ROBOT INTELLIGENCE LAB

Generative Model

Latent Variable Model & GAN & Normalizing Flow

Sungjoon Choi, Korea University

kakaobrain

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Latent Variable Models

Question

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Is an **auto-encoder** a generative model?

Variational Auto-Encoder

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- The objective is simple.

$$\text{Maximize } p_\theta(\mathbf{x})$$

Variational Auto-Encoder

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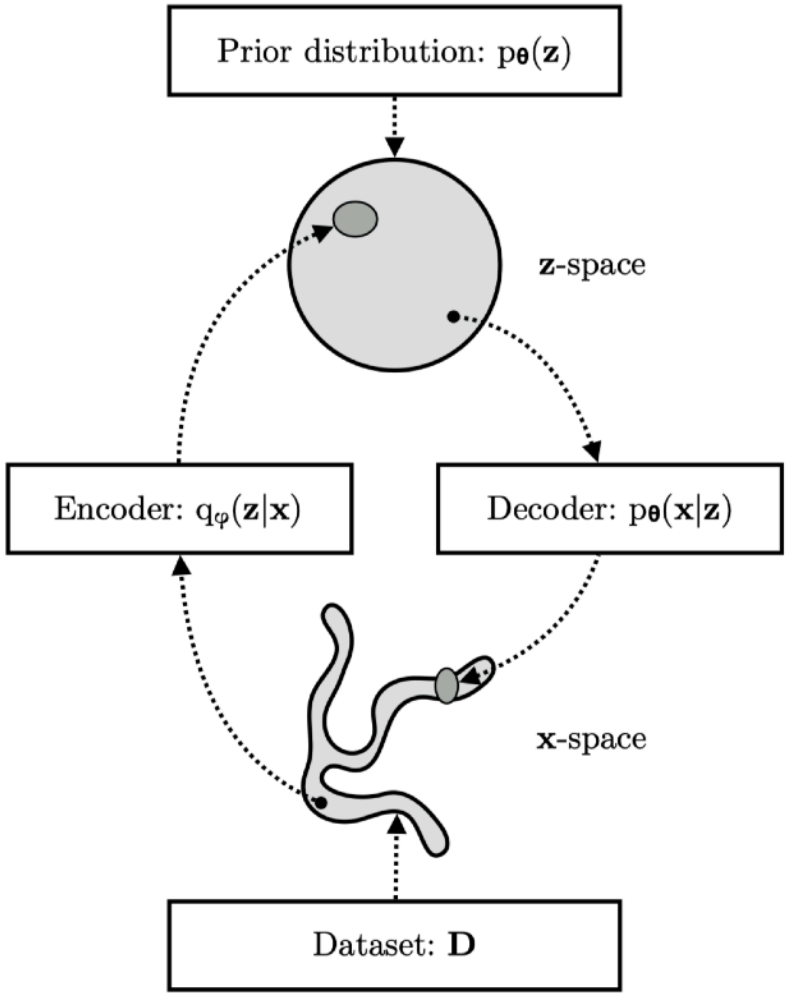

D. Kingma, "Variational Inference and Deep Learning: A New Synthesis," Ph.D. Thesis

Variational Auto-Encoder

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$$
\begin{aligned}
\underbrace{\log p_\theta(x)}_{\text{Maximum Likelihood Learning} \uparrow} &= \int_z \underbrace{q_\phi(z|x)}_{\text{For any } q_\phi} \log p_\theta(x) dz \\
&= \mathbb{E}_{z\sim q_\phi(z|x)}\left[\log \frac{p_\theta(x)p_\theta(z|x)}{p_\theta(z|x)}\right] \\
&= \mathbb{E}_{z\sim q_\phi(z|x)}\left[\log \frac{p_\theta(x,z)}{p_\theta(z|x)}\right] \\
&= \mathbb{E}_{z\sim q_\phi(z|x)}\left[\log \frac{p_\theta(x,z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}\right] \\
&= \mathbb{E}_{z\sim q_\phi(z|x)}\left[\log \frac{p_\theta(x,z)}{q_\phi(z|x)}\right] + \mathbb{E}_{z\sim q_\phi(z|x)}\left[\log \frac{q_\phi(z|x)}{p_\theta(z|x)}\right] \\
&= \underbrace{\mathbb{E}_{z\sim q_\phi(z|x)}\left[\log \frac{p_\theta(x,z)}{q_\phi(z|x)}\right]}_{\text{ELBO} \uparrow} + \underbrace{D_{KL}\left(q_\phi(z|x)\|p_\theta(z|x)\right)}_{\text{Variational Gap} \downarrow}
\end{aligned}
$$

D. Kingma, "Variational Inference and Deep Learning: A New Synthesis," Ph.D. Thesis

Variational Auto-Encoder

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$$\underbrace{\mathbb{E}_{z\sim q_\phi(z|x)}\left[\log \frac{p_\theta(x,z)}{q_\phi(z|x)}\right]}_{\text{ELBO}\uparrow} = \int \log \frac{p_\theta(x|z)p(z)}{q_\phi(z|x)} q_\phi(z|x)dz$$

$$= \underbrace{\mathbb{E}_{q_\phi(z|x)}\left[p_\theta(x|z)\right]}_{\text{Reconstruction Term}} - \underbrace{D_{KL}\left(q_\phi(z|x)\|p(z)\right)}_{\text{Prior Fitting Term}}$$

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Variational Auto-Encoder

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$$\underbrace{\mathbb{E}_{z\sim q_\phi(z|x)}\left[\log \frac{p_\theta(x,z)}{q_\phi(z|x)}\right]}_{\text{ELBO}\uparrow} = \int \log \frac{p_\theta(x|z)p(z)}{q_\phi(z|x)} q_\phi(z|x)dz$$

$$= \underbrace{\mathbb{E}_{q_\phi(z|x)}\left[p_\theta(x|z)\right]}_{\text{Reconstruction Term}} - \underbrace{D_{KL}\left(q_\phi(z|x)\|p(z)\right)}_{\text{Prior Fitting Term}}$$

- Key Limitation
  - It is an **intractable** model (hard to evaluate likelihood).
  - The prior fitting term should be differentiable, hence it is hard to use diverse latent prior distributions.
  - In most cases, we use an isotropic Gaussian where we have a closed-form for the prior fitting term.

$$\underbrace{D_{KL}\left(q_\phi(z|x)\|\mathcal{N}(0,I)\right)}_{\text{Prior Fitting Term}} = \frac{1}{2}\sum_{i=1}^{D}\left(\sigma_{z_i}^2 + \mu_{z_i}^2 - \log(\sigma_{z_i}^2) - 1\right)$$

D. Kingma, "Variational Inference and Deep Learning: A New Synthesis," Ph.D. Thesis

Variational Auto-Encoder

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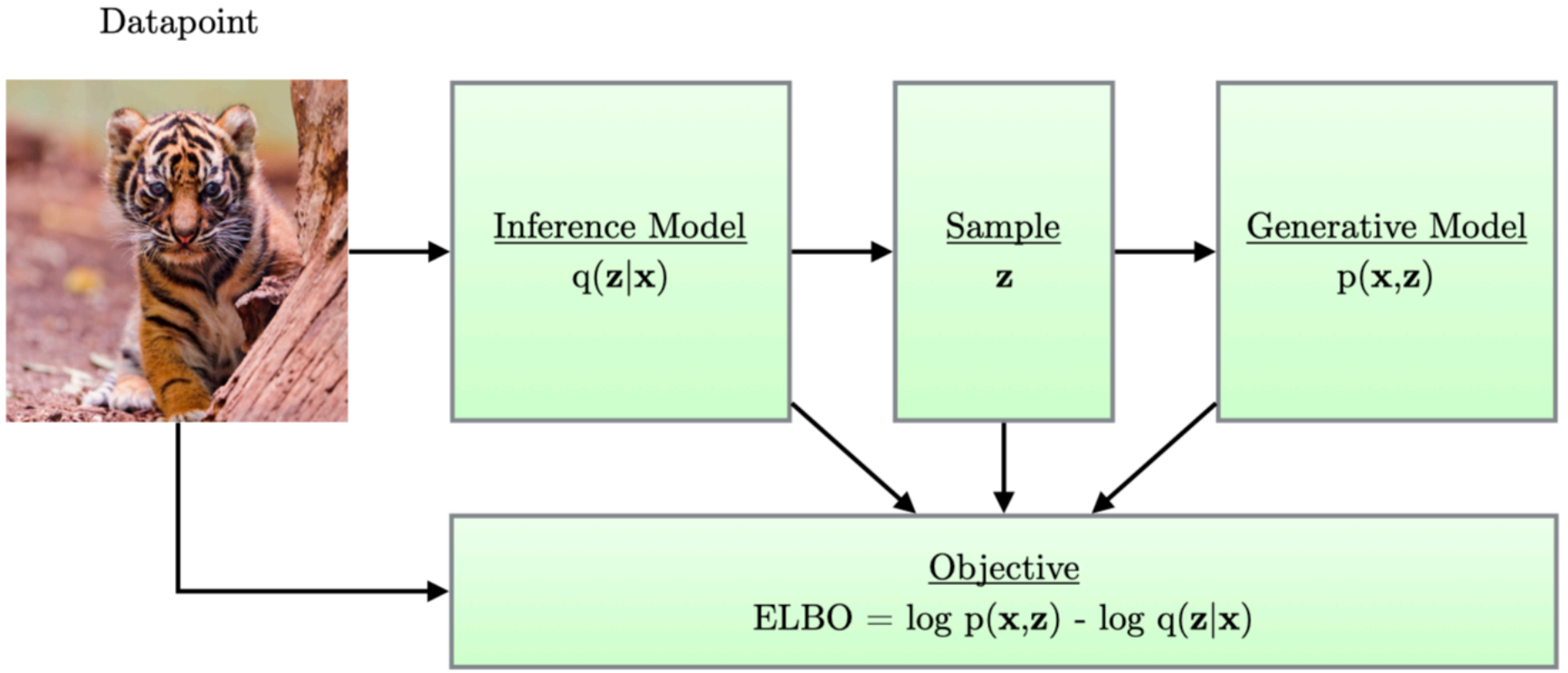

D. Kingma, "Variational Inference and Deep Learning: A New Synthesis," Ph.D. Thesis

Reparametrization Trick

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- Want to compute a gradient with respect to ϕ of

$$E_{q(z;\phi)}[r(z)] = \int q(z;\phi) r(z) dz$$

  where z is continuous.

- Suppose $q(z;\phi) = \mathcal{N}(\mu, \sigma^2)$ is Gaussian with parameters $\phi = (\mu, \sigma)$. These are equivalent ways of sampling:
  - Sample $z \sim q_\phi(z)$
  - Sample $\epsilon \sim \mathcal{N}(0,1)$, then $z = \mu + \sigma\epsilon = g(\epsilon;\phi)$
- Using this equivalence, we compute the expectation is two ways:

$$E_{z\sim q(z;\phi)}[r(z)] = E_{\epsilon\sim\mathcal{N}(0,1)}[r(g(\epsilon;\phi))] = \int p(\epsilon) r(\mu + \sigma\epsilon) d\epsilon$$

$$\nabla_\phi E_{q(z;\phi)}[r(z)] = \nabla_\phi E_\epsilon[r(g(\epsilon;\phi))] = E_\epsilon[\nabla_\phi r(g(\epsilon;\phi))]$$

- Easy to approximate the gradient by

$$E_\epsilon[\nabla_\phi r(g(\epsilon;\phi))] \approx \frac{1}{k}\sum_k \nabla_\phi r(g(\epsilon^k;\phi)) \text{ where } \epsilon^k \sim \mathcal{N}(0,1)$$

Amortizaiton

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$$\max_{\theta} l(\theta; \mathcal{D}) \geq \max_{\theta, \phi^1, \phi^2, \cdots} \sum_{x^i \in \mathcal{D}} \mathcal{L}(x^i; \theta, \phi^i)$$

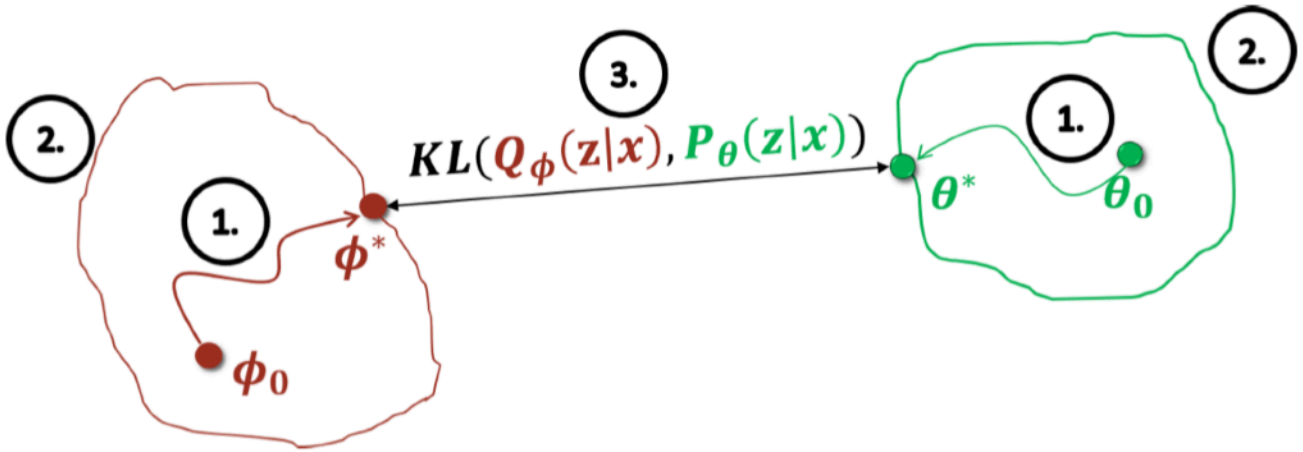
- So far, we have used a set of variational parameters (e.g., μ and σ) ϕ^i for **each** data point x^i. However it does not scale to large datasets.

- **Amortization**: Now we learn a **single** parametric function f_λ that maps each x to a set of (good) variational parameters (i.e., $f_\lambda : x^i \mapsto \phi^i$)
  - For example, if $q(z|x^i)$ are Gaussians with different means and variances, we learn a single neural network f_λ mapping x^i to (μ^i, σ^i).
  - This is an encoder network in VAE.
- We approximate the posteriors $q(z|x^i)$ using the distribution $q_\lambda(z|x)$.

Summary of Latent Variable Models

1. Combine simple models to get a more flexible one (e.g., mixture of Gaussians)
2. Directed model permits ancestral sampling (efficient generation):
    1. $z \sim p(z)$
    2. $x \sim p(x|z;\theta)$
3. However, log-likelihood is generally intractable, hence learning is difficult.
4. Joint learning of a (decoder) model (θ) and an amortized inference component (ϕ) to achieve tractability via ELBO optimization
5. Latent representation for any x can be inferred via $q_\phi(z|x) = q(z; f_\lambda(x))$ (aka an encoder model).

Research Directions



1. Better optimization techniques
2. More expressive approximating (variational) families
3. Alternate loss functions

Adversarial Auto-encoder

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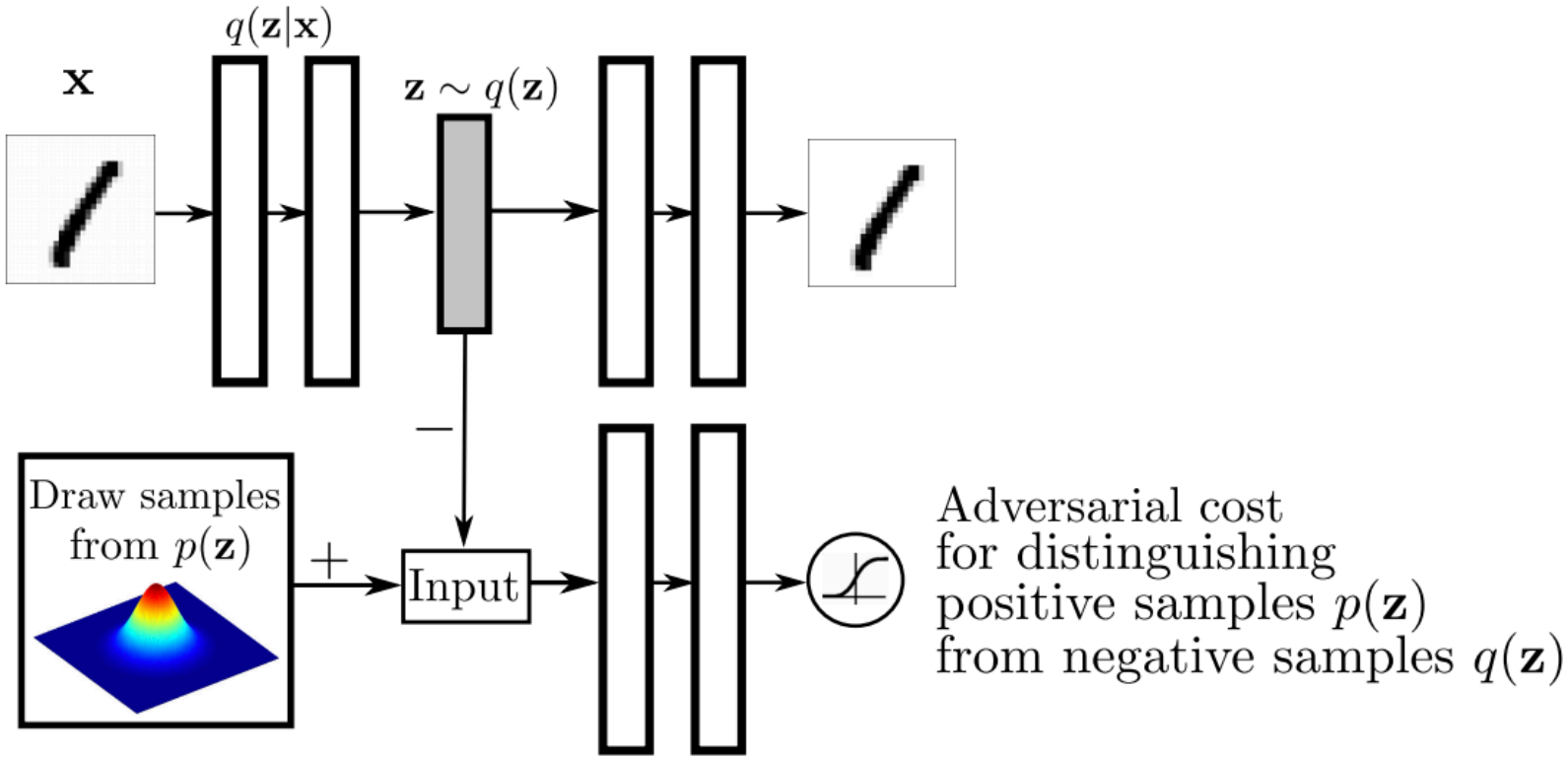
- Let x be the input and z be the latent vector.
- Let $p(z)$ be the prior distribution we want to impose the the latent vectors, $q(z|x)$ be an encoding distribution, and $p(x|z)$ be the decoding distribution.
- Also let $p_d(x)$ be the data distribution, and $p(x)$ be the model distribution.
- The **aggregated posterior distribution** $q(z)$ is defined by the encoder function $q(z|x)$:

$$q(z) = \int_x q(z|x)p_d(x)dx$$

- The adversarial encoder (AAE) is an autoencoder that is **regularized by matching** the aggregated posterior, $q(z)$, to an arbitrary prior, $p(z)$.
- To achieve this, an adversarial network is attached on top of the latent vector of the autoencoder that guides $q(z)$ to match $p(z)$.

https://arxiv.org/abs/1511.05644

Adversarial Auto-encoder



- AAE allows to use any arbitrary latent prior distributions that we can sample.

https://arxiv.org/abs/1511.05644

Wasserstein Auto-encoders

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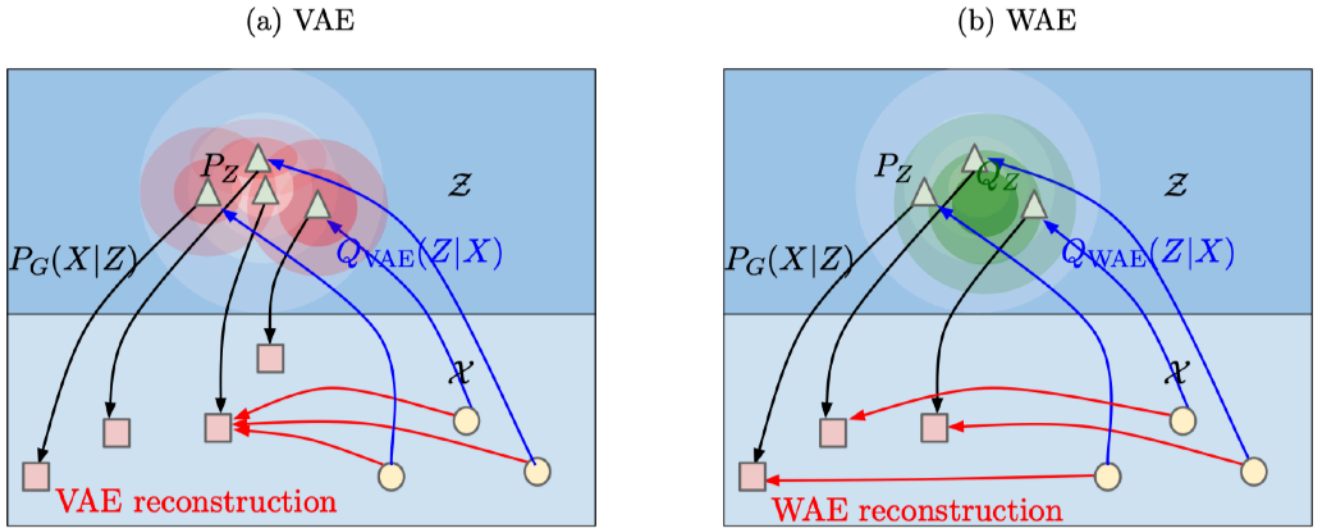

- Both **VAE** and **WAE** minimize two terms: the reconstruction cost and the regularizer penalizing discrepancy between P_Z and distribution induced by the encoder Q.
- VAE forces $Q(Z|X=x)$ to match P_Z for all the different input examples x drawn from P_X.
- This is illustrated on picture (a), where every single red ball is forced to match P_Z depicted as the white shape. Red balls start **intersecting**, which leads to problems with reconstruction.
- In contrast, WAE forces the continuous mixture $Q_Z = \int Q(Z|X)dP_X$ to match P_Z, as depicted with the green ball in picture (b). As a result, latent vectors of different examples get a chance to **stay far way** from each other, promoting a better reconstruction.

https://arxiv.org/abs/1711.01558

Wasserstein Auto-encoders

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- Optimal transport and its dual formulations
  - A rich class of divergences between probability distributions is induces by the optimal transport (OT) problem.

$$W_c(P_X, P_G) = \inf_{\Gamma \in \mathcal{P}(X \sim P_X, Y \sim P_G)} E_{(X,Y)\sim\Gamma}[c(X, Y)]$$

    where $c(x, y) : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+$ is any measurable cost function and $\mathcal{P}(X \sim P_X, Y \sim P_G)$ is a set of all joint distributions of (X, Y) with marginals P_X and P_G, respectively.

  - A particular interesting case is when $(\mathcal{X}, d)$ is a metric space and $c(x, y) = d^p(x, y)$ for $p \geq 1$. In this case, W_c is called the p-Wasserstein distance.

https://arxiv.org/abs/1711.01558

Wasserstein Auto-encoders

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Theorem 1. *For P_G as defined above with deterministic $P_G(X|Z)$ and any function $G: \mathcal{Z} \to \mathcal{X}$*

$$\inf_{\Gamma \in \mathcal{P}(X \sim P_X, Y \sim P_G)} \mathbb{E}_{(X,Y)\sim\Gamma}\left[c(X,Y)\right] = \inf_{Q:\, Q_Z = P_Z} \mathbb{E}_{P_X}\mathbb{E}_{Q(Z|X)}\left[c(X, G(Z))\right],$$

where Q_Z is the marginal distribution of Z when $X \sim P_X$ and $Z \sim Q(Z|X)$.

$$D_{\mathrm{WAE}}(P_X, P_G) := \inf_{Q(Z|X)\in\mathcal{Q}} \mathbb{E}_{P_X}\mathbb{E}_{Q(Z|X)}\left[c(X, G(Z))\right] + \lambda \cdot \mathcal{D}_Z(Q_Z, P_Z), \quad \text{(WAE objective)}$$

- What it means is that
  1. we can reformulate the **optimal transport problem** into the **WAE objective** using its dual formulations.
  2. The WAE objective contains a reconstruction loss and an arbitrary divergence between the aggregated posterior $Q_Z = \int Q(Z|X) dP_X$ and the prior P_Z.
  3. If we use Jensen-Shannon divergence for D_Z (i.e., $D_Z(Q_Z, P_Z) = D_{JS}(Q_Z, P_Z)$, and use the adversarial training to estimate it, it becomes the **adversarial auto-encoder**.

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Generative Adversarial Network

Goodfellow et al., "Generative Adversarial Networks", NIPS, 2014

GAN

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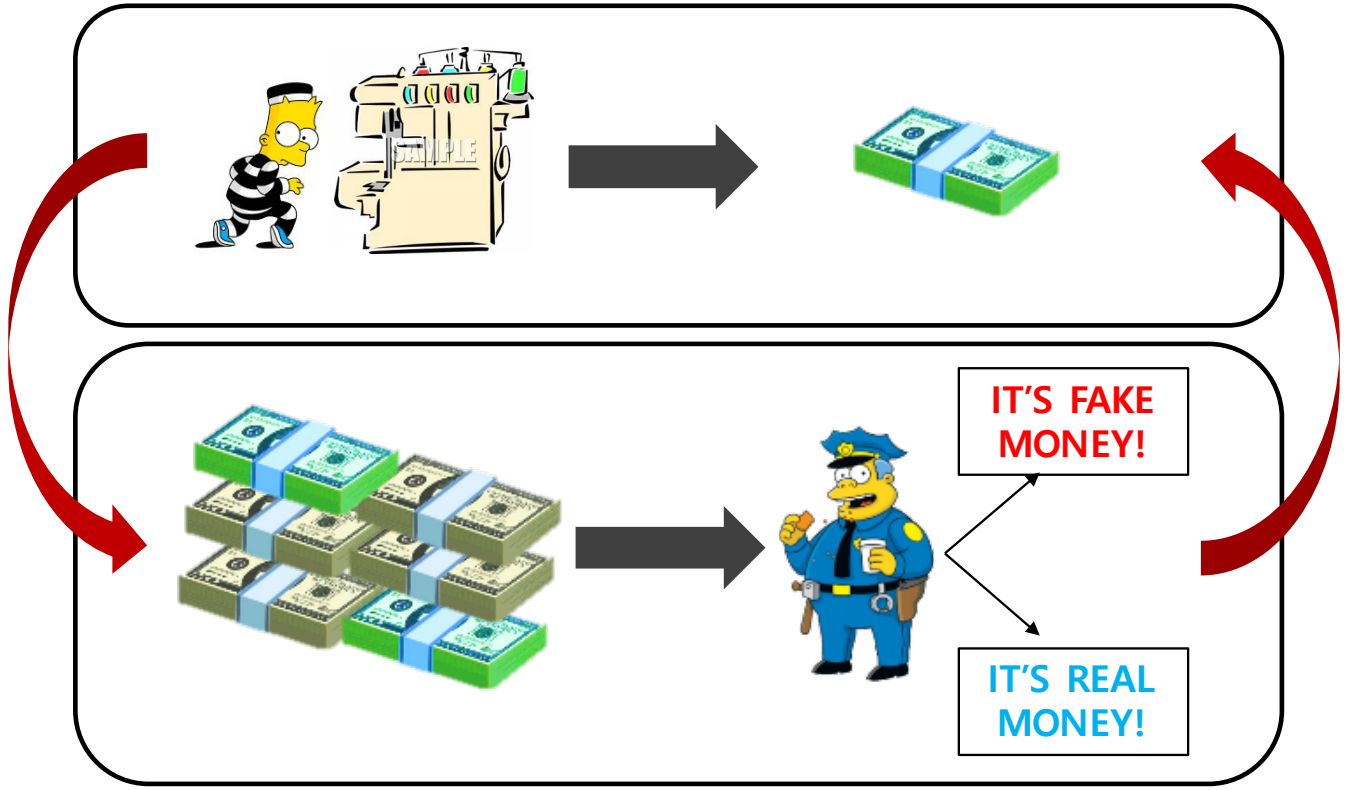
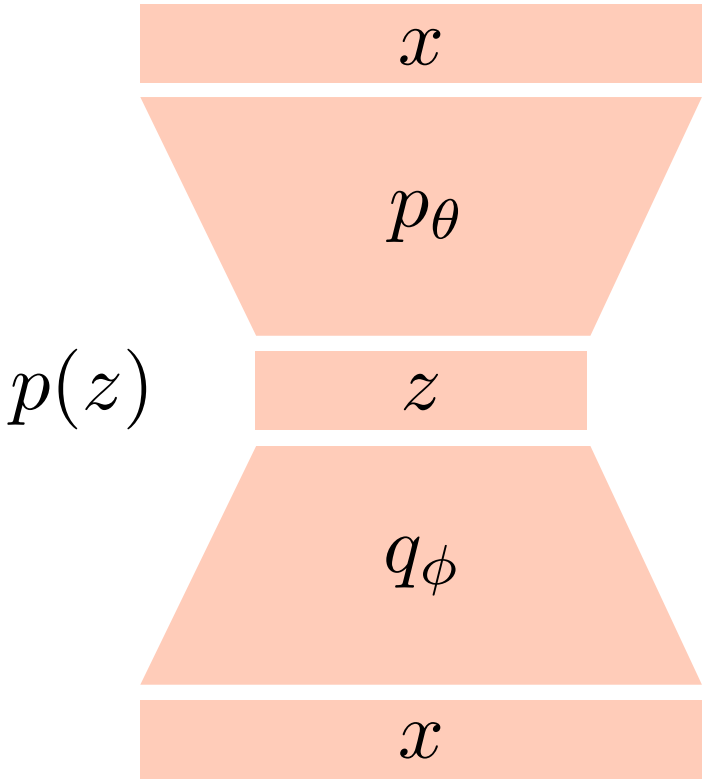


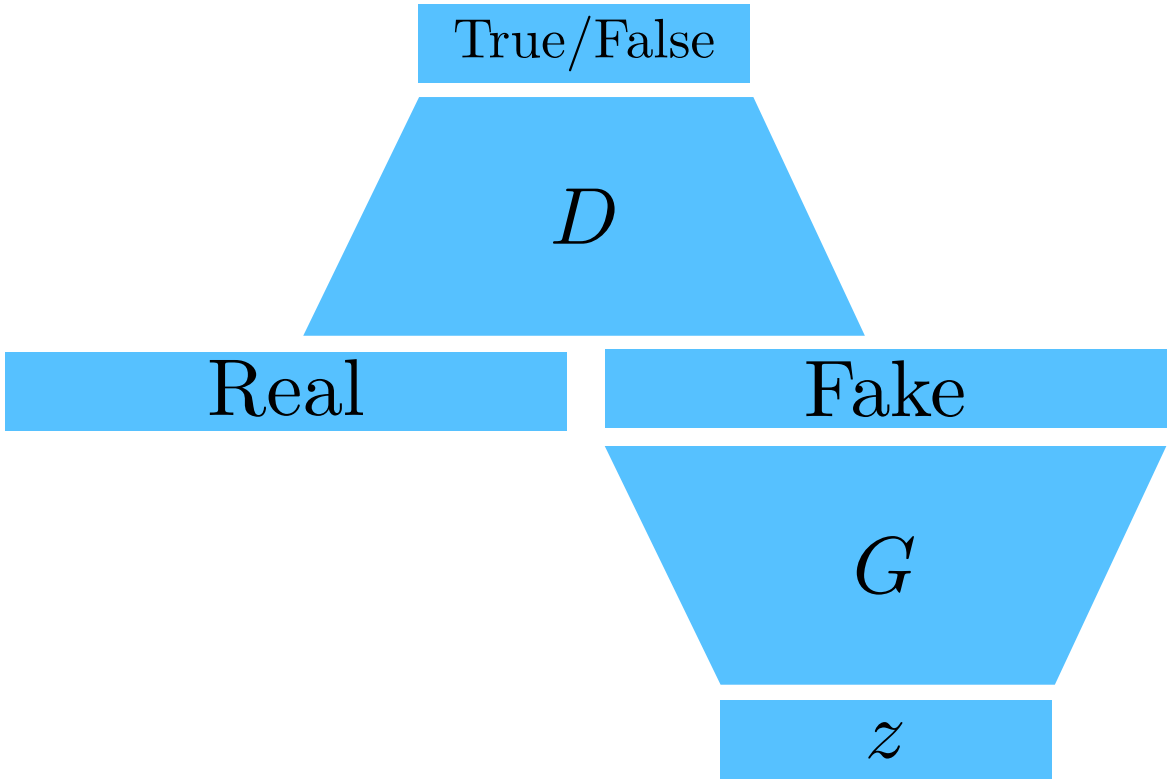
$$\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))].$$

https://arxiv.org/abs/1406.2661

GAN vs. VAE



Variational Auto-encoder



Generative Adversarial Networks

GAN Objective

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- GAN is a two player minimax game between **generator** and **discriminator**.
  - **Discriminator** objective

$$\max_D V(G,D) = E_{\mathbf{x}\sim p_{\text{data}}}[\log D(\mathbf{x})] + E_{\mathbf{x}\sim p_G}[\log(1 - D(\mathbf{x}))]$$

  - The **optimal discriminator** is

$$D_G^*(\mathbf{x}) = \frac{p_{\text{data}}(\mathbf{x})}{p_{\text{data}}(\mathbf{x}) + p_G(\mathbf{x})}$$

https://arxiv.org/abs/1406.2661

GAN Objective

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- GAN is a two player minimax game between **generator** and **discriminator**.
  - **Generator** objective

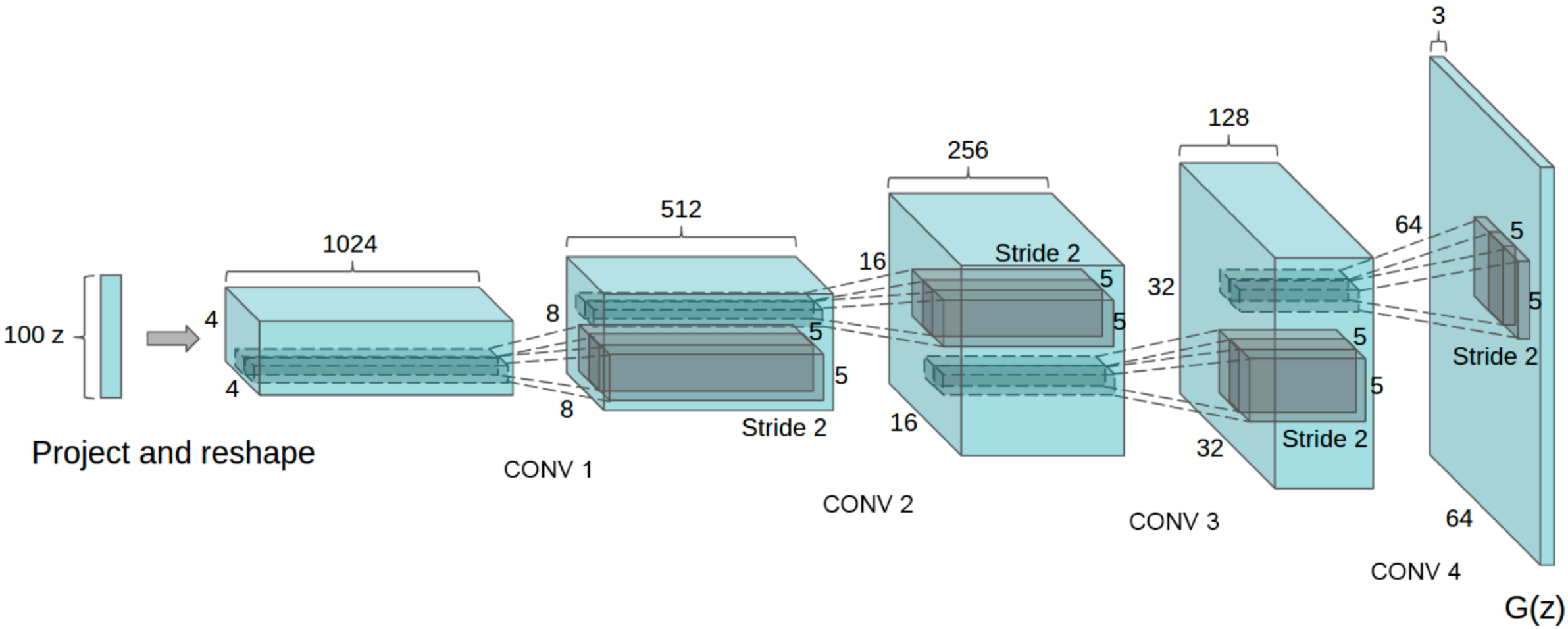
$$\min_G V(G,D) = E_{\mathbf{x}\sim p_{\text{data}}}[\log D(\mathbf{x})] + E_{\mathbf{x}\sim p_G}[\log(1 - D(\mathbf{x}))]$$

  - Plugging in the **optimal discriminator**, we get

$$\begin{aligned} V(G, D_G^*(\mathbf{x})) &= E_{\mathbf{x}\sim p_{\text{data}}}\left[\log \frac{p_{\text{data}}(\mathbf{x})}{p_{\text{data}}(\mathbf{x})+p_G(\mathbf{x})}\right] + E_{\mathbf{x}\sim p_G}\left[\log \frac{p_G(\mathbf{x})}{p_{\text{data}}(\mathbf{x})+p_G(\mathbf{x})}\right] \\ &= E_{\mathbf{x}\sim p_{\text{data}}}\left[\log \frac{p_{\text{data}}(\mathbf{x})}{\frac{p_{\text{data}}(\mathbf{x})+p_G(\mathbf{x})}{2}}\right] + E_{\mathbf{x}\sim p_G}\left[\log \frac{p_G(\mathbf{x})}{\frac{p_{\text{data}}(\mathbf{x})+p_G(\mathbf{x})}{2}}\right] - \log 4 \\ &= \underbrace{D_{KL}\left[p_{\text{data}}, \frac{p_{\text{data}}+p_G}{2}\right] + D_{KL}\left[p_G, \frac{p_{\text{data}}+p_G}{2}\right]}_{2\times\text{Jenson-Shannon Divergence (JSD)}} - \log 4 \\ &= 2D_{JSD}[p_{\text{data}}, p_G] - \log 4 \end{aligned}$$

https://arxiv.org/abs/1406.2661

DCGAN


100 z
Project and reshape
1024
4
4
CONV 1
512
8
8
5
5
Stride 2
CONV 2
256
16
16
5
5
Stride 2
CONV 3
128
32
32
5
5
Stride 2
CONV 4
64
64
3
5
5
Stride 2
G(z)

Info-GAN

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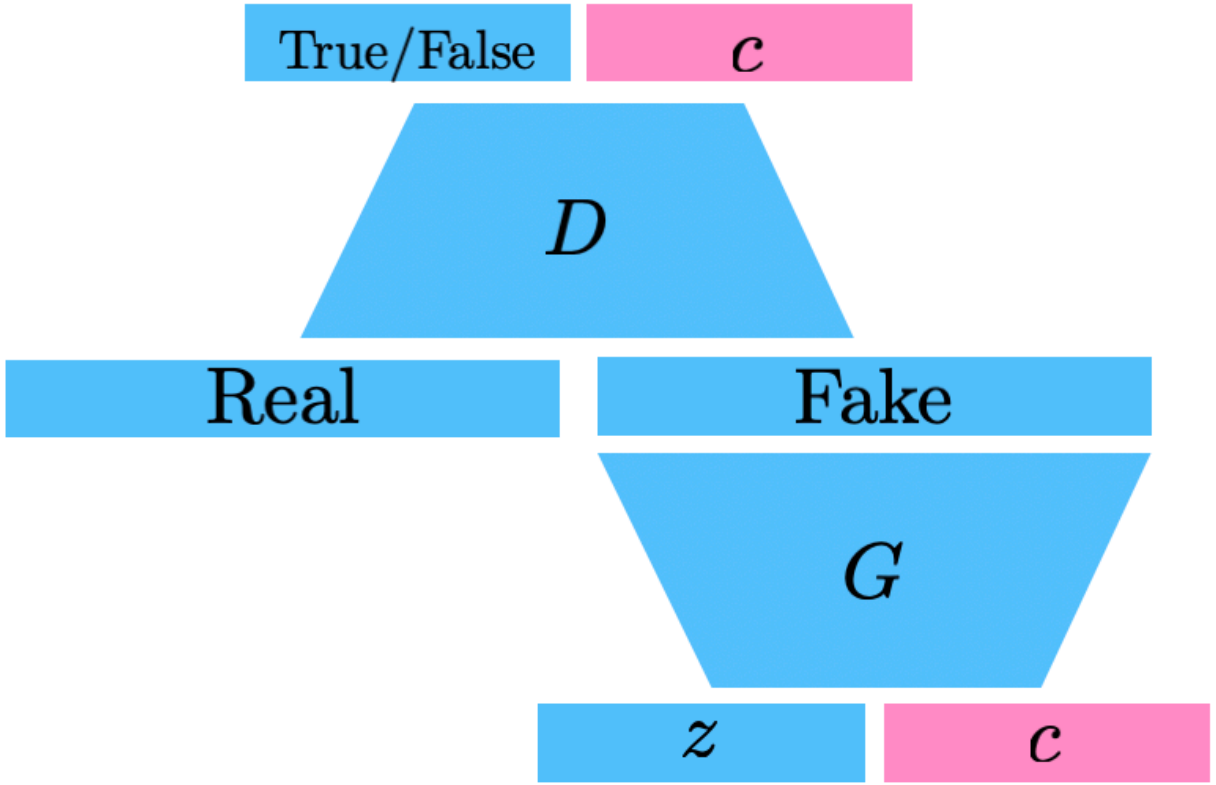

https://arxiv.org/abs/1606.03657

Text2Image

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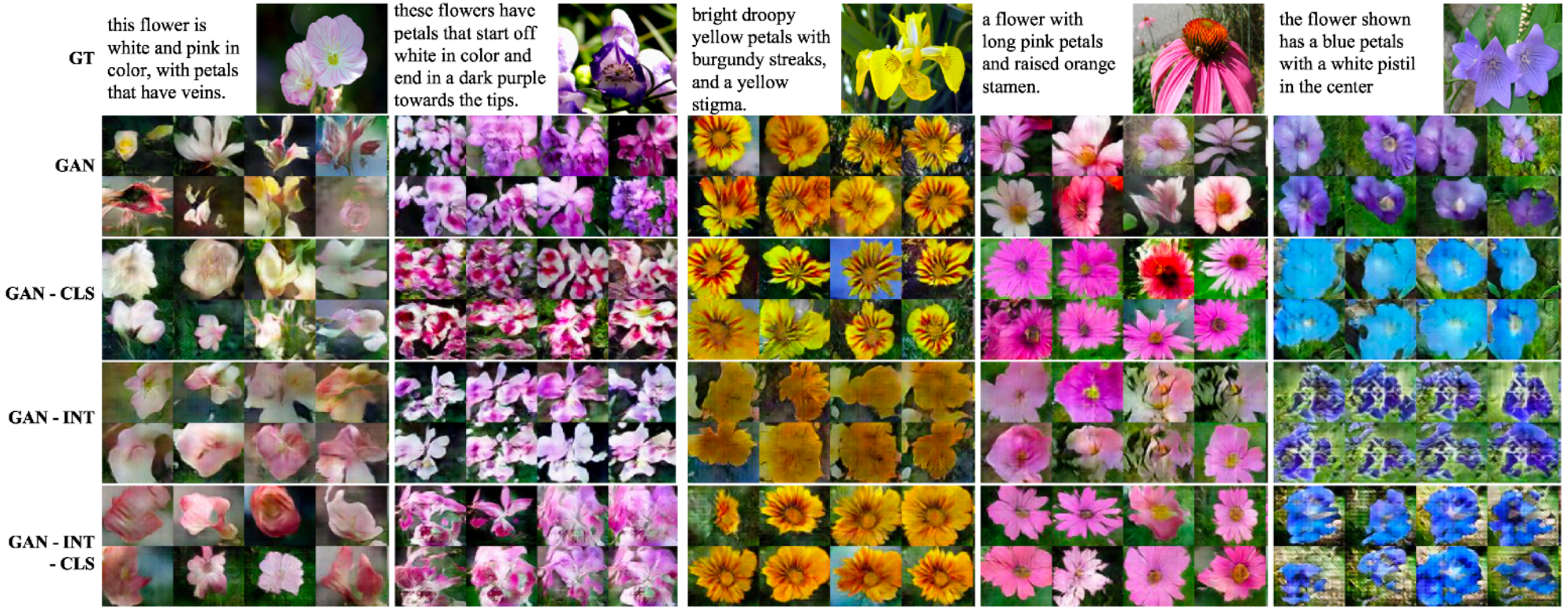
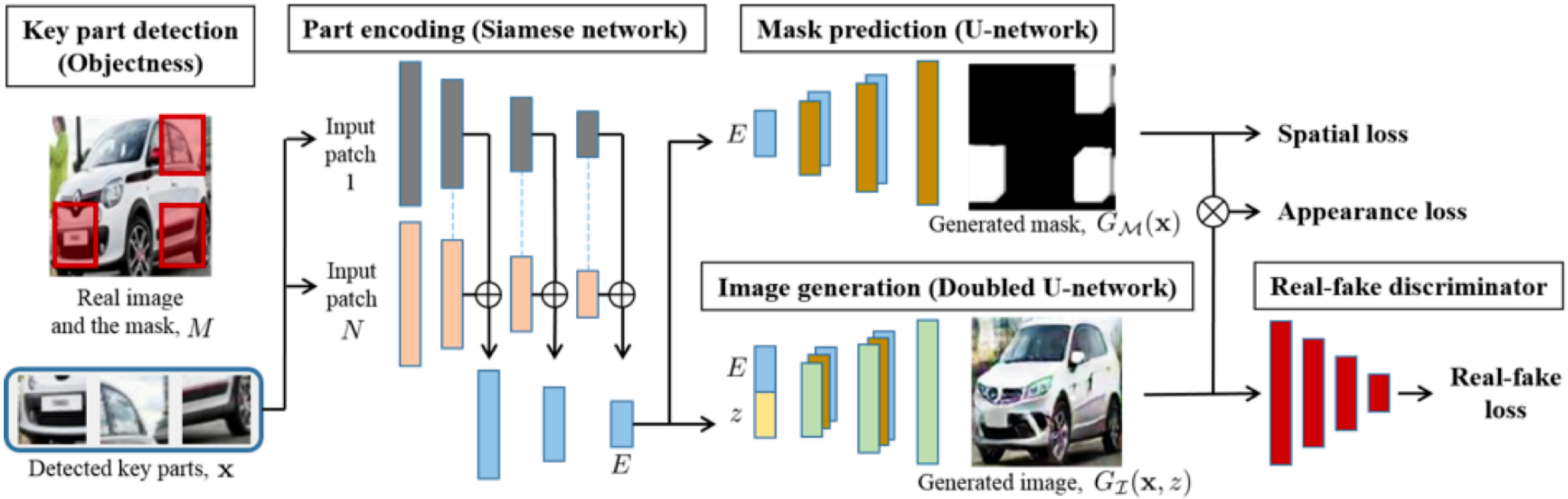


https://arxiv.org/abs/1605.05396

Puzzle-GAN



https://arxiv.org/abs/1703.10730

CycleGAN

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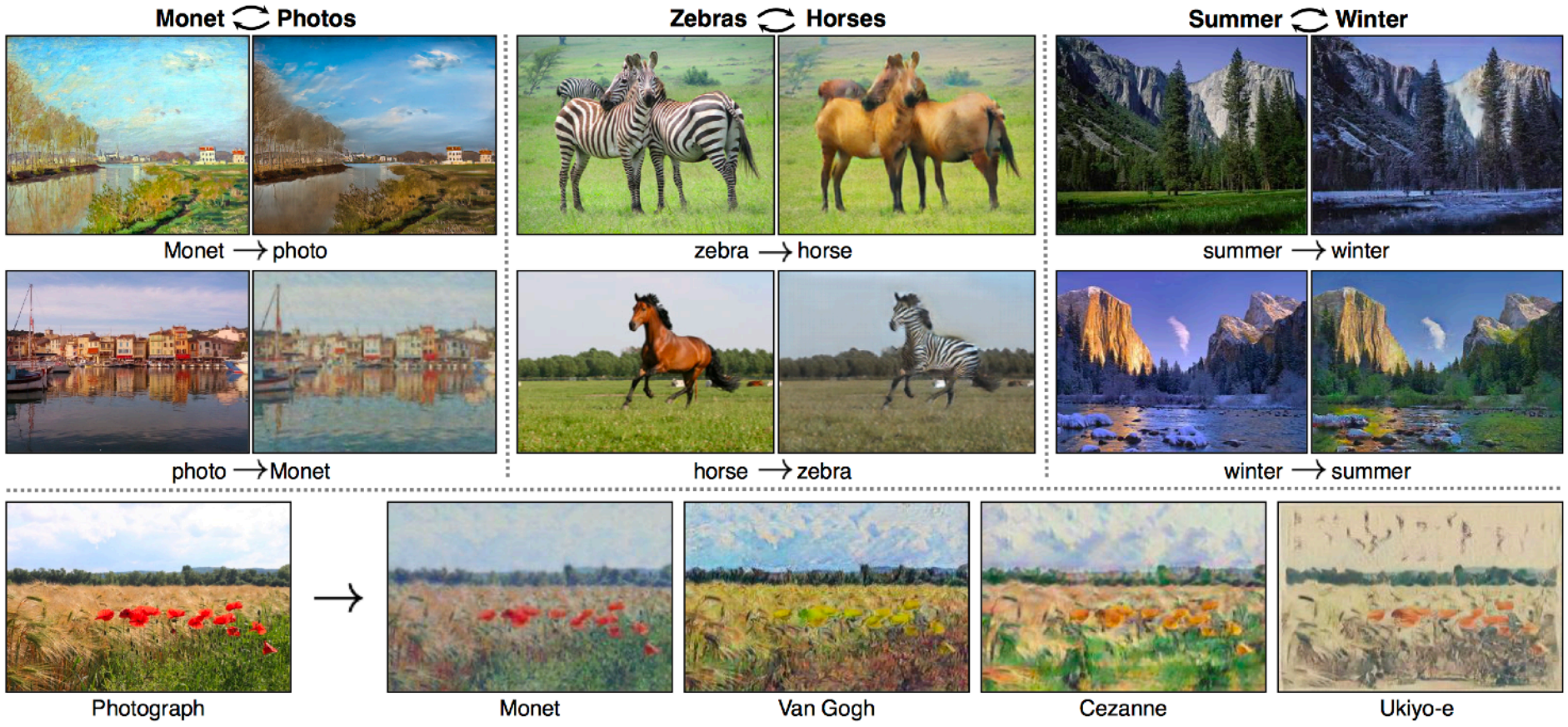

https://arxiv.org/abs/1703.10593

CycleGAN

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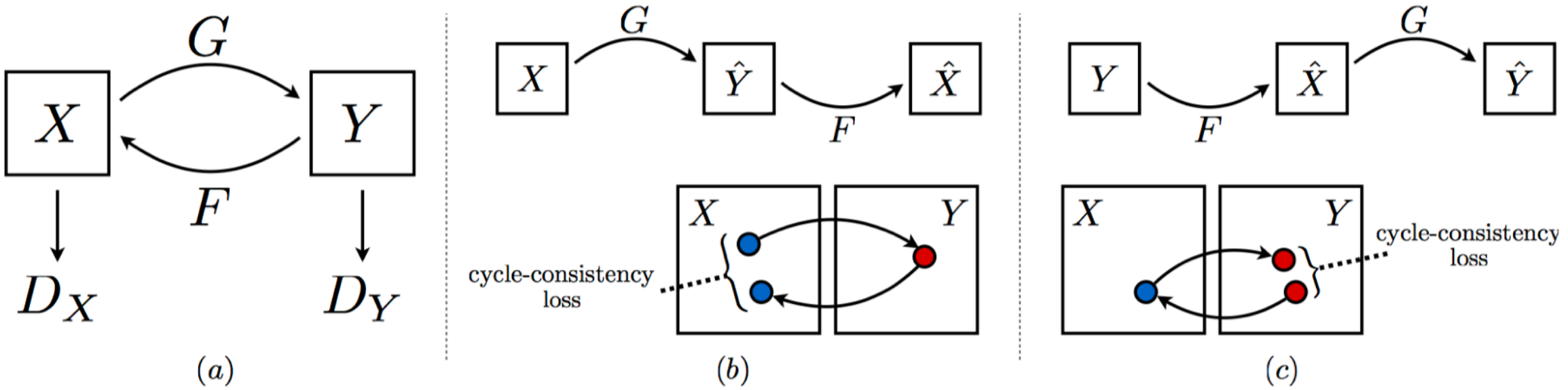
- Cycle-consistency Loss



https://arxiv.org/abs/1703.10593

Star-GAN

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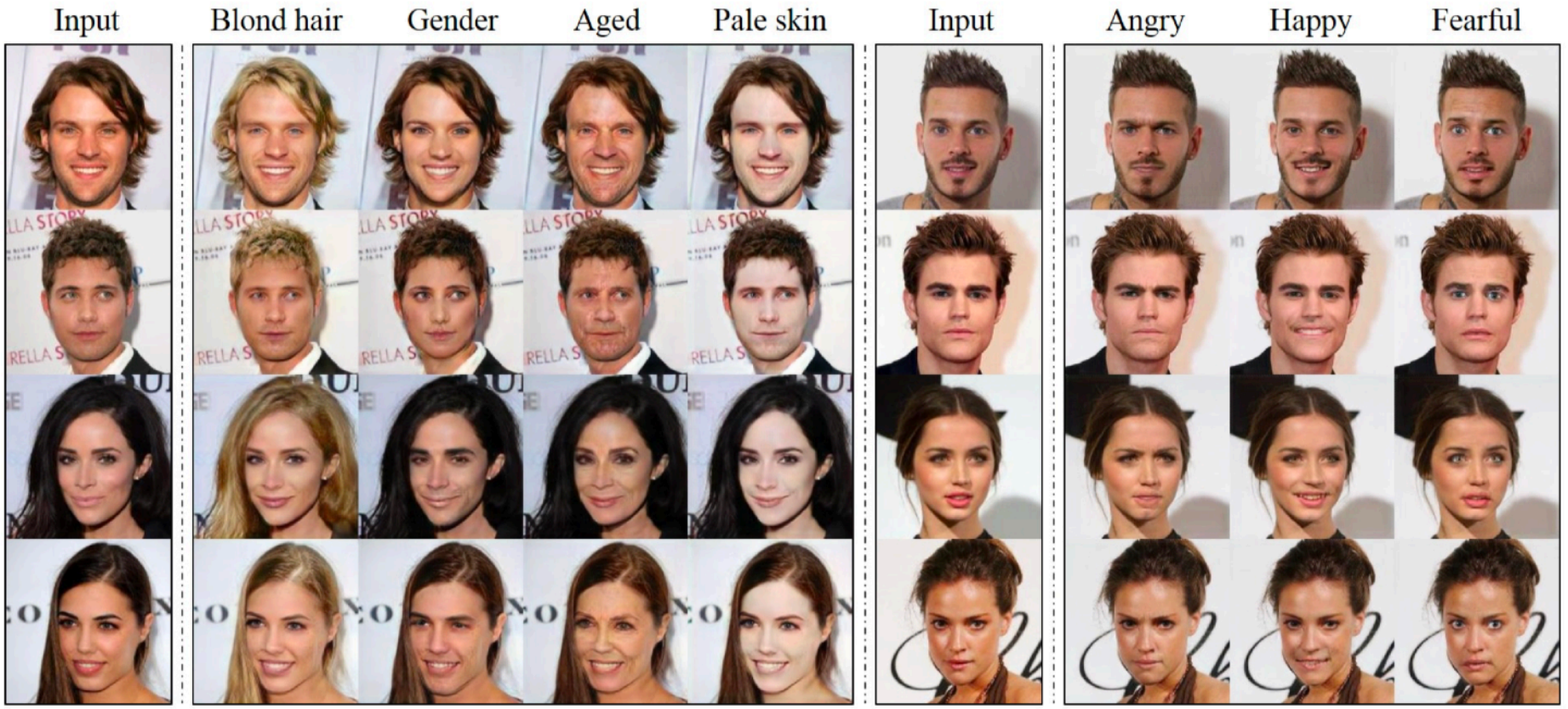

https://arxiv.org/abs/1711.09020

Progressive-GAN

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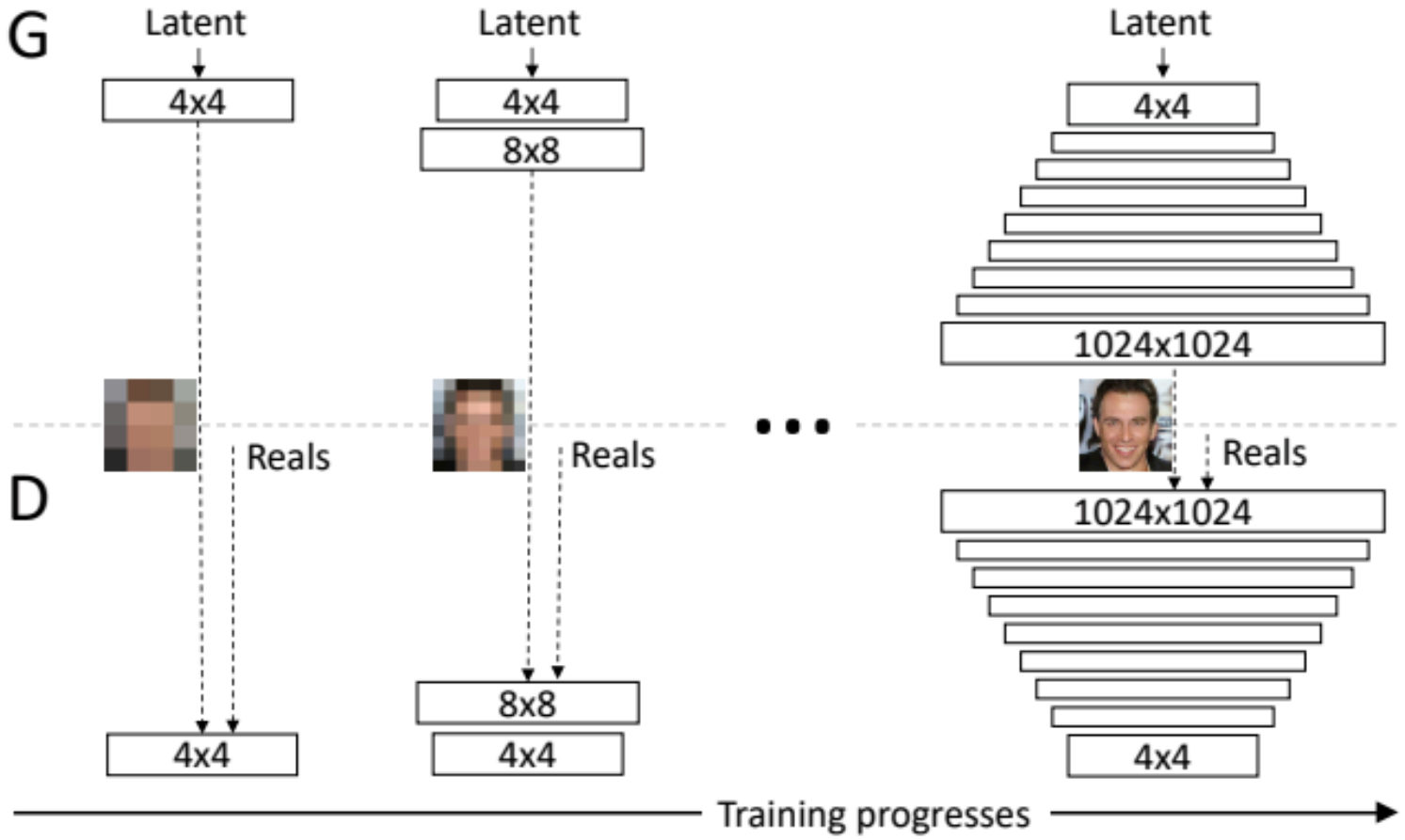
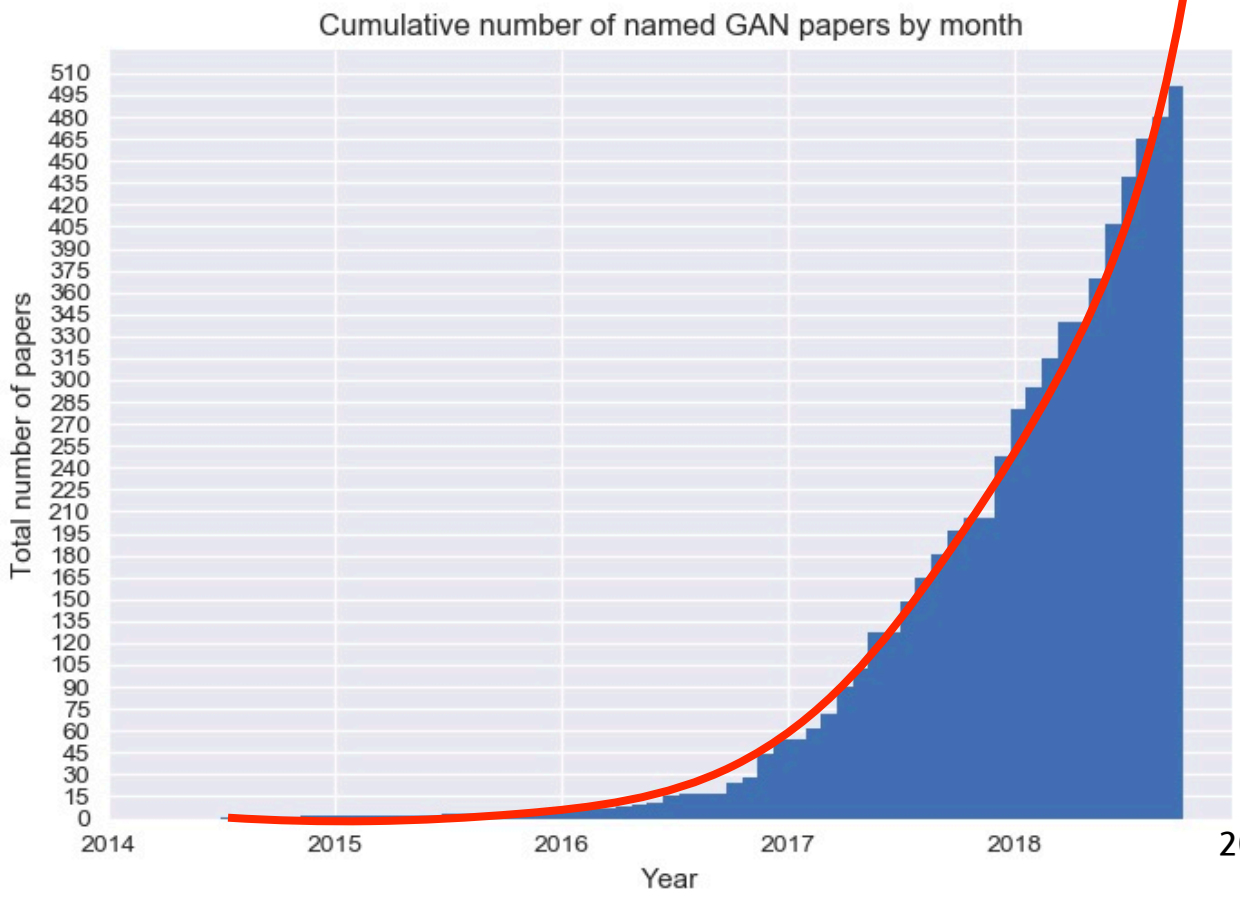
https://arxiv.org/abs/1710.10196

Progressive-GAN



https://arxiv.org/abs/1710.10196

and WAY MORE



2019 2019 2019 2021

?

https://github.com/hindupuravinash/the-gan-zoo

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Normalizing Flow

Normalizing Flow

- Limitations of existing work
  - Autoregressive models provide tractable likelihood but no direct mechanisms for learning features
  - Variational autoencoders can learn feature representations (via latent variables z) but have intractable marginal likelihoods.
- Key question
  - Can we design a latent variable model with tractable likelihoods?
- Desirable properties of any model distribution:
  - Analytic density (explicit model)
  - Easy-to-sample
- Key idea
  - Map simple distributions (easy to sample and evaluate densities) to complex distributions (learned via data) using **change of variables**.

Normalizing Flow

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- Change of Variables Formula
  - Let Z be a uniform random variable $\mathcal{U}[0,2]$ with density p_Z. What is $p_Z(1)$?

Normalizing Flow

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- Change of Variables Formula
  - Let Z be a uniform random variable $\mathcal{U}[0,2]$ with density p_Z. What is $p_Z(1)$?
    - The answer is $\frac{1}{2}$.
  - Let $X = 4Z$ and let p_X be its density. What is $p_X(4)$?

Normalizing Flow

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  - Let Z be a uniform random variable $\mathcal{U}[0,2]$ with density p_Z. What is $p_Z(1)$?
    - The answer is $\frac{1}{2}$.
  - Let $X = 4Z$ and let p_X be its density. What is $p_X(4)$?
    - $p_X(4) = P(X = 4) = P(4Z = 4) = P(Z = 1) = p_Z(1) = 1/2$?

Normalizing Flow

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- Change of Variables Formula
  - Let Z be a uniform random variable $\mathcal{U}[0,2]$ with density p_Z. What is $p_Z(1)$?
    - The answer is $\frac{1}{2}$.
  - Let $X = 4Z$ and let p_X be its density. What is $p_X(4)$?
    - $p_X(4) = P(X = 4) = P(4Z = 4) = P(Z = 1) = p_Z(1) = 1/2$?
    - Unfortunately **Not**.
    - Clearly, X is uniform in $[0,8]$, so $p_X(4) = 1/8$.

Normalizing Flow

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- **Change of variables (1D case)**
  - If $X = f(Z)$ and $f(\cdot)$ is monotone with inverse $Z = f^{-1}(X) = h(X)$, then

$$p_X(x) = p_Z(h(x))\,|h'(x)|$$

- Previous example
  - If $X = 4Z$ and $Z \sim \mathcal{U}[0,2]$, what is $p_X(4)$?
  - Note that $h(X) = X/4$ and $h'(X) = 1/4$.
  - Then, $p_X(4) = p_Z(1)h'(4) = 1/2 \times 1/4 = 1/8$.

Normalizing Flow

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- **Generalized change of variables**
  - The mapping between Z and X, given by $f : \mathbb{R}^n \to \mathbb{R}^n$, is invertible such that $X = f(Z)$ and $Z = f^{-1}(X)$.

$$p_X(x) = p_Z\left(f^{-1}(x)\right) \left| \det \left(\frac{\partial f^{-1}(x)}{\partial x} \right) \right|$$

  - Note 1: x and z need to be continuous and have the same dimension. For example, if $x \in \mathbb{R}^n$ then $z \in \mathbb{R}^n$.
  - Note 2: For any invertible matrix A, $\det(A^{-1}) = \det(A)^{-1}$, then

$$p_X(x) = p_Z(z) \left| \det \left(\frac{\partial f(z)}{\partial z} \right) \right|^{-1}$$

Normalizing Flow

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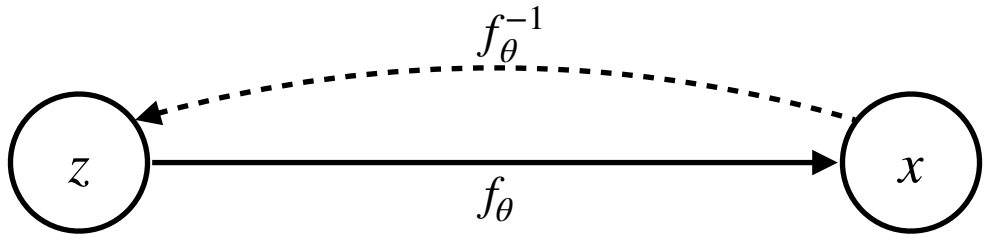
- Normalizing flow models
  - Consider a directed, latent-variable model over observed variables X and latent variables Z.
  - In a **normalizing flow model**, the mapping between Z and X, given by $f_\theta : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is deterministic and invertible such that $X = f_\theta(Z)$ and $Z = f_\theta^{-1}(X)$



  - Using change of variables, the marginal likelihood $p(x)$ is given by

$$p_X(x;\theta) = p_Z\left(f_\theta^{-1}(x)\right)\left|\det\left(\frac{\partial f_\theta^{-1}(x)}{\partial x}\right)\right|$$

Normalizing Flow

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- Normalizing flow models
  - **Normalizing**: Change of variables gives a normalized density after applying an invertible transformation
  - **Flow**: Invertible transformations can be composed with each other

$$z_m \equiv f_\theta^m \circ \cdots \circ f_\theta^1(z_0) = f_\theta^m(f_\theta^{m-1}(\cdots(f_\theta^1(z_0)))) \equiv f_\theta(z_0)$$

  - Start with a simple distribution for z_0 (e.g., Gaussian)
  - Apply a sequence of M invertible transformations $x \equiv z_M$
  - By change of variables

$$p_X(x;\theta) = p_Z\left(f_\theta^{-1}(x)\right)\prod_{m=1}^{M}\left|\det\left(\frac{\partial(f_\theta^m)^{-1}(z_m)}{\partial z_m}\right)\right|$$

(Note: determinant of product equals product of determinants)

Planar flows

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- **Planar flow**
- Invertible transformation

$$\mathbf{x} = f_\theta(\mathbf{z}) = \mathbf{z} + \mathbf{u}h(\mathbf{w}^T\mathbf{z} + b)$$

parametrized by $\theta = (\mathbf{w}, \mathbf{u}, b)$ where $h(\cdot)$ is a non-linearity.

- Absolute value of the determinant of the Jacobian is given by

$$\left|\det \frac{\partial f_\theta(\mathbf{z})}{\partial \mathbf{z}}\right| = \left|\det\left(I + h'(\mathbf{w}^T\mathbf{z} + b)\mathbf{u}\mathbf{w}^T\right)\right| = \left|1 + h'(\mathbf{w}^T\mathbf{z} + b)\mathbf{u}^T\mathbf{w}\right|$$

(matrix determinant lemma)

Planar flows

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- **Learning** via **maximum likelihood** over the dataset $\mathscr{D}$.

$$\max_{\theta} \log p_X(\mathscr{D};\theta) = \sum_{x\in\mathscr{D}} \log p_Z\left(f_\theta^{-1}(x)\right) + \log \left| \det\left(\frac{\partial f_\theta^{-1}(x)}{\partial x}\right)\right|$$

- **Exact likelihood evaluation** via inverse transform $\mathbf{x} \mapsto \mathbf{z}$ and change of variables formula
- Sampling via forward transformation $\mathbf{z} \mapsto \mathbf{x}$

$$\mathbf{z} \sim p_Z(\mathbf{z}) \quad \mathbf{x} = f_\theta(\mathbf{z})$$

- **Latent representations** inferred via inverse transformation (in inference network required!)

$$\mathbf{z} = f_\theta^{-1}(\mathbf{x})$$

https://arxiv.org/pdf/1505.05770

Thank You