datasets in high energy physics, arXiv:2002.06307 [hep-ph]

Quite a developing field!

Important note: one cannot increase the statistics with GANs

GANs rather memorize and interpolate the available data

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(Shameless plug)

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Thank you!

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