

# GENERATIVE ADVERSARIAL NETWORKS

## GAN, WGAN AND SIG-WGAN

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# GAN AND WGAN

<b>1</b>	<b>Generative Adversarial Networks</b>	<b>4</b>
1.1	Motivations	4
1.2	Framework	5
1.3	Loss Functions	7
1.4	Training Process	12
1.5	Problems	18
1.6	More about GAN	20
<b>2</b>	<b>Wasserstein Generative Adversarial Networks</b>	<b>22</b>
2.1	Likelihood and KL divergence	22
2.2	Motivation	28
2.3	$W_1$ Distance	29
2.4	WGAN	33
2.5	Comparison	37

# SIG-WGAN

<b>1</b>	<b>Sig-WGAN</b>	<b>40</b>
1.1	Log-signature	40
1.2	Sig- $W_1$ Distance	44
1.3	Logsig-RNN	46
1.4	RNN and LSTM	52
<b>2</b>	<b>References</b>	<b>58</b>

Part I

# GENERATIVE MODELS

# GENERATIVE ADVERSARIAL NETWORKS

## MOTIVATIONS

- ▶ Model-based reinforcement learning
- ▶ Simulate possible futures
- ▶ Generate good examples for training

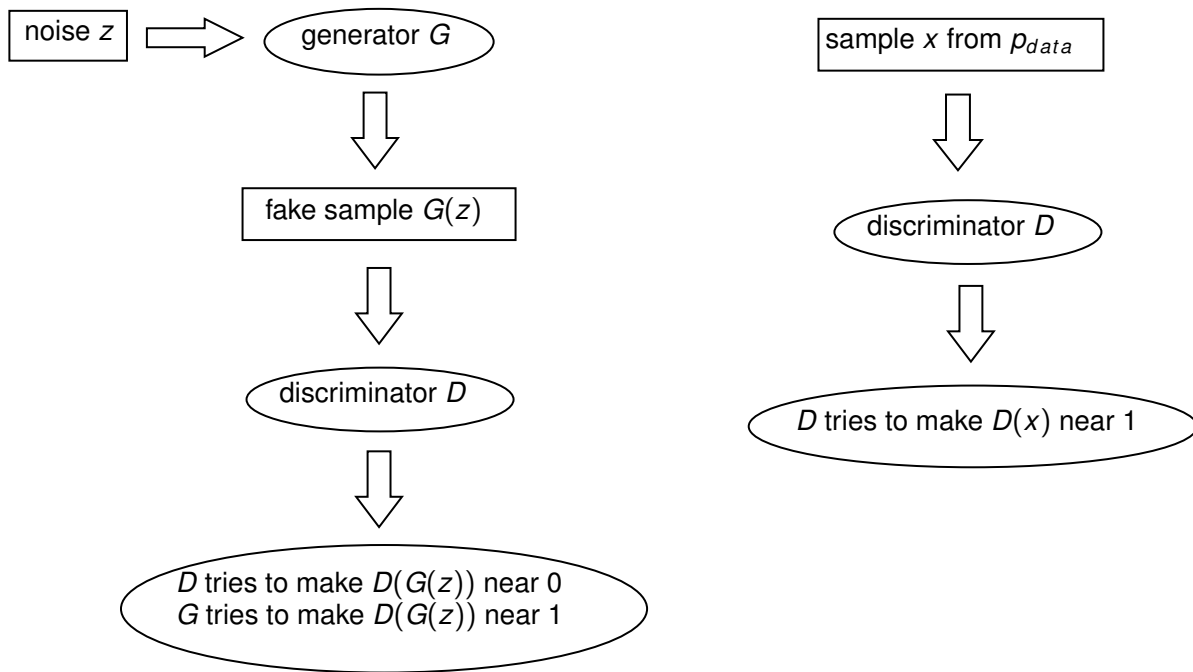
# GENERATIVE ADVERSARIAL NETWORKS

## FRAMEWORK

- ▶ **generator** : counterfeiter, trying to make fake money
  - $G: \mathcal{Z} \rightarrow \mathcal{X}$  inputs a latent vector (or noise)  $z$  and outputs a fake sample
  - $\mathcal{Z}$ : latent space
  - $z$  variable in  $\mathcal{Z}$  with known distribution  $\mathbb{P}_Z$
- ▶ **discriminator** : police, trying to allow legitimate money and catch counterfeit money
  - $D$ : inputs a fake or real sample and outputs the probability that the sample is **real**
- ▶ **differentiable**
- ▶  $p_{data}$ : data generating distribution
- ▶  $G$  (and also  $D$ ) is a neural network

# GENERATIVE ADVERSARIAL NETWORKS

## FRAMEWORK



# GENERATIVE ADVERSARIAL NETWORKS

## LOSS FUNCTIONS

- ▶ The discriminator wishes to minimize  $J^{(D)}(\theta^{(D)}, \theta^{(G)})$ .
- ▶ The generator wishes to minimize  $J^{(G)}(\theta^{(D)}, \theta^{(G)})$ .
- ▶ All of the different games designed for GANs so far use the same cost for the discriminator,  $J^{(D)}$ . They differ only in terms of the cost used for the generator,  $J^{(G)}$ . (Ian Goodfellow, 2016)

For discriminator:

$$J^{(D)}(\theta^{(D)}, \theta^{(G)}) = -\frac{1}{2} \mathbb{E}_{x \sim p_{data}} \log D(x) - \frac{1}{2} \mathbb{E}_z \log(1 - D(G(z)))$$



# GENERATIVE ADVERSARIAL NETWORKS

## LOSS FUNCTIONS

$$\mathcal{J}^{(D)}(\theta^{(D)}, \theta^{(G)}) = -\frac{1}{2}\mathbb{E}_{x \sim p_{data}} \log D(x) - \frac{1}{2}\mathbb{E}_z \log(1 - D(G(z)))$$

- ▶  $\log$ : negative on  $(0, 1]$ , avoid too long precision
- ▶  $D(x)$ : the probability that  $x$  is real
- ▶  $1 - D(G(z))$ : the probability that  $D$  tells the fake sample  $G(z)$
- ▶ We take all data into our consideration  $\rightarrow$  expectation
- ▶ If the probability is close to 1, then  $J$  is close to 0

# GENERATIVE ADVERSARIAL NETWORKS

## LOSS FUNCTIONS

In the zero-sum game, the loss function of the generator could be

$$J^{(G)} = -J^{(D)}.$$

In this case, we can describe the entire game by a value function  $V(\theta^{(D)}, \theta^{(G)})$ , defined by

$$V(\theta^{(D)}, \theta^{(G)}) = -J^{(D)}(\theta^{(D)}, \theta^{(G)}).$$

The optimal parameters of  $G$  is thus

$$\theta^{(G)*} = \arg \min_{\theta^{(G)}} \max_{\theta^{(D)}} V(\theta^{(D)}, \theta^{(G)})$$

# GENERATIVE ADVERSARIAL NETWORKS

## LOSS FUNCTIONS

### What is the problem?

- ▶ Note that the protagonist of GAN is the generator.
- ▶ At the starting stage, the generator is poor. The discriminator can tell the fake samples easily.
- ▶ If the discriminator is able to tell the real data with high probability, that is, the loss  $J^{(D)}$  is small, then the gradient of  $J^{(G)} = -J^{(D)}$  vanishes.
- ▶ Cannot improve the generator

# GENERATIVE ADVERSARIAL NETWORKS

## LOSS FUNCTIONS

Thus, we often choose

$$J^{(G)} = -\frac{1}{2} \mathbb{E}_z \log D(G(z))$$

where  $D(G(z))$  is the probability that the discriminator believes that the fake sample is real. The generator aims to **maximize** this probability so that  $-\log D(G(z))$  is small, i.e. minimize  $J^{(G)}$ .

More precisely, if the discriminator can tell with high confidence, then  $D(G(z))$  is small. In other words,  $-\log D(G(z))$  is large.

# GENERATIVE ADVERSARIAL NETWORKS

## TRAINING PROCESS

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### Algorithm General GAN training algorithm with alternating updates

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Initialize  $\theta^{(D)}, \theta^{(G)}$

**for** each training iteration **do**

**for**  $K$  steps **do**

        Update the discriminator parameters  $\theta^{(D)}$  using the gradient  $\nabla J^{(D)}(\theta^{(D)}, \theta^{(G)})$

**end for**

        Update the generator parameters  $\theta^{(G)}$  using the gradient  $\nabla J^{(G)}(\theta^{(D)}, \theta^{(G)})$

**end for**

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# GENERATIVE ADVERSARIAL NETWORKS

## TRAINING PROCESS

### How to calculate the gradient?

We want to update  $\theta^{(D)}$  and  $\theta^{(G)}$ , so we take the gradient with respect to  $\theta^{(D)}$  and  $\theta^{(G)}$ . The expectation is taken over all  $x$  or  $z$ .

### Theorem 1 (Leibniz integral rule)

If  $a(x)$  and  $b(x)$  and  $f(x, y)$  are  $C^1$ , then

$$\frac{d}{dx} \int_{a(x)}^{b(x)} f(x, y) dy = f(x, b(x))b'(x) - f(x, a(x))a'(x) + \int_{a(x)}^{b(x)} \frac{\partial f}{\partial x}(x, y) dy.$$

Special case:  $a(x)$  and  $b(x)$  are constant. Then

$$\frac{d}{dx} \int_a^b f(x, y) dy = \int_a^b \frac{\partial f}{\partial x}(x, y) dy.$$

# GENERATIVE ADVERSARIAL NETWORKS

## TRAINING PROCESS

### How to calculate the gradient?

The above theorem also holds for random variable  $y = X$  similarly.

### Theorem 2

*Let  $X$  be a random variable,  $g: \mathbb{R} \times \mathcal{X} \rightarrow \mathbb{R}$  a function such that  $g(t, X)$  is integrable for all  $t$  and  $g$  is continuously differentiable w.r.t.  $t$ . Assume that there is a random variable  $Z$  such that  $\frac{\partial}{\partial t}g(t, X) \leq Z$  a.s. for all  $t$  and  $\mathbb{E}Z < \infty$ . Then*

$$\frac{\partial}{\partial t}\mathbb{E}[g(t, X)] = \mathbb{E}\left[\frac{\partial}{\partial t}g(t, X)\right]$$

- ▶ You can replace  $t$  by parameters  $\theta$
- ▶ There's a more general theorem with similar form of the conditions, but we're going to mention it.

# GENERATIVE ADVERSARIAL NETWORKS

## TRAINING PROCESS

Thus, we have

$$\begin{aligned}\nabla J^{(D)}(\theta^{(D)}, \theta^{(G)}) &= \nabla \left( -\frac{1}{2} \mathbb{E}_{x \sim p_{data}} \log D(x) - \frac{1}{2} \mathbb{E}_z \log(1 - D(G(z))) \right) \\ &= -\frac{1}{2} \mathbb{E}_{x \sim p_{data}} \nabla \log D(x) - \frac{1}{2} \mathbb{E}_z \nabla \log(1 - D(G(z)))\end{aligned}$$

and

$$\begin{aligned}\nabla J^{(G)} &= \nabla \left( -\frac{1}{2} \mathbb{E}_z \log D(G(z)) \right) \\ &= -\frac{1}{2} \mathbb{E}_z \nabla \log D(G(z))\end{aligned}$$

$\nabla \log D(x)$  and  $\nabla \log D(G(z))$  can be calculated with **backpropagation** , and each expectation can be estimated using **Monte Carlo estimation** .



# GENERATIVE ADVERSARIAL NETWORKS

## TRAINING PROCESS

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### Algorithm GAN training algorithm

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Initialize  $\theta^{(D)}, \theta^{(G)}$

**for** each training iteration **do**

**for**  $K$  steps **do**

        Sample batch of  $m$  noise vectors  $z_i$

        Sample batch of  $m$  examples  $x_i$

        Update the discriminator by performing stochastic gradient descent using

$$\nabla_{\theta^{(D)}} \frac{1}{m} \sum_{i=1}^m \left[ -\frac{1}{2} \log D(x_i) - \frac{1}{2} \log(1 - D(G(z_i))) \right]$$

**end for**

    Sample batch of  $m$  noise vectors  $z_i$

    Update the generator by performing stochastic gradient descent using

$$\nabla_{\theta^{(G)}} \frac{1}{m} \sum_{i=1}^m \left[ -\frac{1}{2} \log(D(G(z_i))) \right]$$

**end for**

---

# GENERATIVE ADVERSARIAL NETWORKS

## TRAINING PROCESS

In practice, there are better choices of the training algorithm

- ▶ Adam gradient descent
- ▶ Simultaneous gradient descent: one step for each player (Ian Goodfellow (2016) thinks this is the best one)

# GENERATIVE ADVERSARIAL NETWORKS

## PROBLEMS

There are some theoretical and practical problems of training GAN:

► Non-convergence:

- GANs require finding the equilibrium to a game with two players.
- In practice, GANs often seem to oscillate. The equilibrium is like the saddle point.
- There is neither a theoretical argument that GAN games should converge when the updates are made to parameters of deep neural networks, nor a theoretical argument that the games should not converge.

► Balance  $D$  and  $G$

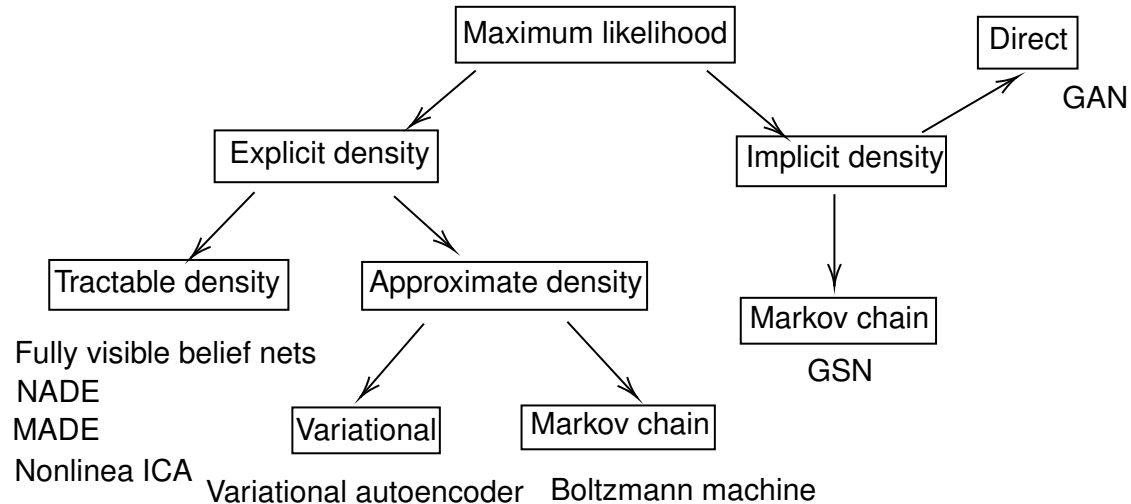
# GENERATIVE ADVERSARIAL NETWORKS

## PROBLEMS

- ▶ Mode collapse
  - The generator learns to map several different input  $z$  values to the same output point.
  - Lack diversity
  - Mode collapse does not seem to be caused by any particular cost function
  - Limited to problems where it is acceptable for the model to produce a small number of distinct outputs

# GENERATIVE ADVERSARIAL NETWORKS

## MORE ABOUT GAN



# GENERATIVE ADVERSARIAL NETWORKS

## MORE ABOUT GAN

- ▶ Boltzmann machines: few probability distributions admit tractable Markov chain sampling
- ▶ Nonlinear independent component analysis: generator must be invertible;  $z$  must have the same dimension as the samples  $x$ 
  - GAN admits  $z$  with larger dimension
- ▶ No Markov chains are needed
  - slow convergence, inefficient in high-dimensional spaces
- ▶ No variational bound is needed
  - Good likelihood but bad samples
- ▶ GANs are subjectively regarded as producing better samples than other methods.

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## LIKELIHOOD AND KL DIVERGENCE

For generative models,

- ▶ maximize the **likelihood** of our training data, that is, to generate training data as possible
- ▶ minimize the **distance** of the two distributions

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## LIKELIHOOD

### What is likelihood?

- ▶ 4 patients among 10 people
- ▶ infected patients  $X \sim \text{Bin}(10, \theta)$
- ▶ Patients are independent

$$\mathbb{P}(X = 4|\theta) = \binom{10}{4} \theta^4 (1 - \theta)^{10-4}$$

**What is the  $\theta$  such that  $\mathbb{P}(X = 4|\theta)$  is largest?**



# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## LIKELIHOOD

- ▶ **Likelihood** :  $L(\theta|X = 4) = \mathbb{P}(X = 4|\theta)$ 
  - a function of  $\theta$ , determining the probability of the observation  $X = 4$
  - $\mathbb{P}(X = 4|\theta)$ : given  $\theta$ , the probability of 4 infected patients
- ▶ **Maximum likelihood** :  $\max_{\theta} L(\theta|X = 4)$

In this problem, the optimal parameter  $\theta$  is  $\arg \max_{\theta} L(\theta|X = 4) = 4$ .

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## LIKELIHOOD IN GENERATIVE MODELS

- ▶ training data:  $x^i, i = 1, \dots, m$
- ▶ likelihood: the probability that the model assigns to the training data  
 $\prod_{i=1}^m p_{model}(x^i; \theta)$
- ▶ take log

$$\begin{aligned}\theta^* &= \arg \max_{\theta} \prod_{i=1}^m p_{model}(x^i; \theta) \\ &= \arg \max_{\theta} \sum_{i=1}^m \log p_{model}(x^i; \theta)\end{aligned}$$

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## KL DIVERGENCE

Intuitively, the purpose of KL divergence is to measure the **difference** or "**distance**" of two probability distributions.

### Definition 2.1 (KL divergence)

*Given two distributions  $p(x)$  and  $q(x)$ . The discrete KL divergence is defined by*

$$KL(p||q) \doteq \sum_{k=1}^m \log \frac{p_k}{q_k},$$

*and the continuous KL divergence is*

$$\begin{aligned} KL(p||q) &\doteq \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} d\mu(x) \\ &= \mathbb{E}_{x \sim p(x)} \log \frac{p(x)}{q(x)} \end{aligned}$$

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## LIKELIHOOD AND KL DIVERGENCE

### Proposition 1

*Minimizing KL divergence is equivalent to maximizing likelihood.*

### Proof.

Let  $\theta^*$  be the optimal parameters and  $\hat{\theta}$  be the approximate parameters.

$$\begin{aligned} & \arg \min_{\hat{\theta}} KL(p(x|\theta^*) || p(x|\hat{\theta})) \\ &= \arg \min_{\hat{\theta}} \mathbb{E}_{x \sim p(x|\theta^*)} \left[ \log \frac{p(x|\theta^*)}{p(x|\hat{\theta})} \right] \\ &= \arg \min_{\hat{\theta}} \mathbb{E}_{x \sim p(x|\theta^*)} \left[ \log p(x|\theta^*) - \log p(x|\hat{\theta}) \right] \\ &= \arg \min_{\hat{\theta}} \mathbb{E}_{x \sim p(x|\theta^*)} \left[ -\log p(x|\hat{\theta}) \right] \\ &= \arg \max_{\hat{\theta}} \mathbb{E}_{x \sim p(x|\theta^*)} \left[ \log p(x|\hat{\theta}) \right] \end{aligned}$$

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## MOTIVATION

Why does the choice of distance matter?

### Theorem 3

*A sequence of distributions  $\mathbb{P}_t$  converges with respect to  $\rho$  if and only if there exists a distribution  $\mathbb{P}_\infty$  such that  $\rho(\mathbb{P}_t, \mathbb{P}_\infty) \rightarrow 0$  as  $t \rightarrow \infty$ .*

- ▶ In order to optimize the parameter  $\theta$ , we hope the distance of distributions is **continuous**, that is, if  $\theta$  converges to  $\theta^*$ , then  $\mathbb{P}_\theta$  converges to  $\mathbb{P}_{\theta^*}$ .
- ▶ Gradient descent on KL divergence? No, we'll give a counterexample later.

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## $W_1$ DISTANCE

Let  $\mathcal{X}$  be a compact metric set and let  $\Sigma$  denote the set of all the Borel subsets of  $\mathcal{X}$ .

- ▶ The *Total Variation* (TV) distance

$$\delta(\mathbb{P}_r, \mathbb{P}_g) = \sup_{A \in \Sigma} |\mathbb{P}_r(A) - \mathbb{P}_g(A)|$$

- ▶ The KL divergence

$$KL(\mathbb{P}_r || \mathbb{P}_g) = \int \log \frac{P_r(x)}{P_g(x)} P_r(x) d\mu(x)$$

This is asymmetric.

- ▶ The *Jensen-Shannon* (JS) divergence

$$JS(\mathbb{P}_r, \mathbb{P}_g) = KL(\mathbb{P}_r || \mathbb{P}_m) + KL(\mathbb{P}_g || \mathbb{P}_m)$$

where  $\mathbb{P}_m = \frac{\mathbb{P}_r + \mathbb{P}_g}{2}$ . This divergence is symmetrical and always defined because we can choose  $\mu = \mathbb{P}_m$ .

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## EM DISTANCE

- The *Earth-Mover* (EM) distance or Wasserstein-1

$$W(\mathbb{P}_r, \mathbb{P}_g) = \inf_{\gamma \sim \Pi(\mathbb{P}_r, \mathbb{P}_g)} \mathbb{E}_{(x,y) \sim \gamma} [\|x - y\|]$$

where  $\Pi(\mathbb{P}_r, \mathbb{P}_g)$  denotes the set of all joint distributions  $\gamma(x, y)$  whose marginals are respectively  $\mathbb{P}_r$  and  $\mathbb{P}_g$ . Intuitively,  $\gamma(x, y)$  indicates how much “mass” must be transported from  $x$  to  $y$  in order to transform the distributions  $\mathbb{P}_r$  into the distribution  $\mathbb{P}_g$ . The EM distance then is the “**cost**” of the optimal transport plan.

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## EM DISTANCE

### Example

- ▶  $Z \sim U[0, 1]$
- ▶  $\mathbb{P}_0 = (0, Z)$
- ▶  $g_\theta = (\theta, z), z \sim Z$

In this case,

▶

$$W(\mathbb{P}_0, \mathbb{P}_g) = |\theta|$$

▶

$$JS(\mathbb{P}_0, \mathbb{P}_g) = \begin{cases} \log 2 & \text{if } \theta \neq 0 \\ 0 & \theta = 0 \end{cases}$$

▶

$$KL(\mathbb{P}_0 || \mathbb{P}_g) = KL(\mathbb{P}_g || \mathbb{P}_0) \begin{cases} \infty & \text{if } \theta \neq 0 \\ 0 & \theta = 0 \end{cases}$$

▶

$$\delta(\mathbb{P}_0, \mathbb{P}_g) = \begin{cases} 1 & \text{if } \theta \neq 0 \\ 0 & \theta = 0 \end{cases}$$



# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## EM DISTANCE

- ▶ Among all distances, only Wasserstein-1 distance is continuous in this example.

Fix a distribution  $\mathbb{P}_r$  and let  $\mathbb{P}_\theta$  denote the distribution of  $g_\theta(Z)$ .

## Proposition 2 (easily understood version)

*For any feedforward neural network parametrized by  $\theta$ , noise  $z$  sampled from a desired distribution (e.g. Gaussian),  $W(\mathbb{P}_r, \mathbb{P}_\theta)$  is continuous everywhere and differentiable almost everywhere.*

- ▶ desired distribution  $\longrightarrow \mathbb{E}_{z \sim p(z)}[\|z\|] < \infty$

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## WGAN

By the Kantorovich-Rubinstein duality,

$$W(\mathbb{P}_r, \mathbb{P}_\theta) = \sup_{\|f\|_L \leq 1} \mathbb{E}_{x \sim \mathbb{P}_r}[f(x)] - \mathbb{E}_{x \sim \mathbb{P}_\theta}[f(x)].$$

If we replace  $\|f\|_L \leq 1$  by  $\|f\|_L \leq K$ , then we end up with  $K \cdot W(\mathbb{P}_r, \mathbb{P}_\theta)$ . The gradient is scaled but its direction does not change.

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## WGAN

Let  $f_w$  denote the neural network with parameters  $w$ . We could consider solving

$$\max_{w \in \mathcal{W}} \mathbb{E}_{x \sim \mathbb{P}_r}[f_w(x)] - \mathbb{E}_{z \sim \mathbb{P}_z}[f_w(g_\theta(z))]$$

where we restrict the range of parameters. For example, we restrict  $\mathcal{W} \in [-0.01, 0.01]^l$  so that  $\frac{\partial f_w}{\partial w_i}$  are bounded and the gradient is Lipschitz.

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## WGAN

---

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

---

Initialize  $\alpha$ : learning rate,  $c$ : clipping parameter,  $m$ : batch size,  $n_{critic}$ : the number of iterations of the critic per generator iteration

Initialize  $w_0$ : discriminator parameters,  $\theta_0$ : generator parameters

**for** each training iteration **do**

**for**  $t=0,1,\dots,n_{critic}$  **do**

        Sample  $\{x^{(i)}\}_{i=1}^m \sim \mathbb{P}_r$  a batch of 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

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

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

**end for**

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# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## WGAN

- ▶ We clip the domain of parameters to enforce Lipchitz
- ▶ We **get rid of the sigmoid** in the last layer since the discriminator of **WGAN is not a logistic regression**. Instead, the discriminator is an approximate to  $W_1$  distance, so this is a regression and we don't need sigmoid.
- ▶ No log

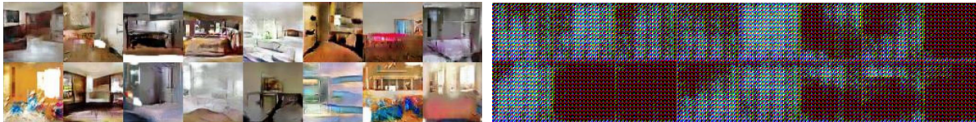
# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

## COMPARISON

- In no experiment did we see evidence of mode collapse for the WGAN algorithm.



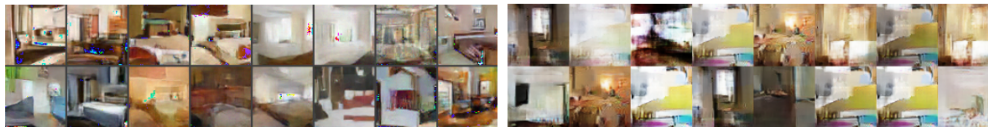
**Figure.** Algorithms trained with a DCGAN generator. Left: WGAN algorithm. Right: standard GAN formulation. Both algorithms produce high quality samples.



**Figure.** Algorithms trained with a generator without batch normalization and constant number of filters at every layer. Standard GAN failed to learn while the WGAN still was able to produce samples.

# WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS

WGAN



**Figure.** Algorithms trained with an MLP generator with 4 layers and 512 units with ReLU nonlinearities. WGAN: lower quality, GAN: worse quality and mode collapse

## Part II

# SIGNATURE AND GAN



# SIG-WGAN

## LOG-SIGNATURE

### Piecewise linear transformation

- ▶ time-joined transformation
- ▶ lead-lag transformation (uniquely determines the path)
- ▶ rectlinear interpolation

# SIG-WGAN

## LOG-SIGNATURE

### Definition 1.1 (Signature)

*For a continuous path  $X = (f_1(t), \dots, f_d(t)) : [0, 1] \longrightarrow \mathbb{R}^d$ , the signature of  $X$  is defined by an infinite sequence*

$$S(X) = \left( \int_0^1 \cdots \int_0^{t_{k-1}} dX_{t_1} \cdots dX_{t_k} \right)_{k \in \mathbb{N}} \in (\mathbb{R}^d)^{\otimes k}$$

# SIG-WGAN

## LOG-SIGNATURE

### Definition 1.2 (Logarithm map)

Let  $a = (a_0, a_1, \dots) \in T((\mathbb{R}^d))$  be such that  $a_0 = 1$ ,  $t = a - 1$ . Then the logarithm map denoted by  $\log$  is defined as follows:

$$\log(a) = \log(1 + t) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} t^{\otimes n}$$

- $a$  can be viewed as the signature of a path

### Definition 1.3 (The Log Signature of a Path)

The log signature of path  $X$  by  $\log S(X)$  is the logarithm of the signature of the path  $X$ , denoted by  $\text{LogSig}(X)$ .

- degree  $M \longrightarrow \text{LogSig}^M(X)$

# SIG-WGAN

## LOG-SIGNATURE

- ▶ **Uniqueness** : the log-signature is bijective to the signature
- ▶ **Dimension reduction** : the dimension of the truncated log-signature is no greater than that of the truncated signature
- ▶ Invariance under time parameterization
- ▶ Missing Data and unequally time spacing

# SIG-WGAN

## SIG- $W_1$ DISTANCE

- ▶  $\mathcal{X} = \Omega_0^1(J, \mathbb{R}^d)$ : all paths with 1-variation that maps a compact interval  $J$  to  $\mathbb{R}^d$
- ▶  $\mu, \nu$ : measures (probability distributions) on  $\Omega_0^1(J, \mathbb{R}^d)$

The  $W_1$  distance on the signature space is

$$W_1^{\text{Sig space}}(\mu, \nu) = \sup_{\|f\|_{\text{Lip}} \leq 1} \mathbb{E}_{X \sim \mu}[f(S(X))] - \mathbb{E}_{X \sim \nu}[f(S(X))].$$

**universality**  $\implies$

$$\text{Sig-}W_1^{\text{Sig space}}(\mu, \nu) = \sup_{L \text{ is linear, } \|L\| \leq 1} \mathbb{E}_{X \sim \mu}[L(S(X))] - \mathbb{E}_{X \sim \nu}[L(S(X))].$$

# SIG-WGAN

## SIG- $W_1$ DISTANCE

**Factorial decay**  $\implies$

$$\text{Sig-}W_1^{(M)}(\mu, \nu) = \sup_{L \text{ is linear, } \|L\| \leq 1} L(\mathbb{E}_{X \sim \mu}[S^M(X)] - \mathbb{E}_{X \sim \nu}[S^M(X)]) .$$

When the norm of  $L$  is chosen as the  $l_2$  norm of the linear coefficients of  $L$ , this reduced optimization problem admits the analytic solution

$$\text{Sig-}W_1^{(M)}(\mu, \nu) := |\mathbb{E}_\mu[S^M(X)] - \mathbb{E}_\nu[S^M(X)]|$$

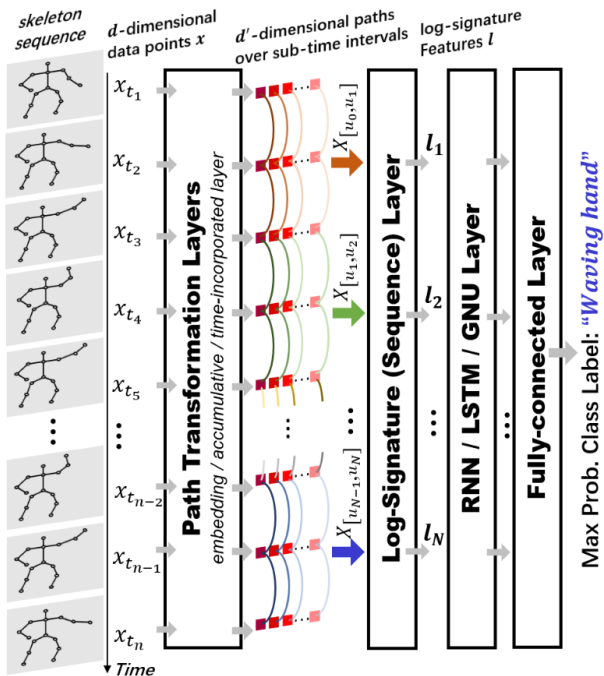
# SIG-WGAN

## LOGSIG-RNN

- ▶ time-series data  $\longrightarrow$  path transformation  $\longrightarrow$  log-signature transformation  
 $\longrightarrow$  RNN/LSTM

# SIG-WGAN

## LOGSIG-RNN





# SIG-WGAN

## PATH TRANSFORMATION LAYER

- ▶ **Embedding Layer** : maps  $(X_{t_i})_{i=1}^n$  to  $(LX_{t_i})_{i=1}^n$ , where  $X_{t_i} \in \mathbb{R}^d$ ,  $LX_{t_i} \in \mathbb{R}^{d'}$  with  $d' < d$ ,  $L$  trainable matrix (dimension reduction)
- ▶ **Accumulative Layer** :  $Y_i = \sum_{j=1}^i X_{t_j}$ ,  $i = 1, \dots, n$  (extract the quadratic variation and other higher order statistics of an input path  $X$  effectively)
- ▶ **Time-incorporated Layer** :  $(t_i, X_{t_i})_{i=1}^n$

# SIG-WGAN

## LOG-SIGNATURE LAYER

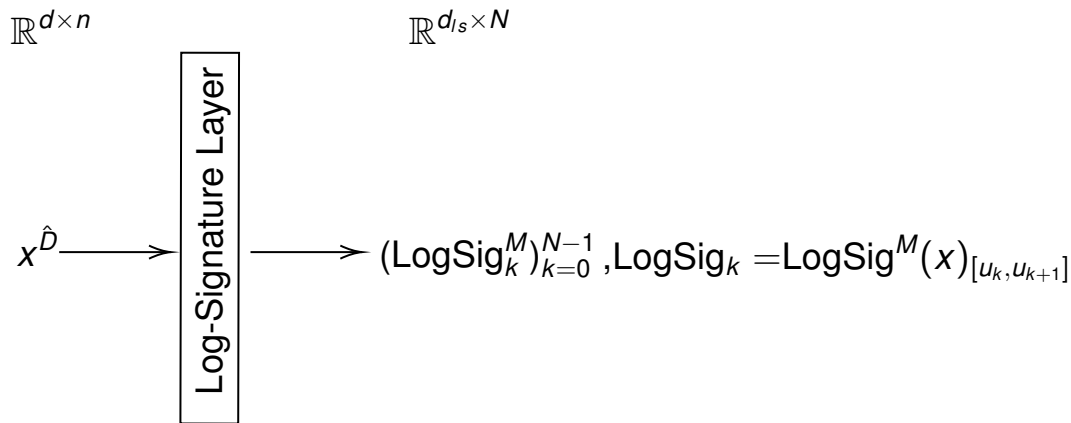
Consider

- ▶  $x^{\hat{\mathcal{D}}} = (x_{t_i})_{i=1}^n$ : discrete  $d$ -dimensional time series over some time interval  $J$ ,  $\hat{\mathcal{D}}$  partition of  $J$
- ▶ linear interpolation
- ▶  $\mathcal{D} := (u_k)_{k=0}^N \subset \hat{\mathcal{D}}$ : coarser partition of  $J$

The Log-Signature Layer transforms an input  $x^{\hat{\mathcal{D}}}$  to a sequence of the log signature of  $x^{\hat{\mathcal{D}}}$  over a coarser time partition  $\mathcal{D}$ .

# SIG-WGAN

## LOG-SIGNATURE LAYER



- ▶  $d_{ls}$ : dimension of truncated log-signature
- ▶ No weights
- ▶  $(d, n) \longrightarrow (d_{ls}, N)$  where  $N \leq n$  and  $d_{ls} \geq d$ 
  - shrinks time dimension by using the more informative spatial features of a higher dimension

# SIG-WGAN

## BACKPROPOGATION

By chain rule, the derivative of  $F$  is

$$\frac{\partial F(l_0, \dots, l_{N-1})}{\partial x_{t_i}} = \sum_{k=0}^{N-1} \frac{\partial F(l_0, \dots, l_{N-1})}{\partial l_k} \frac{\partial l_k}{\partial x_{t_i}}.$$

- ▶ If  $t_i \notin [u_k, u_{k+1}]$ ,  $\frac{\partial l_k}{\partial x_{t_i}} = 0$ . Otherwise,  $\frac{\partial l_k}{\partial x_{t_i}}$  is the derivative of the single log-signature  $l_k$  w.r.t. path  $x_{u_k, u_{k+1}}$  where  $t_i \in \mathcal{D} \cap [u_k, u_{k+1}]$ .
- ▶ The log signature  $\text{LogSig}(x^{\hat{\mathcal{D}}})$  with respect to  $x_{t_i}$  is proved differentiable.

# SIG-WGAN

## RNN

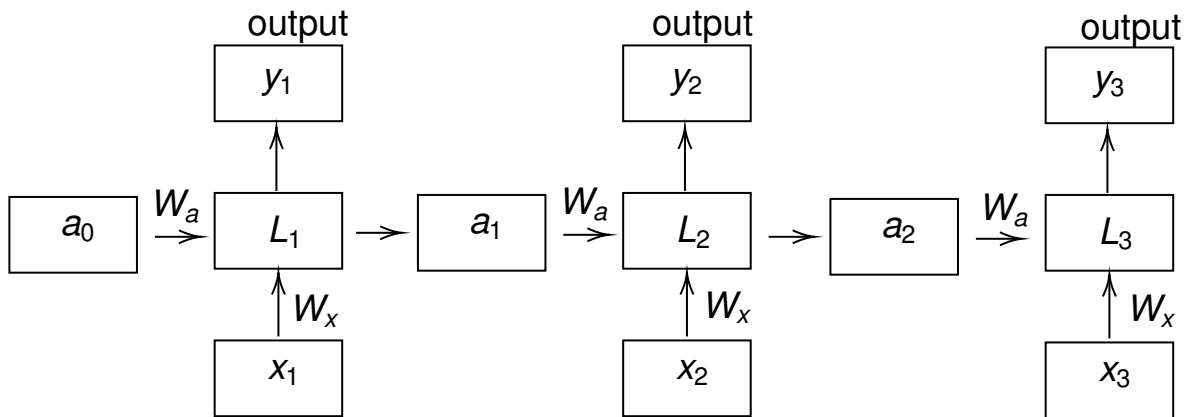
- ▶ The inspiration of Logsig-RNN comes from the numerical approximation of SDE, which is of the form

$$a_{n+1} = f_{\theta}(a_n, x_n).$$

- ▶ Backpropagation
- ▶ Gradient vanishing/exploding

# SIG-WGAN

## RNN



►  $a_1 = \sigma(W_a \cdot a_0 + W_x \cdot x_1 + b_1)$

►  $a_2 = \sigma(W_a \cdot a_1 + W_x \cdot x_2 + b_2)$

►  $\vdots$

# SIG-WGAN

## RNN

- ▶ The same weight matrices are multiplied many times in the hidden layers.
- ▶ The gradient decays/cumulates

# SIG-WGAN

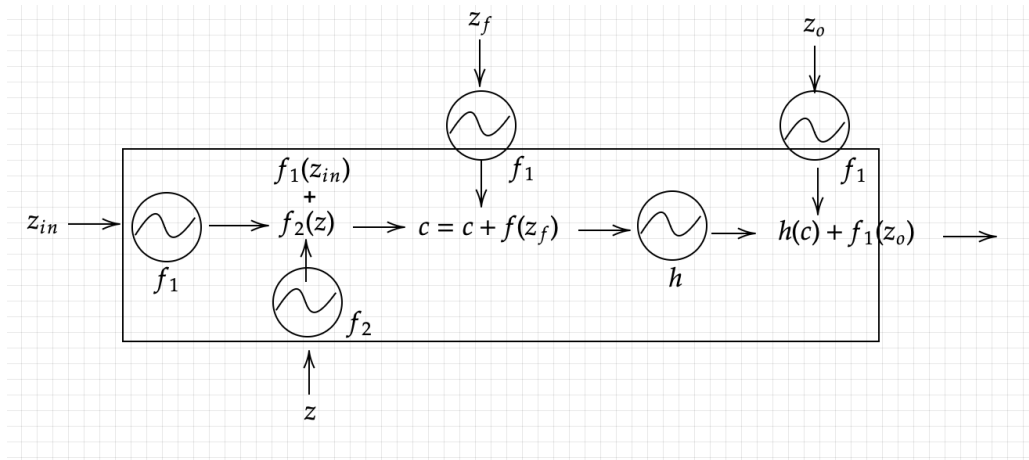
## LSTM

- ▶ Long Short-term memory (LSTM) is a unit ( $\approx$  neuron).
- ▶ Use gates to control input



# SIG-WGAN

## LSTM



- sigmoid: between 0 and 1, the degree of opening

# SIG-WGAN

## LOGSIG-RNN vs. LSTM

- ▶ few time steps  $\longrightarrow$  LSTM is better
- ▶ high frequency  $\longrightarrow$  Logsig-RNN is better

# REFERENCES

- ▶ Probabilistic Machine Learning: Advanced Topics, MIT Press, 2023.
- ▶ NIPS 2016 Tutorial: Generative Adversarial Networks. arXiv:1701.00160
- ▶ Wasserstein GAN. arXiv:1701.07875
- ▶ Learning from the past, predicting the statistics for the future, learning an evolving system. arXiv:1309.0260
- ▶ Sig-Wasserstein GANs for Time Series Generation. arXiv:2111.01207
- ▶ Learning stochastic differential equations using RNN with log signature features. arXiv:1908.08286
- ▶ zhihu