EECE 571F: Deep Learning with Structures

Lecture 8 I: Generative Adversarial Networks

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Outline

- Generative Adversarial Networks (GANs)
  - Zero-sum game & min-max loss
  - Optimal discriminator
  - Global minimum
  - Architectures
  - Results & Challenges
- Variants
  - Wasserstein GANs
  - Progressive GANs
  - Cycle GANs
  - MolGANs

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Generative Adversarial Networks (GANs)

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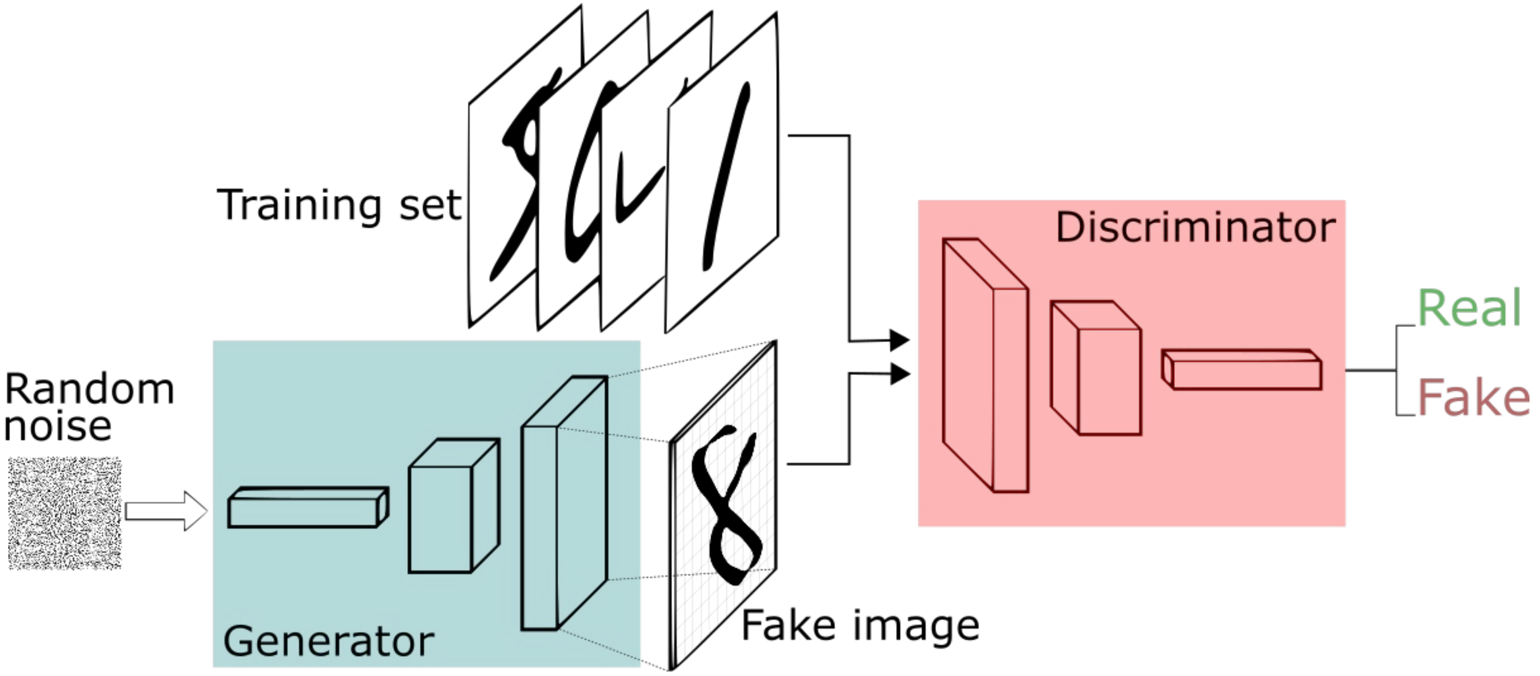

Image Credit: [2]

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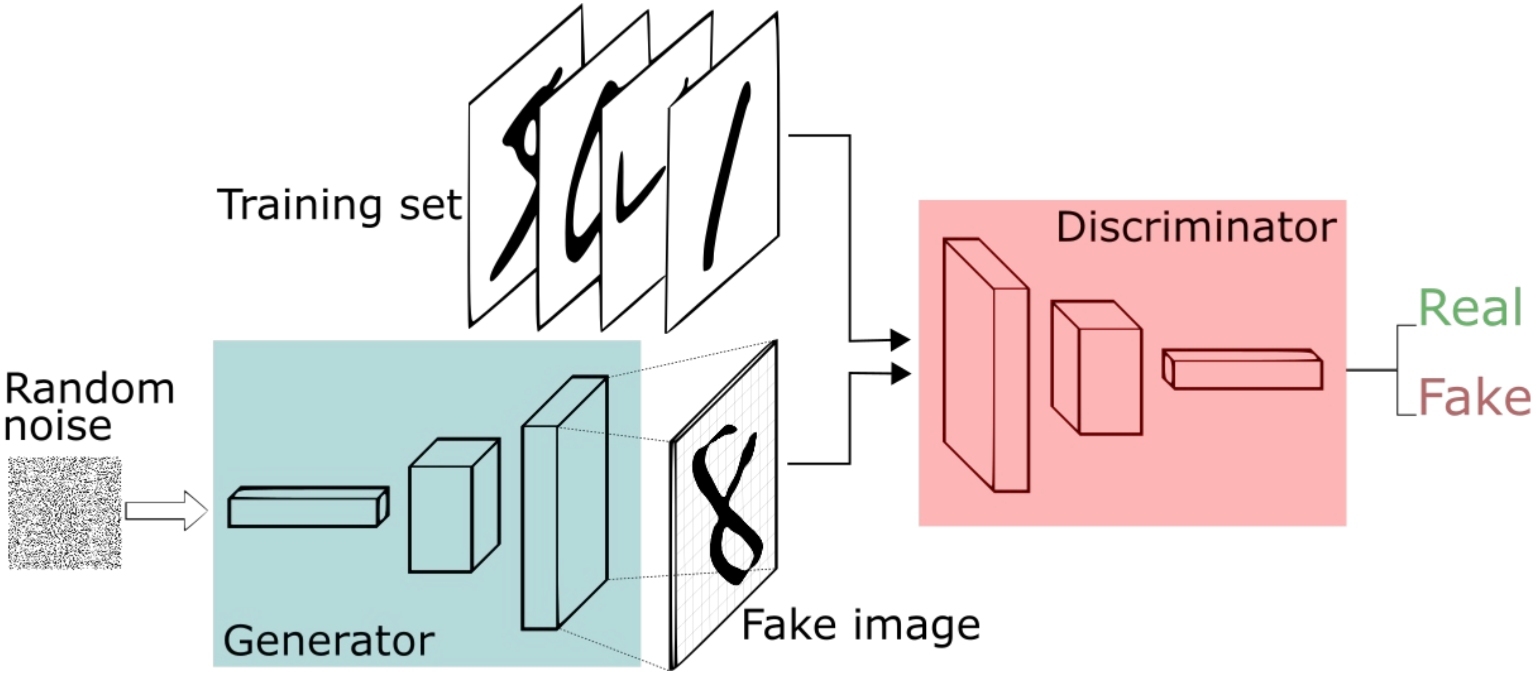

Min-max loss:

$$\min_{\theta} \max_{\phi} \quad \mathbb{E}_{X \sim p_{\text{data}}(X)}[\log D_\phi(X)] + \mathbb{E}_{Z \sim p(Z)}[\log(1 - D_\phi(G_\theta(Z)))]$$

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Optimal Discriminator of GANs

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$$\begin{aligned}
\ell(G_\theta, D_\phi) &= \mathbb{E}_{X \sim p_{\mathrm{data}}(X)}[\log D_\phi(X)] + \mathbb{E}_{Z \sim p(Z)}[\log(1 - D_\phi(G_\theta(Z))] \\
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Law Of The Unconscious Statistician (LOTUS)

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Law Of The Unconscious Statistician (LOTUS)

Set the gradient of loss w.r.t. D to be zero, we obtain the optimal discriminator

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Global Minimum of Min-Max Loss

Suppose we found the optimal discriminator, our loss function becomes

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\begin{aligned}
C(G_\theta) &= \max_{D_\phi} \quad \ell(G_\theta, D_\phi) \\
&= \mathbb{E}_{X \sim p_{\text{data}}(X)} \left[\log D_\phi^*(X)\right] + \mathbb{E}_{X \sim p_{G_\theta}(X)} \left[\log(1 - D_\phi^*(X))\right] \\
&= \mathbb{E}_{X \sim p_{\text{data}}(X)} \left[\log \left(\frac{p_{\text{data}}(X)}{p_{\text{data}}(X) + p_{G_\theta}(X)}\right)\right] + \mathbb{E}_{X \sim p_{G_\theta}(X)} \left[\log \left(\frac{p_{G_\theta}(X)}{p_{\text{data}}(X) + p_{G_\theta}(X)}\right)\right]
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Why?

$$
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C(G_\theta) &= \mathbb{E}_{X \sim p_{\text{data}}(X)} \left[\log \left(\frac{p_{\text{data}}(X)}{(p_{\text{data}}(X) + p_{G_\theta}(X))/2} \right) \right] \\
&\quad + \mathbb{E}_{X \sim p_{G_\theta}(X)} \left[\log \left(\frac{p_{G_\theta}(X)}{(p_{\text{data}}(X) + p_{G_\theta}(X))/2} \right) \right] + 2 \log(\frac{1}{2}) \\
&= \text{JSD}(p_{\text{data}}(X) \| p_{G_\theta}(X)) - \log(4)
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Global Minimum of Min-Max Loss

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Jensen–Shannon divergence (JSD) is in $[0, \log_b 2]$ (base b) and is zero iff. P = Q

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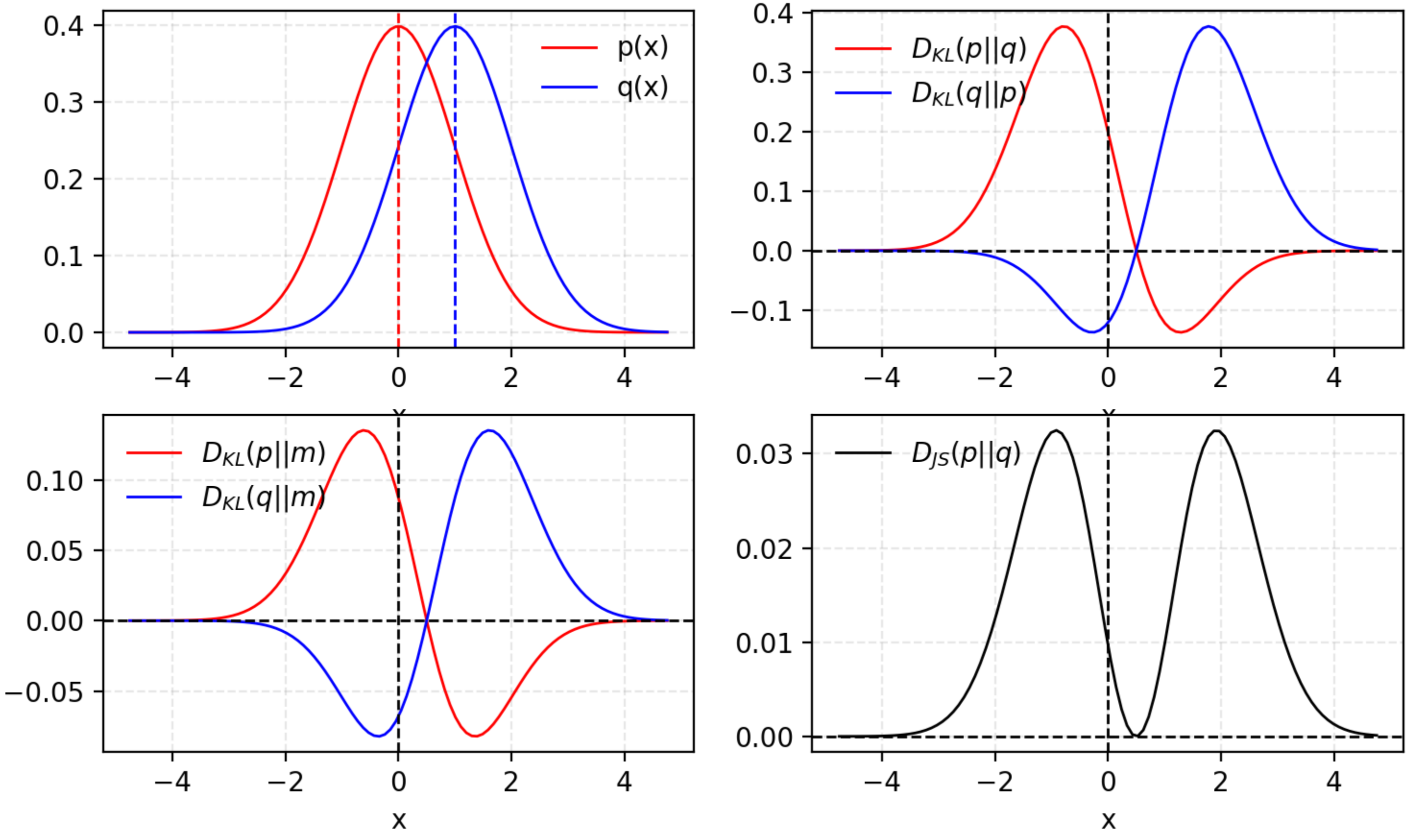

Given two Gaussian distribution, p with mean=0 and std=1 and q with mean=1 and std=1. The average of two distributions is labelled as m. KL divergence is asymmetric but JS divergence is symmetric.

Image Credit: [3]

Global Minimum of Min-Max Loss

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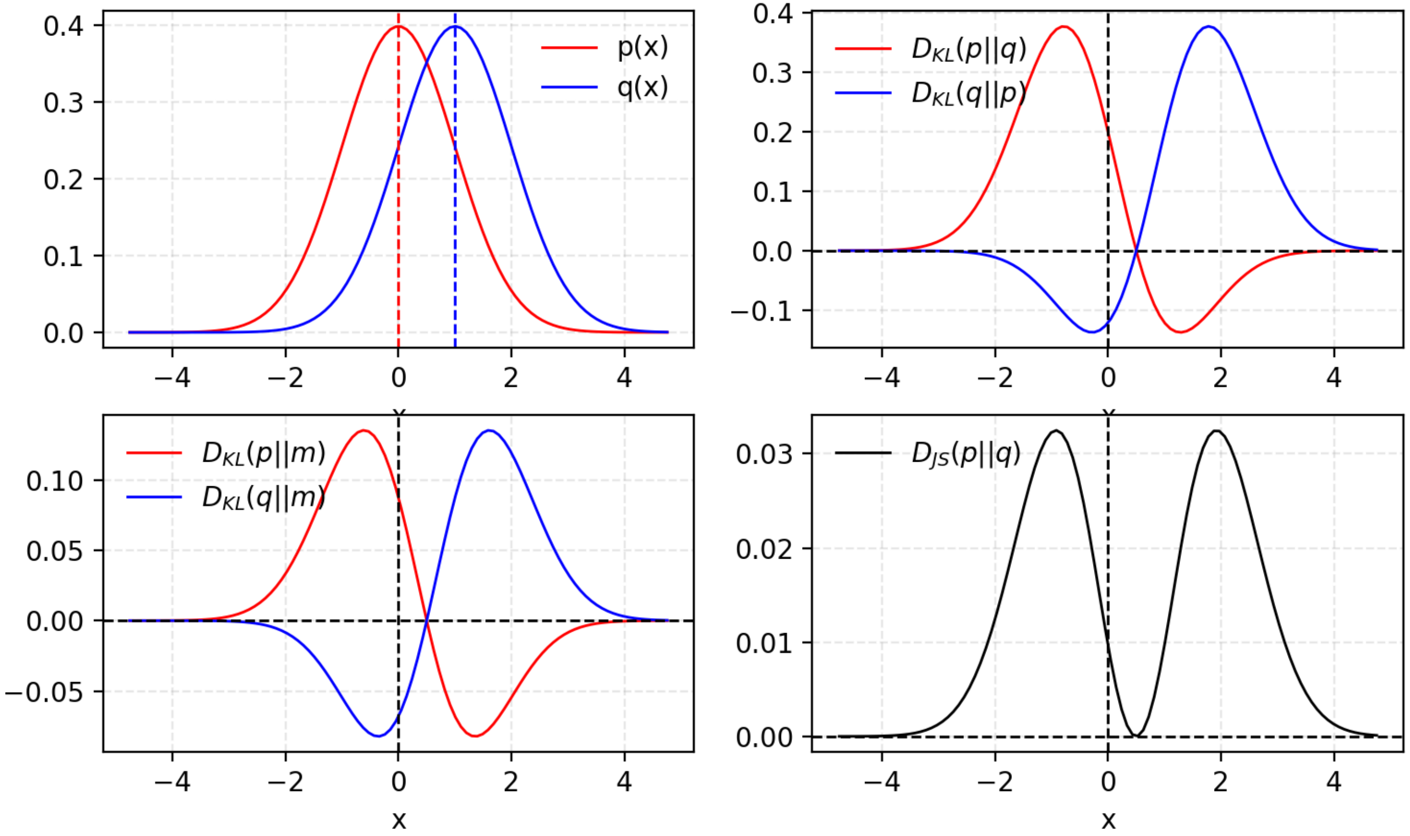

Given two Gaussian distribution, p with mean=0 and std=1 and q with mean=1 and std=1. The average of two distributions is labelled as m. KL divergence is asymmetric but JS divergence is symmetric.

If high density areas of data and model (generator) distributions have less overlap, JSD is not a good objective!

Image Credit: [3]

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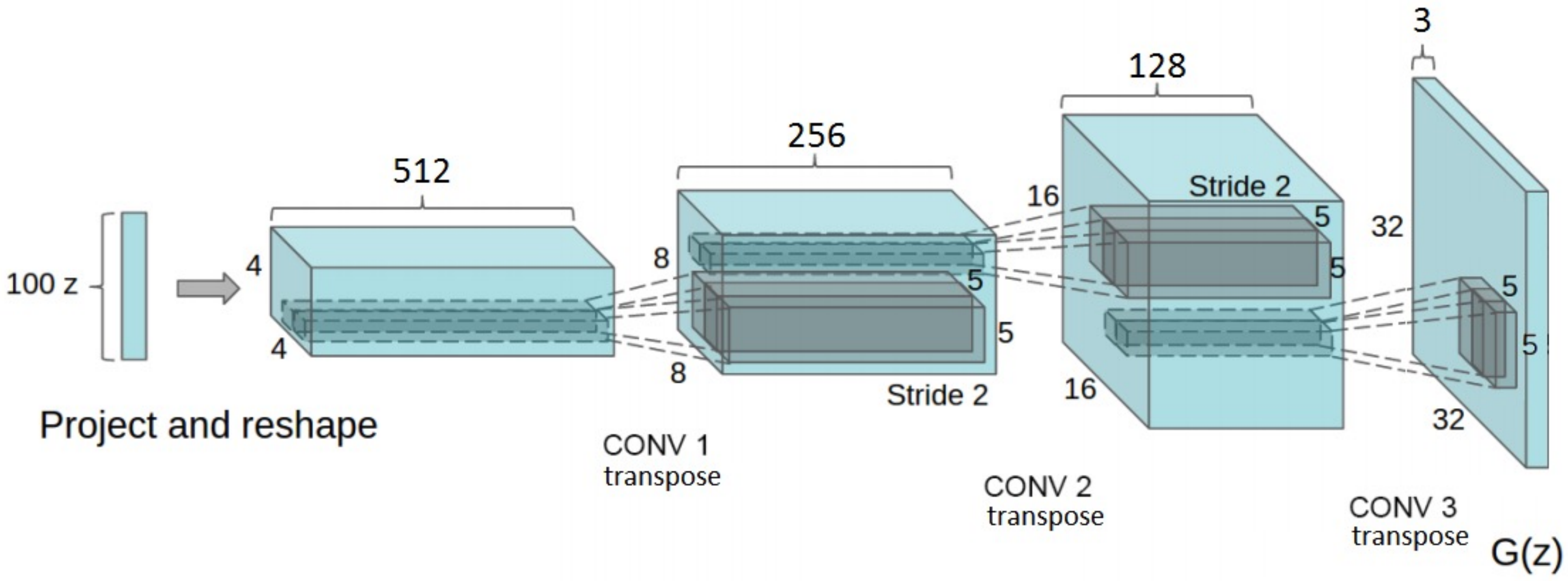
Architectures

Deep Convolutional Generative Adversarial Network (DCGANs) [4] : using CNNs as both Generator and Discriminator.



Generator

Image Credit: [2]

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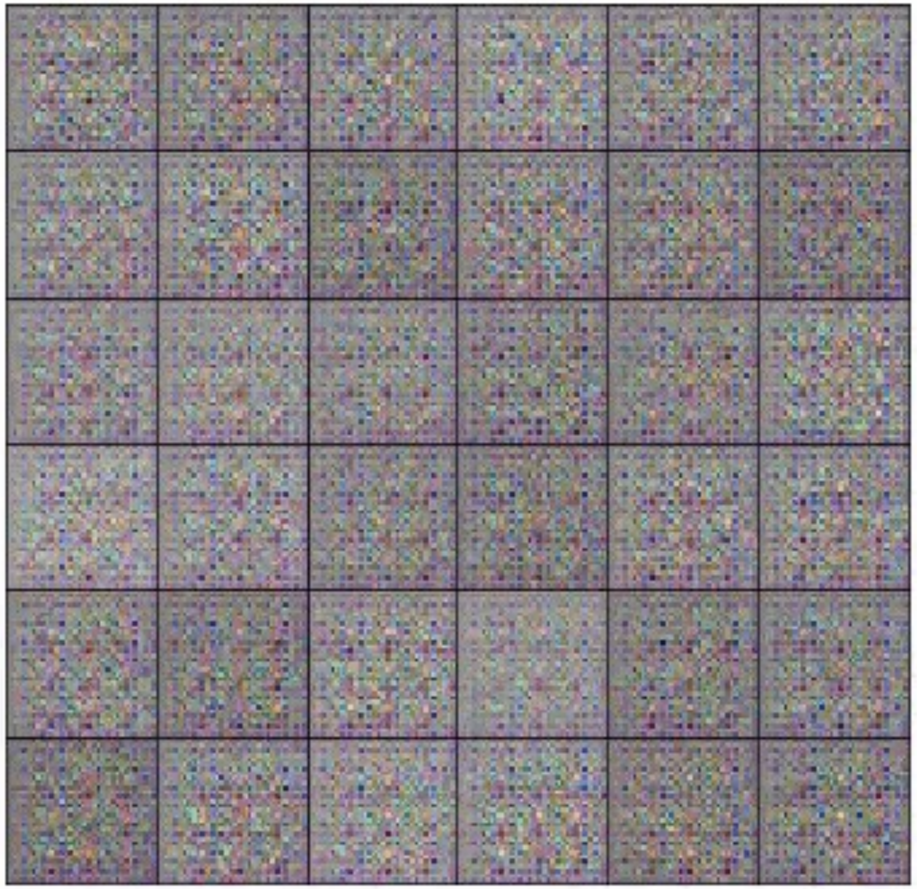
Results

Samples from GANs during training on SVHNs (left) and MNIST (right)



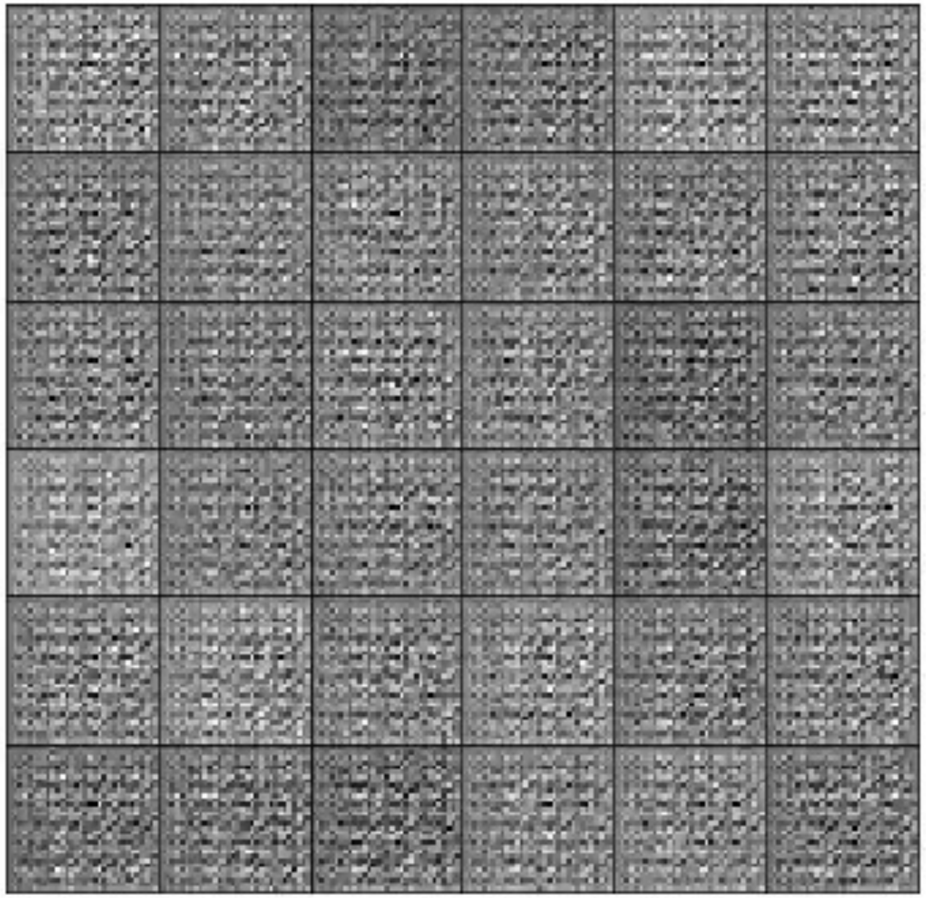
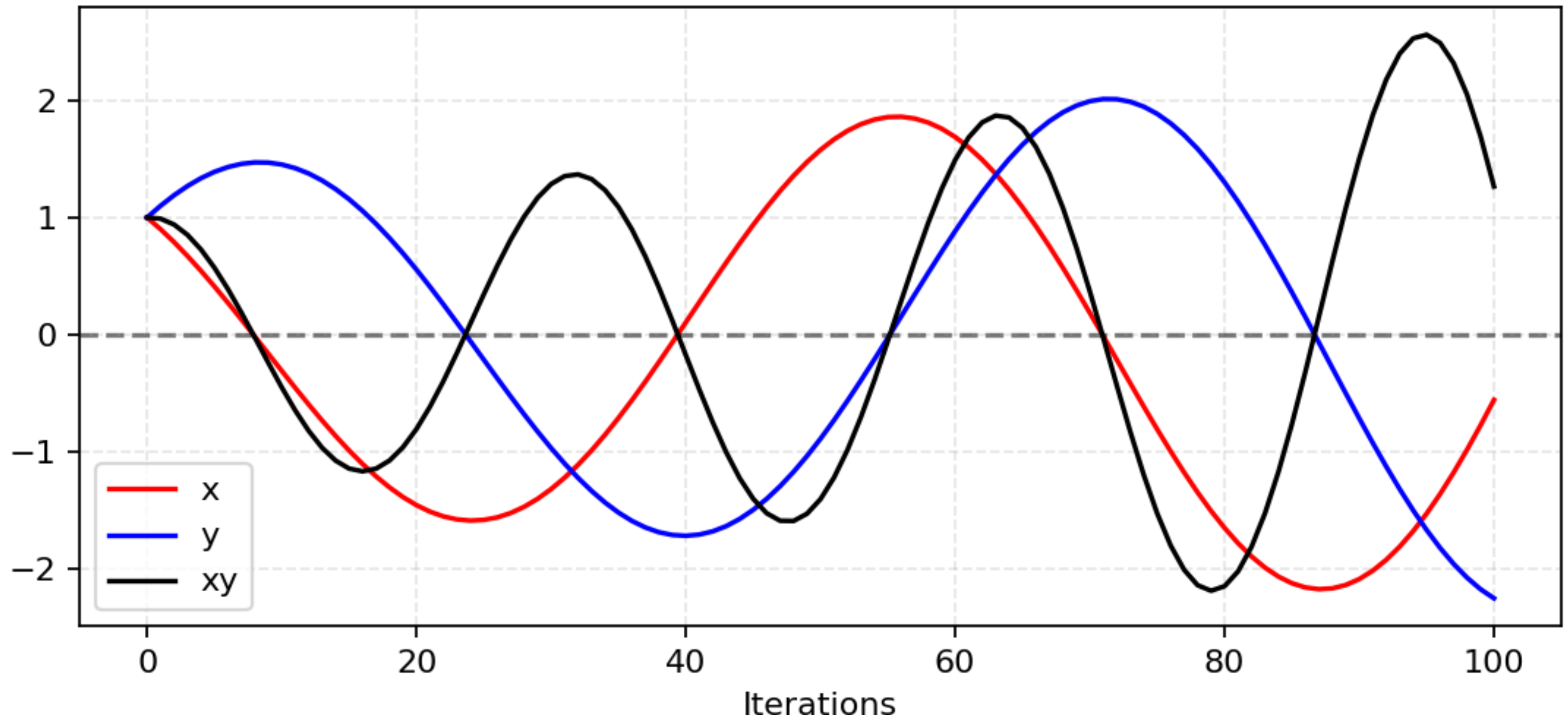


Image Credit: [2]

Challenges in Training GANs

1) ***Training instability***

Hard to reach Nash Equilibrium:



A simulation for updating x to minimize xy and updating y to minimize $-xy$. The learning rate $\eta = 0.1$. With more iterations, the oscillation grows more and more unstable.

Image & Example Credit: [3]

Challenges in Training GANs

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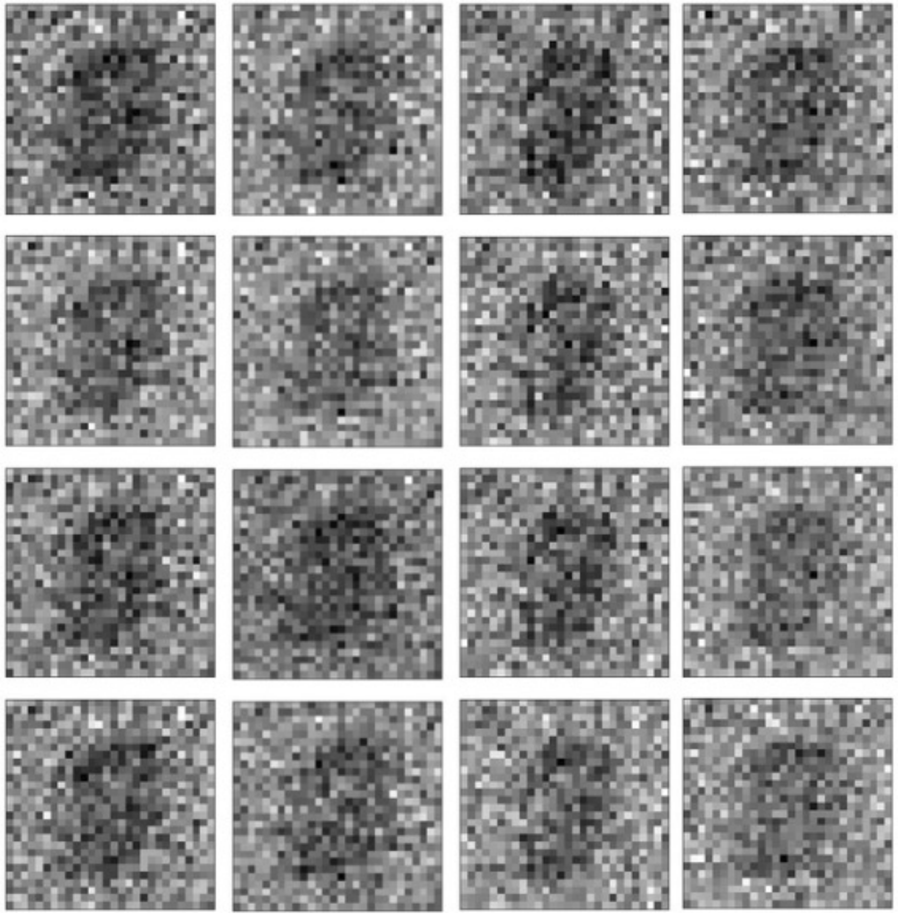


Convergence Failure: e.g., caused by imbalance training of generator and discriminator

Image Credit: [5]

Challenges in Training GANs

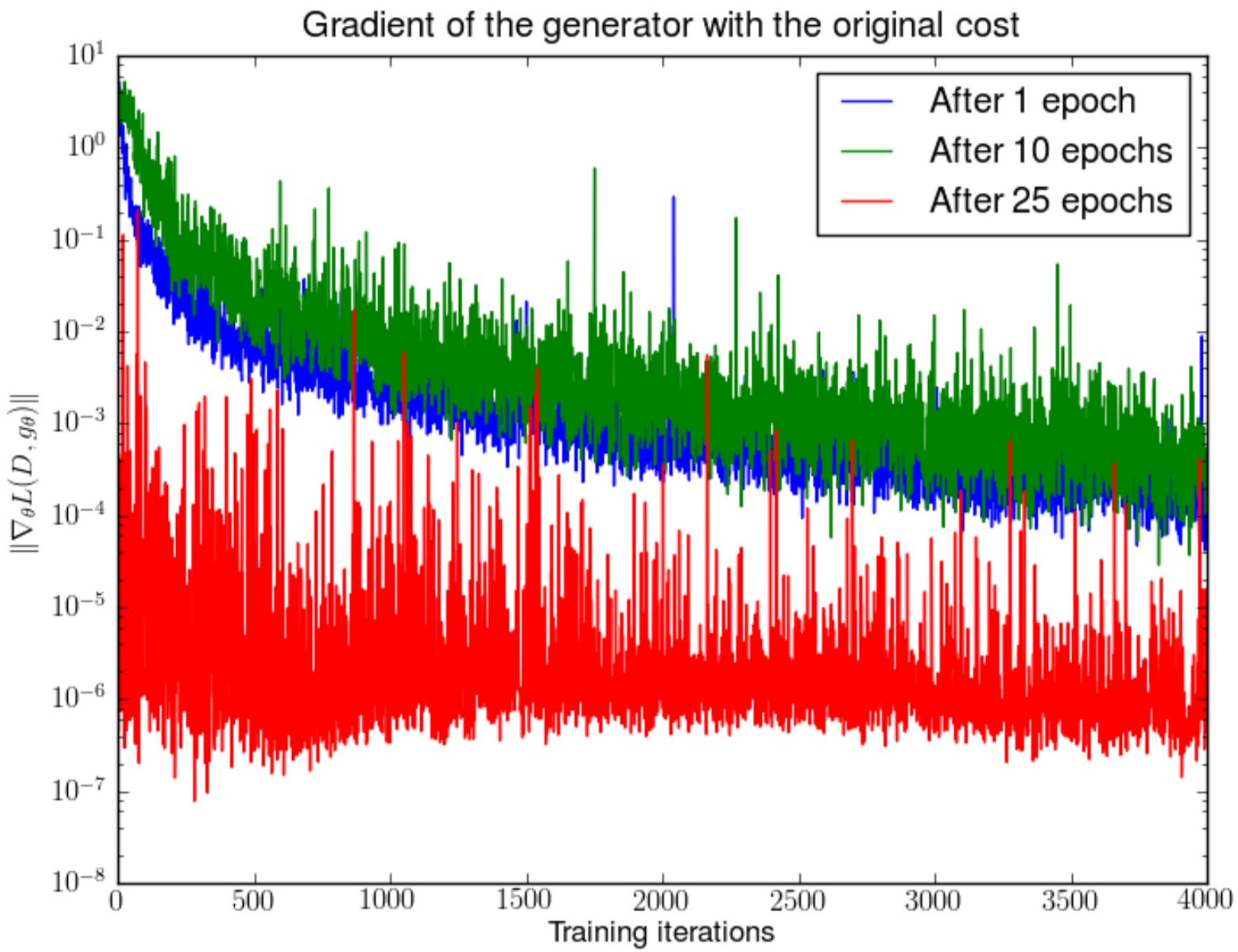
1) *Training instability, 2)* ***Mode collapse***

Mode Collapse: generating samples that are very similar or even identical

Image Credit: [5]

Challenges in Training GANs

1) *Training instability, 2) Mode collapse,* ***3) Vanishing gradient***



First, a DCGAN is trained for 1, 10 and 25 epochs. Then, with **the generator fixed**, a discriminator is trained from scratch and measure the gradients with the original cost function. We see the gradient norms **decay quickly** (in log scale), in the best case 5 orders of magnitude after 4000 discriminator iterations.

Image & Example Credit: [6]

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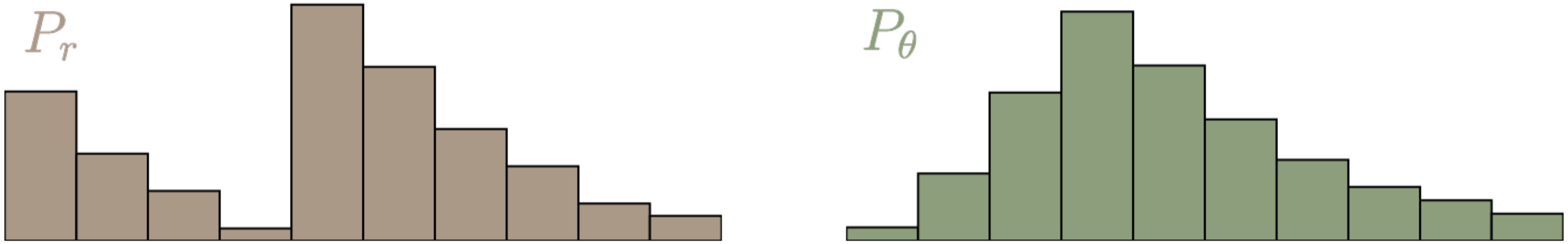
Earth Mover Distance (Wasserstein-1 Distance)

Suppose we have two distributions P_r and P_θ, we want to match them by “moving dirt” from P_r to P_θ.



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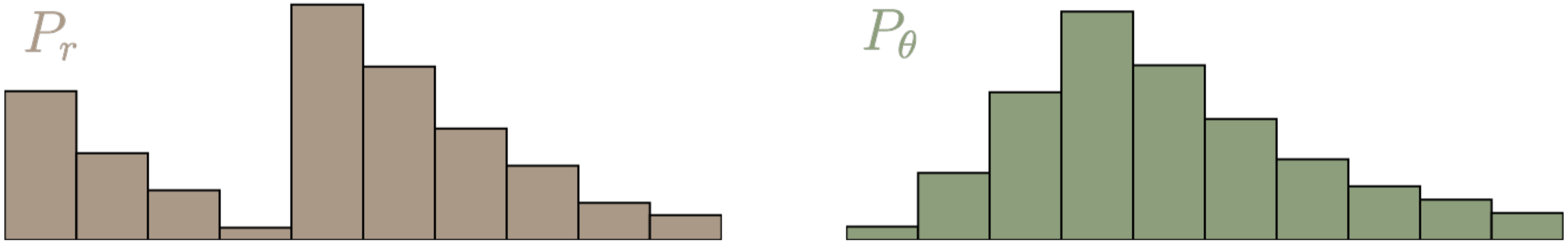
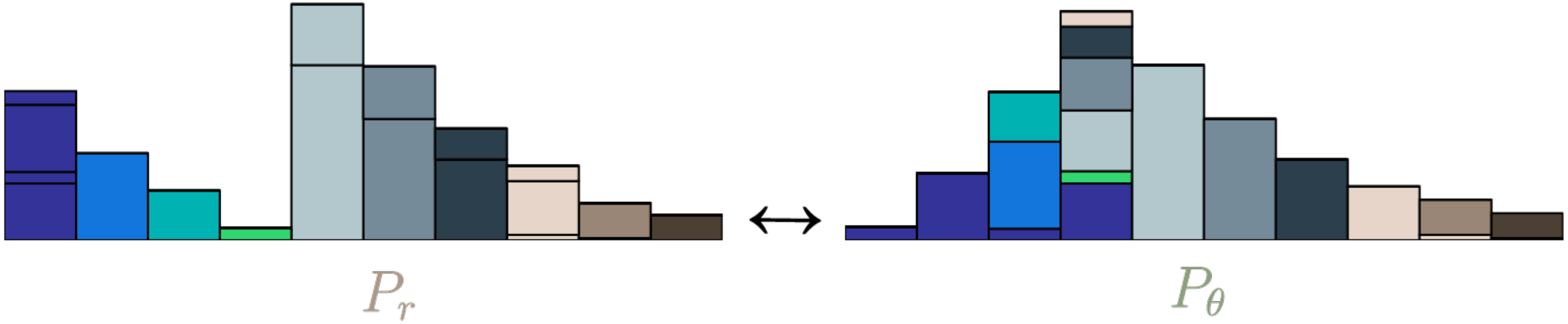


Transportation Plan: we split the "dirt" (probability) and move it to different locations to match them.



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Earth Mover Distance (Wasserstein-1 Distance)

$$\mathrm{EMD}(P_r, P_\theta) = \inf_{\gamma \in \Pi} \sum_{x,y} \|x - y\| \gamma(x, y) = \inf_{\gamma \in \Pi} \mathbb{E}_{(x,y)\sim\gamma} \|x - y\| = \inf_{\gamma \in \Pi} \langle \mathbf{D}, \mathbf{\Gamma} \rangle_{\mathrm{F}}$$

$\prod$ is the set of all distributions whose marginals are P_r, P_θ respectively, called *couplings*.

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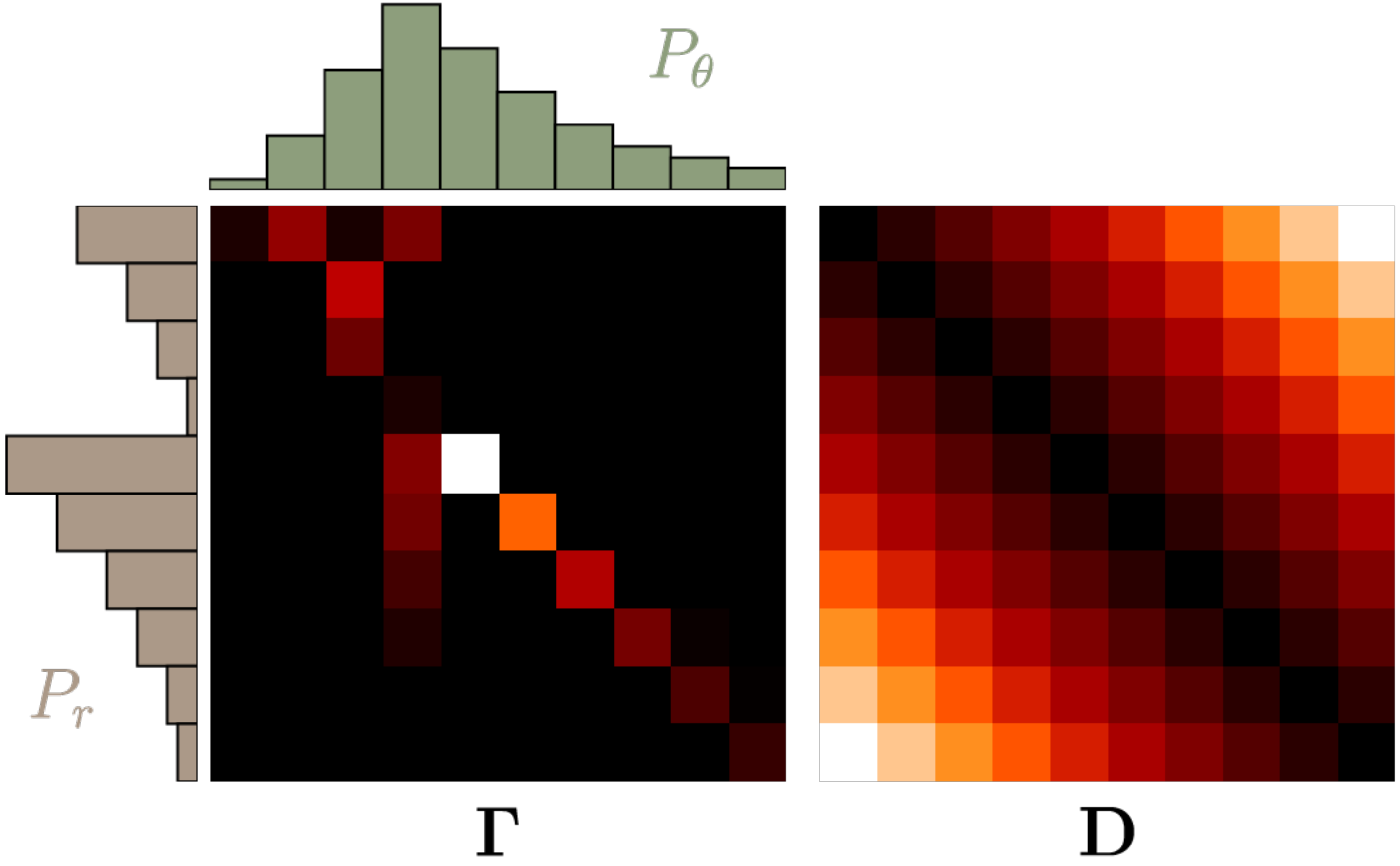

$\mathbf{\Gamma} = \gamma(x,y)$ $\mathbf{D} = \|x - y\|$

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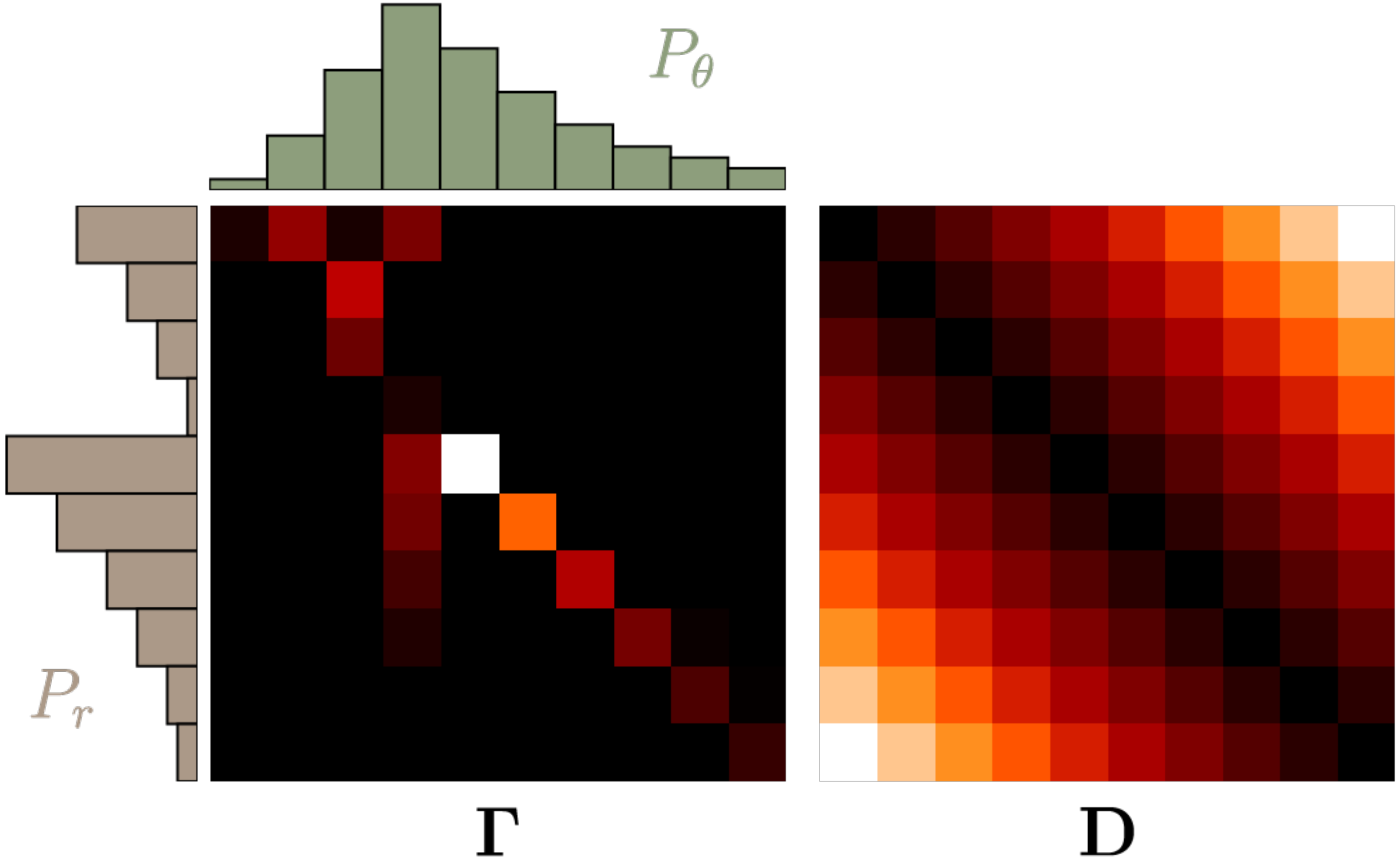

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Transportation Plan

$\mathbf{D} = \|x-y\|$

Cost

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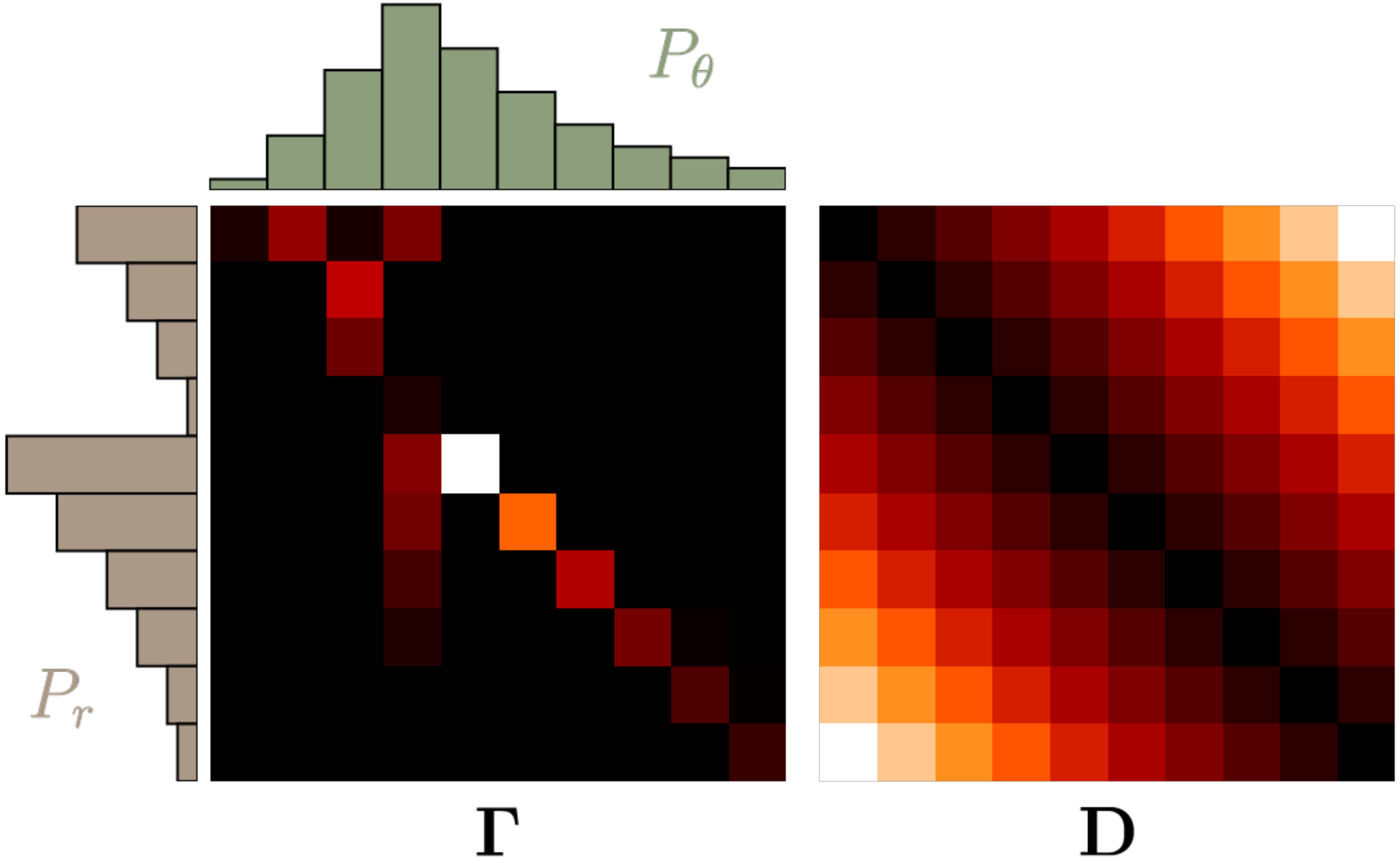

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One can generalize it to Wasserstein-p Distance:

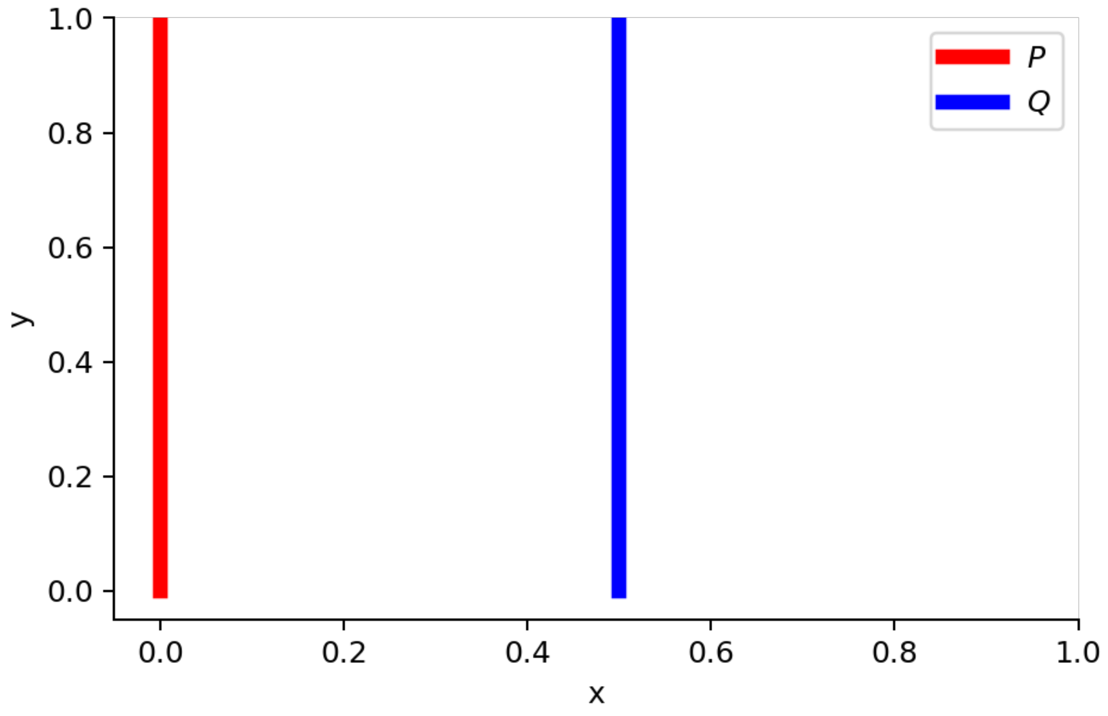
$$W_p(P_r, P_\theta) = \left(\inf_{\gamma \in \Pi} \mathbb{E}_{(x,y)\sim\gamma} d(x, y)^p \right)^{1/p}$$

Image Credit: [7]

Why Wasserstein Distance?

Consider two distributions:

$$\forall (x, y) \in P \quad x = 0, \quad y \sim U(0, 1)$$
$$\forall (x, y) \in Q \quad x = \theta \ (0 \leq \theta \leq 1), \quad y \sim U(0, 1)$$



Example & Image Credit: [3]

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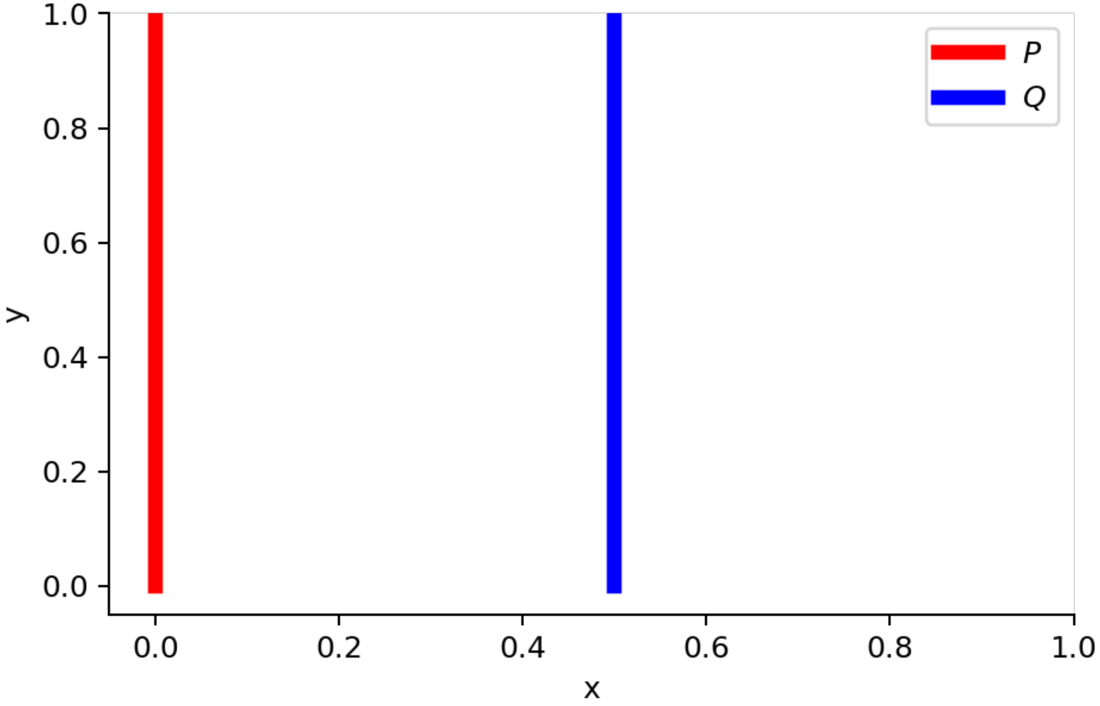

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If $\theta \neq 0$:

$$D_{KL}(P \| Q) = \sum_{\substack{x=0 \\ y \sim U(0,1)}} 1 \cdot \log \frac{1}{0} = +\infty$$

$$D_{KL}(Q \| P) = \sum_{\substack{x=\theta \\ y \sim U(0,1)}} 1 \cdot \log \frac{1}{0} = +\infty$$

$$D_{JS}(P, Q) = \frac{1}{2}\Big(\sum_{\substack{x=0 \\ y \sim U(0,1)}} 1 \cdot \log \frac{1}{1/2} + \sum_{\substack{x=\theta \\ y \sim U(0,1)}} 1 \cdot \log \frac{1}{1/2} \Big) = \log 2$$

$$W(P, Q) = |\theta|$$

Example & Image Credit: [3]

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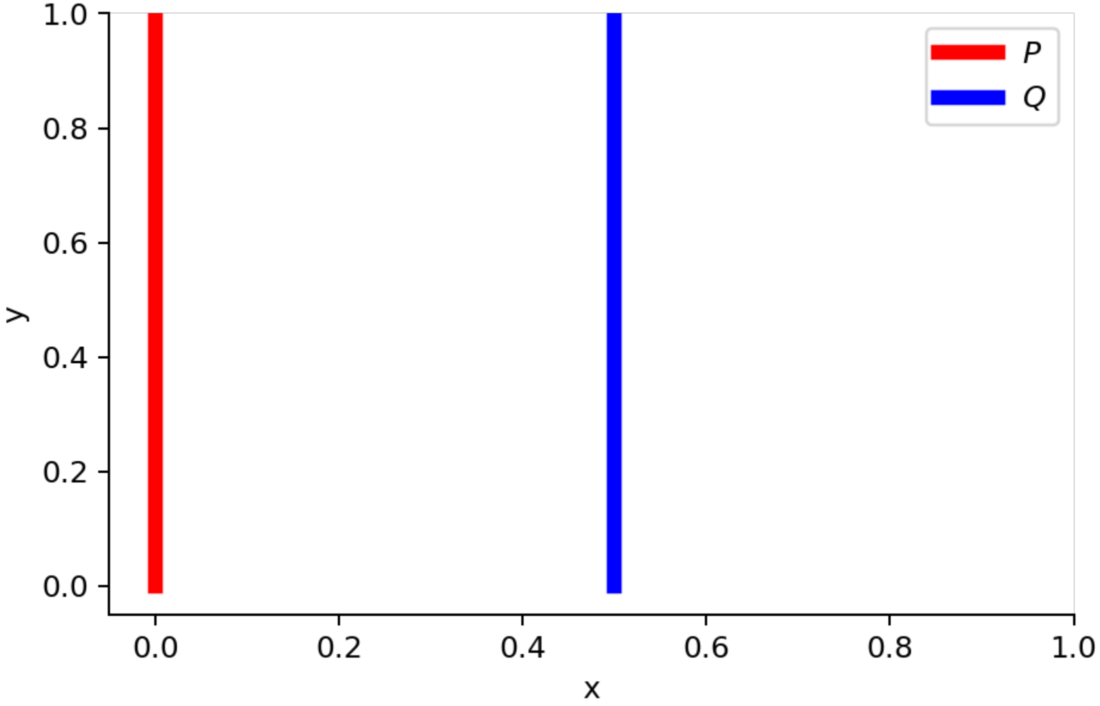

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Else:

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$$W(P,Q) = 0 = |\theta|$$

Example & Image Credit: [3]

Why Wasserstein Distance?

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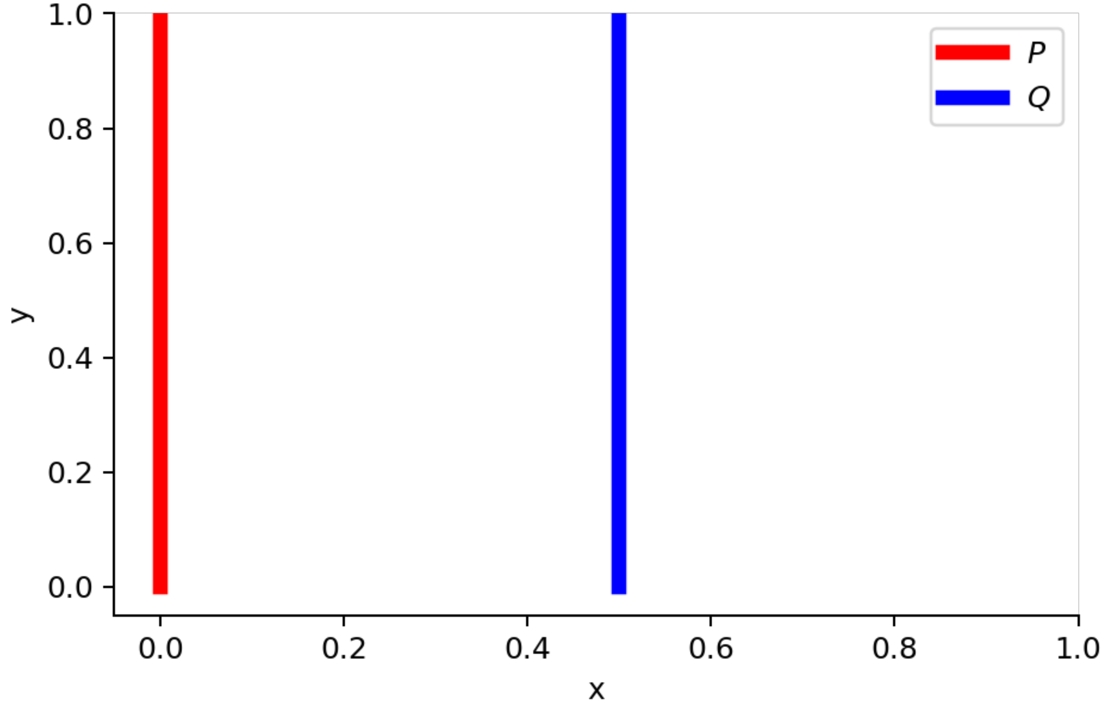

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$$W(P,Q)=|\theta|$$

Else:

$$D_{KL}(P\|Q)=D_{KL}(Q\|P)=D_{JS}(P,Q)=0$$
$$W(P,Q)=0=|\theta|$$

Wasserstein distance is smooth, which is helpful for gradient based learning!

Example & Image Credit: [3]

Wasserstein GANs

Earth Mover Distance / Wasserstein Metric:

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$$= \inf_{\gamma \in \Pi} \langle \mathbf{D}, \mathbf{\Gamma} \rangle_{\mathrm{F}}$$

It is typically hard to compute (need to solve linear programming for discrete distributions)!

Wasserstein GANs

Earth Mover Distance / Wasserstein Metric:

$$\mathrm{EMD}(P_r, P_\theta) = \inf_{\gamma \in \Pi} \sum_{x,y} \|x - y\| \gamma(x, y) = \inf_{\gamma \in \Pi} \mathbb{E}_{(x,y)\sim\gamma} \|x - y\|$$
$$= \inf_{\gamma \in \Pi} \langle \mathbf{D}, \mathbf{\Gamma} \rangle_{\mathrm{F}}$$

It is typically hard to compute (need to solve linear programming for discrete distributions)!

Wasserstein distance (using Kantorovich-Rubinstein duality, see, e.g., [8]):

$$\mathrm{EMD}(P_r, P_\theta) = \sup_{\|f\|_{L \leq 1}} \mathbb{E}_{x \sim P_r} f(x) - \mathbb{E}_{x \sim P_\theta} f(x).$$

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Wasserstein-GAN [8] proposes a unified objective:

Learn Discriminator via $\quad \max_{\phi} \quad \mathbb{E}_{X\sim p_{\mathrm{data}}(X)}[D_\phi(X)] - \mathbb{E}_{\epsilon\sim p(\epsilon)}[D_\phi(G_\theta(\epsilon))]$

Learn Generator via $\quad \min_{\theta} \quad \mathbb{E}_{X\sim p_{\mathrm{data}}(X)}[D_\phi(X)] - \mathbb{E}_{\epsilon\sim p(\epsilon)}[D_\phi(G_\theta(\epsilon))]$

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To enforce Lipschitz condition, one can clip weights [8], add gradient penalty (WGAN-GP) [9], and use spectral normalization [10]

Wasserstein GANs

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

Image Credit: [8]

Wasserstein GANs

Image Credit: [9]

Outline

- Generative Adversarial Networks (GANs)
    - Zero-sum game & min-max loss
    - Optimal discriminator
    - Global minimum
    - Architectures
    - Results & Challenges
- Variants
    - Wasserstein GANs
    - **Progressive GANs**
    - Cycle GANs
    - MolGANs

Progressive GANs

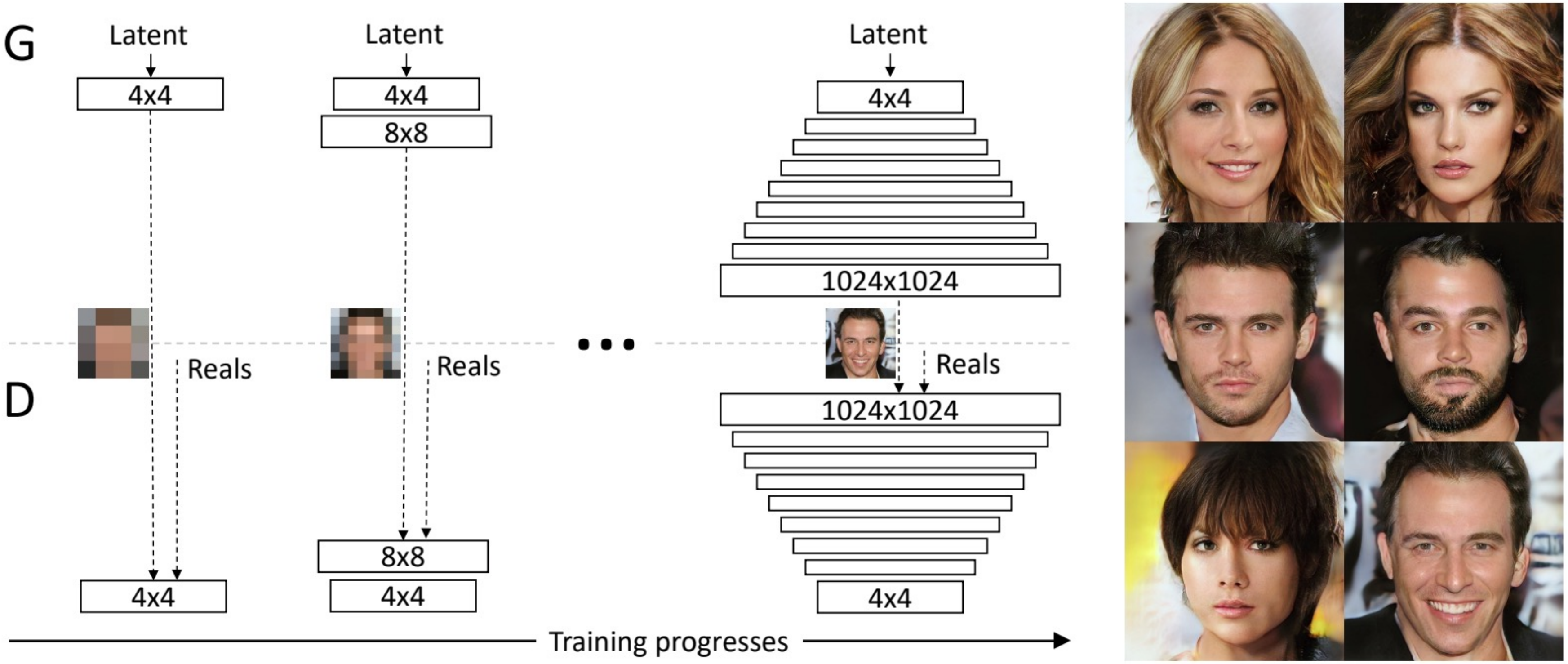

Figure 1: Our training starts with both the generator (G) and discriminator (D) having a low spatial resolution of 4×4 pixels. As the training advances, we incrementally add layers to G and D, thus increasing the spatial resolution of the generated images. All existing layers remain trainable throughout 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.

Image Credit: [11]

Progressive GANs

Figure 5: 1024 × 1024 images generated using the CELEBA-HQ dataset. See Appendix F for a larger set of results, and the accompanying video for latent space interpolations.

Image Credit: [11]

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Cycle GANs

Cycle-Consistent Generative Adversarial Networks [12] learn the image-to-image translation without a training set of aligned image pairs

Image Credit: [13]

Cycle GANs

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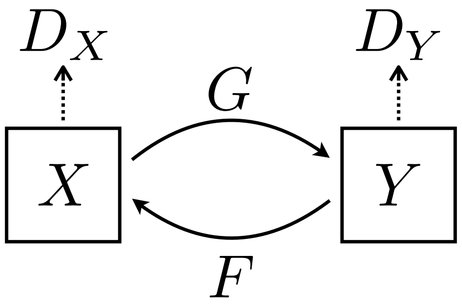

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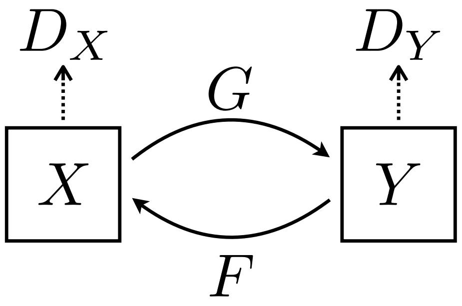

$$\mathcal{L}_{\text{GAN}}(F, D_X, X, Y) = \mathbb{E}_{x \sim p_{\text{data}}(x)}[\log D_X(x)] + \mathbb{E}_{y \sim p_{\text{data}}(y)}[\log(1 - D_X(F(y))]$$

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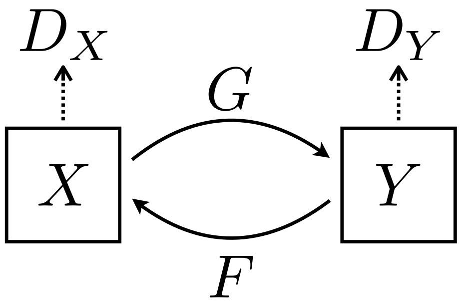

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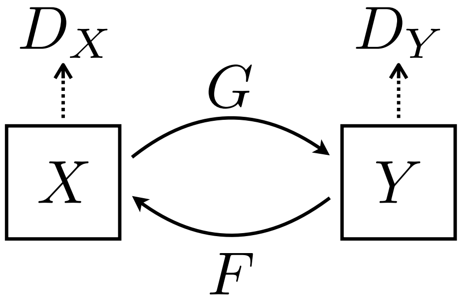

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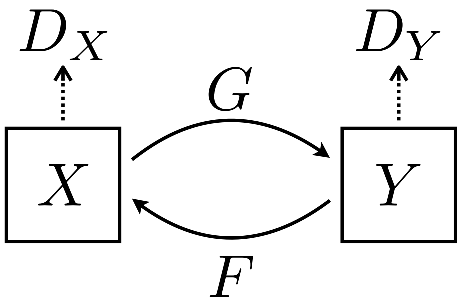

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$$\mathcal{L}(G, F, D_X, D_Y) = \mathcal{L}_{\text{GAN}}(G, D_Y, X, Y) + \mathcal{L}_{\text{GAN}}(F, D_X, Y, X) + \lambda\mathcal{L}_{\text{cyc}}(G, F)$$

Image Credit: [12,13]

Cycle GANs

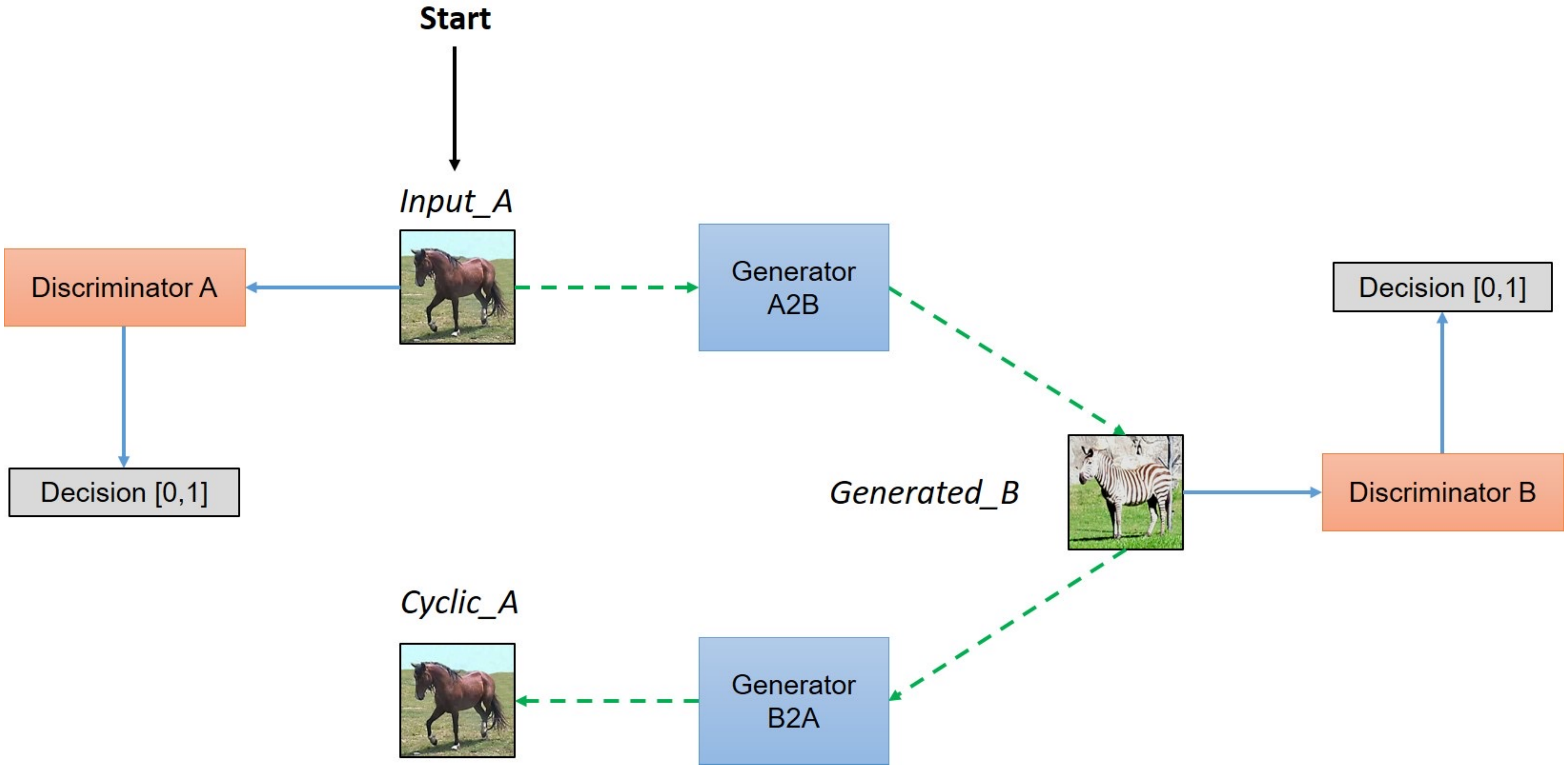


Image Credit: [14]

Cycle GANs

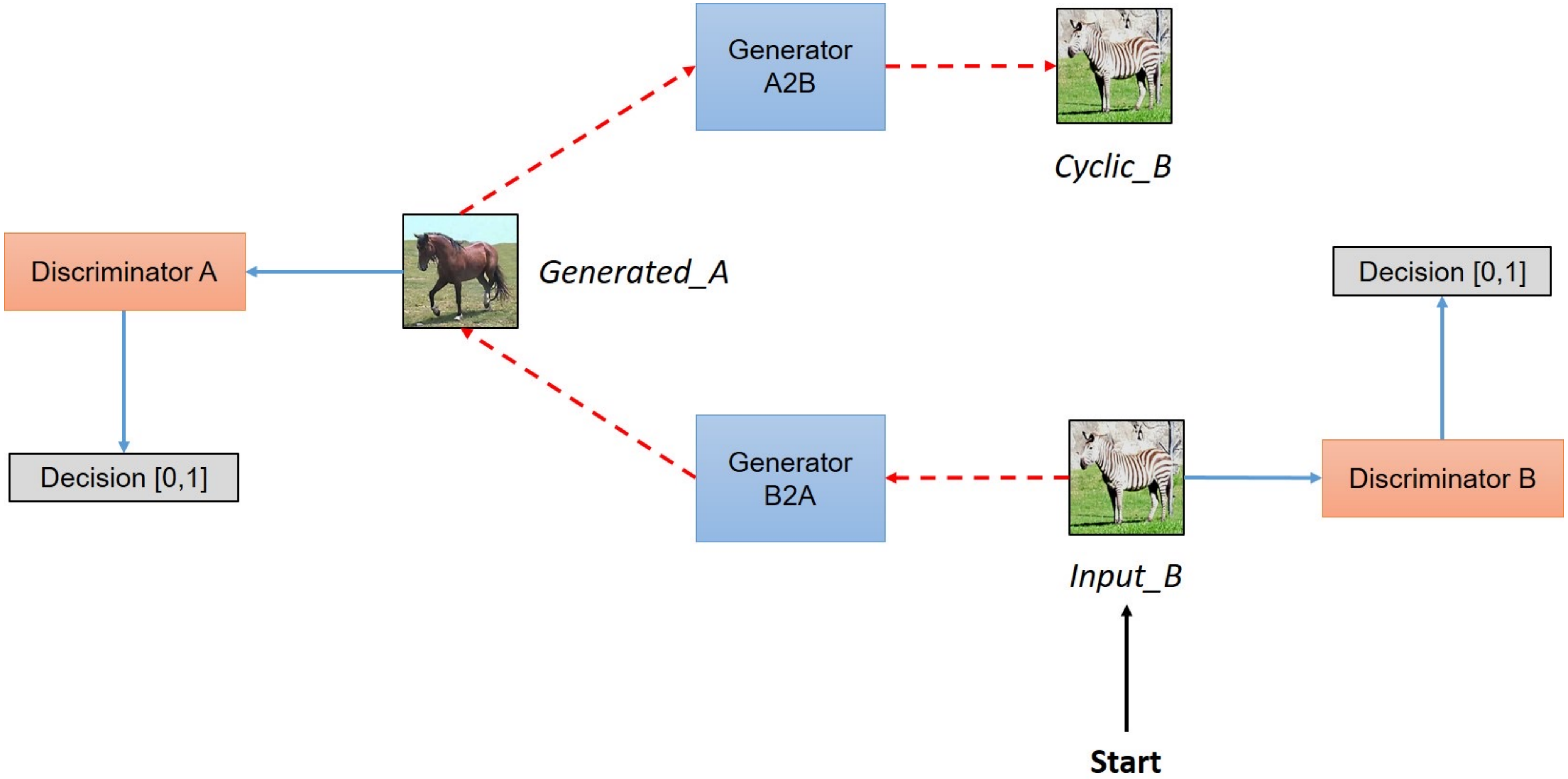
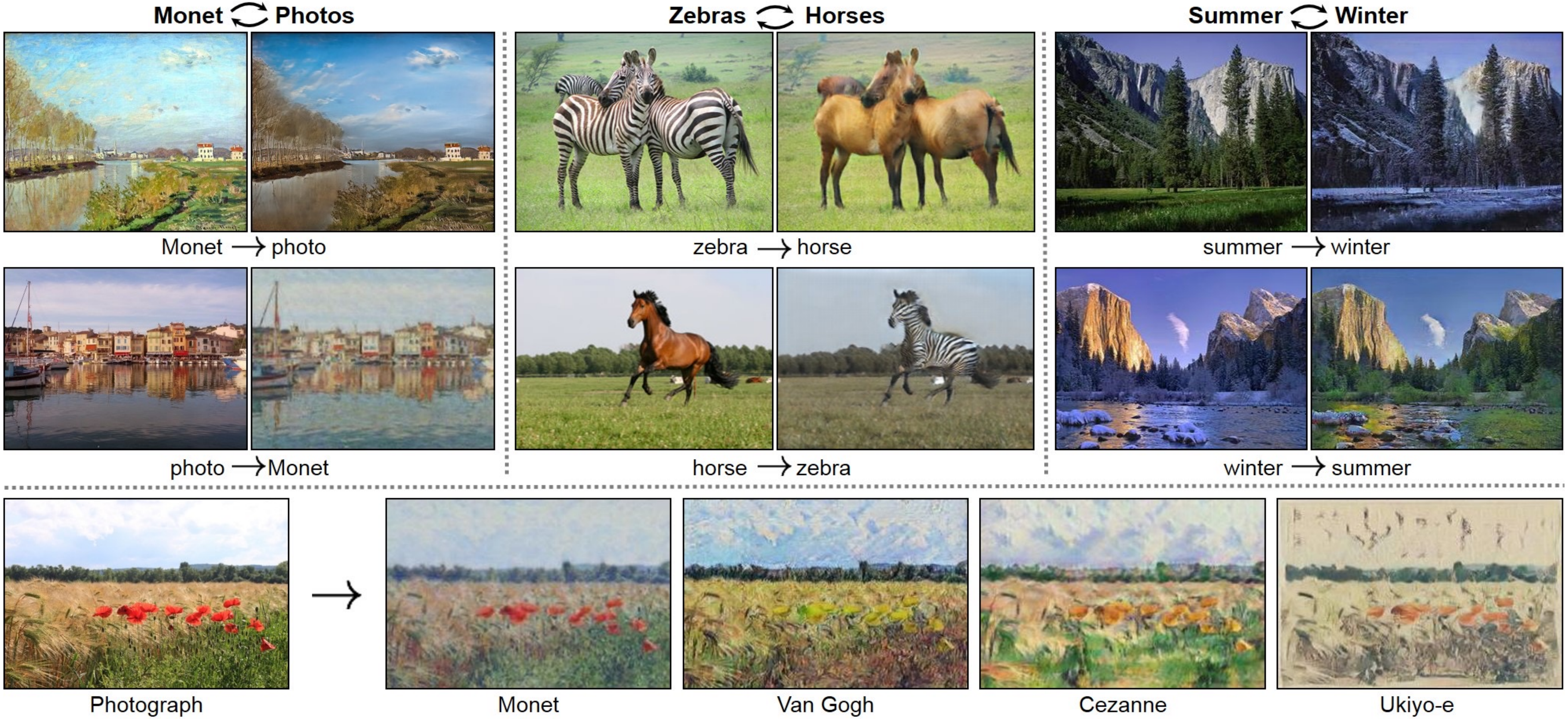


Image Credit: [14]

Cycle GANs



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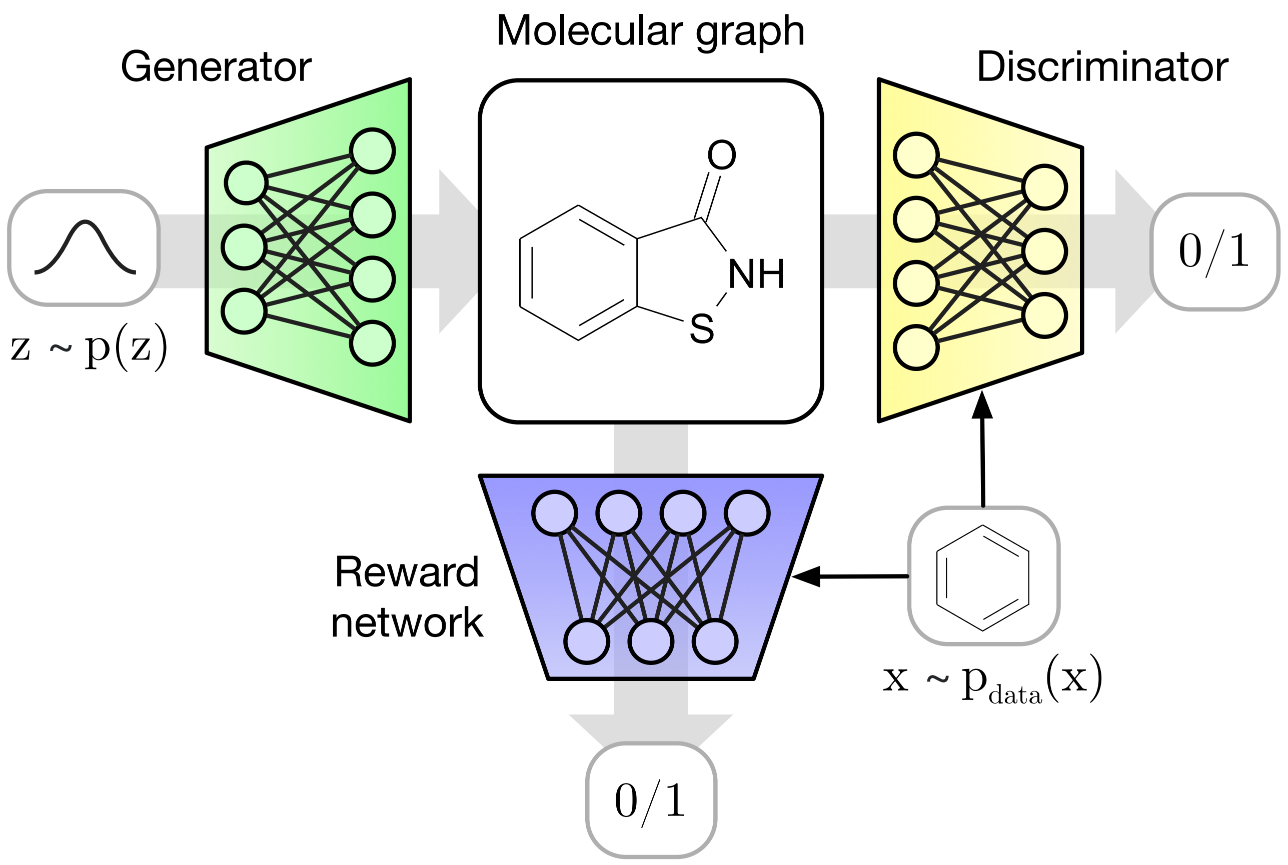
  - **MolGANs**

MolGANs

MolGANs [15] generate molecular graphs without graph matching:



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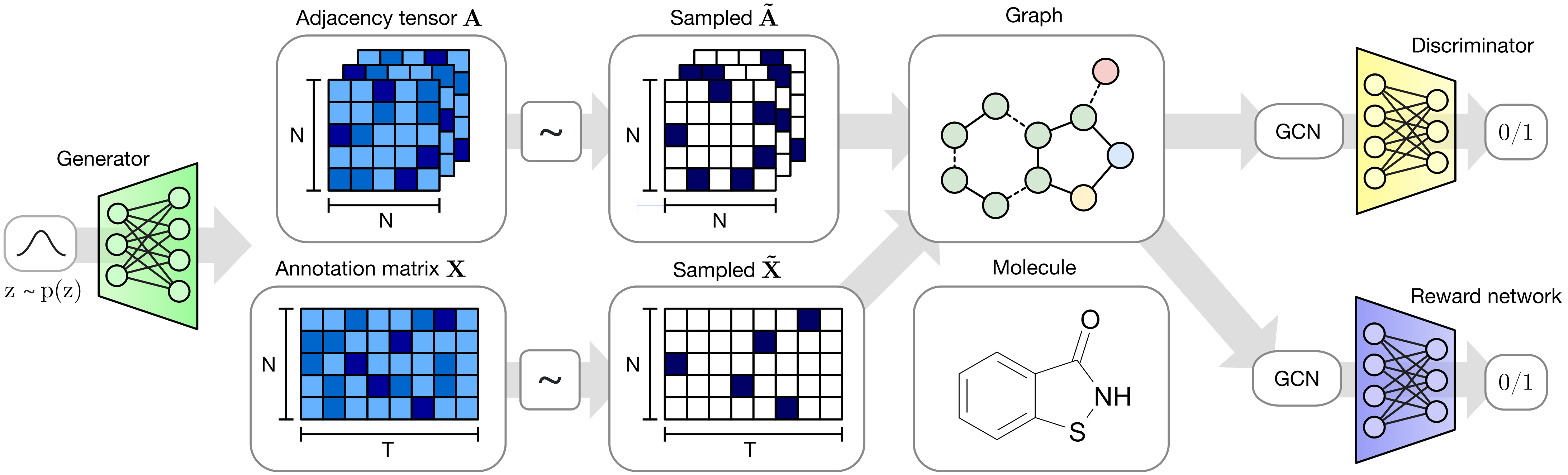

Image Credit: [15]

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Questions?