Wasserstein GAN

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Improved Training of Wasserstein GANs

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GAN Reading Group

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Goal - Convince you that WGAN is the "best" GAN

Outline

Introduction

Different Distances

Standard GAN

Wasserstein GAN

Improved Wasserstein GAN

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What does it mean to learn a probability distribution?

When learning generative models, we assume the data we have comes from some unknown distribution \mathbb{P}_r .

Want to learn a distribution \mathbb{P}_{θ} that approximates \mathbb{P}_{r} , where θ are the parameters of the distribution.

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There are two approaches for doing this:

- 1. Directly learn the probability density function \mathbb{P}_{θ} and then optimize through maximum likelihood estimation
- 2. Learn a function that transforms an existing distribution Z into \mathbb{P}_{θ} . Here, g_{θ} is some differentiable function, Z is a common distribution (usually uniform or Gaussian), and $\mathbb{P}_{\theta} = g_{\theta}(Z)$

Recall that for continuous distributions \mathbb{P} and \mathbb{Q} the KL divergence is:

$$\mathit{KL}(\mathbb{P}||\mathbb{Q}) = \int_{\mathcal{X}} \mathbb{P}(x) \log \frac{\mathbb{P}(x)}{\mathbb{Q}(x)} dx$$

and given function \mathbb{P}_{θ} , the MLE objective is

$$\max_{\theta \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1}^m \log \mathbb{P}_{\theta}(x^{(i)})$$

In the limit (as $m \to \infty$), samples will appear based on the data distribution \mathbb{P}_r , so

$$\lim_{m \to \infty} \max_{\theta \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1}^m \log \mathbb{P}_{\theta}(x^{(i)}) = \max_{\theta \in \mathbb{R}^d} \int_{x} \mathbb{P}_{r}(x) \log \mathbb{P}_{\theta}(x) dx$$

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$$= \min_{\theta \in \mathbb{R}^d} KL(\mathbb{P}_r || \mathbb{P}_{\theta})$$

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- This unfortunately introduces some error, and empirically people have needed to add a lot of random noise to make models train

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GANs offer much more flexibility but their training is unstable.

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How do we define *d*?

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 χ - compact metric set (such as the space of images $[0,1]^d$)

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Kullback-Leibler (KL) divergence

$$\mathit{KL}(\mathbb{P}_r||\mathbb{P}_{ heta}) = \int_{x} \mathbb{P}_r(x) \log rac{\mathbb{P}_r(x)}{\mathbb{P}_{ heta}(x)} d\mu(x)$$

where both \mathbb{P}_r and \mathbb{P}_θ are assumed to be absolutely continuous with respect to a same measure μ defined on χ .

Jensen-Shannon (JS) Divergence

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

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Earth-Mover (EM) distance or Wasserstein-1

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

where $\Pi(\mathbb{P}_r, \mathbb{P}_{\theta})$ denotes the set of all join distributions $\gamma(x, y)$ whose marginals are respectively \mathbb{P}_r and \mathbb{P}_{θ}

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Transport Plan

Each $\gamma \in \Pi$ is a transport plan and to execute the plan, for all x, y move $\gamma(x, y)$ mass from x to y.

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This shows why the marginals of $\gamma \in \Pi$ must be \mathbb{P}_r and \mathbb{P}_{θ} . For scoring, the effort spent is

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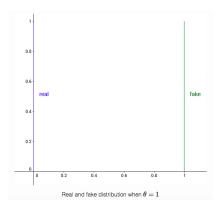
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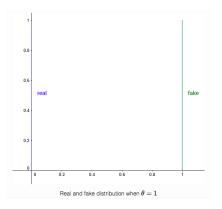
Computing the infimum of this over all valid γ gives the earth mover distance

Let $Z \sim U[0,1]$ and let \mathbb{P}_0 be the distribution of $(0,Z) \in \mathbb{R}^2$, uniform on a straight vertical line passing through the origin. Now let $g_{\theta}(z) = (\theta,z)$ with θ a single real parameter.

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We'd like our optimization algorithm to learn to move θ to 0. As $\theta \to 0$, the distance $d(\mathbb{P}_0, \mathbb{P}_{\theta})$ should decrease.

For many common distance functions, this doesn't happen.

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

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

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

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

Theoretical Justification

Theorem (1)

Let \mathbb{P}_r be a fixed distribution over χ . Let Z be a random variable over another space \mathcal{Z} . Let $g: \mathcal{Z} \times \mathbb{R}^d \to \chi$ be a function, that will be denote $g_{\theta}(z)$ with z the first coordinate and θ the second. Let \mathbb{P}_{θ} denote the distribution of $g_{\theta}()$. Then,

- 1. If g is continuous in θ , so is $W(\mathbb{P}_r, \mathbb{P}_{\theta})$.
- 2. If g is locally Lipschitz and satisfies regularity assumption 1, then $W(\mathbb{P}_r, \mathbb{P}_{\theta})$ is continuous everywhere, and differentiable almost everywhere
- 3. Statements 1-2 are false for the Jensen-Shannon divergence $JS(\mathbb{P}_r, \mathbb{P}_{\theta})$ and all the KLs.

Theoretical Justification

Theorem (2)

Let $\mathbb P$ be a distribution on a compact space χ and $(\mathbb P_n)_{n\in\mathbb N}$ be a sequence of distributions on χ . Then, considering all limits as $n\to\infty$,

- 1. The following statements are equivalent
 - $\delta(\mathbb{P}_n,\mathbb{P}) \to 0$
 - ▶ $JS(\mathbb{P}_n,\mathbb{P}) \to 0$
- 2. The following statements are equivalent
 - $W(\mathbb{P}_n,\mathbb{P}) \to 0$
 - ▶ $\mathbb{P}_n \stackrel{D}{\to} \mathbb{P}$ where $\stackrel{D}{\to}$ represents convergence in distribution for random variables
- 3. $KL(\mathbb{P}_n||\mathbb{P}) \to 0$ or $KL(\mathbb{P}||\mathbb{P}_n) \to 0$ imply the statements in (1).
- 4. The statements in (1) imply the statements in (2).

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The discriminator network D receives either a generated sample or a true data sample and must distinguish between the two.

The generator is trained to fool the discriminator.

Formally we can express the game between the generator G and the discriminator D with the minimax objective:

$$\min_{G} \max_{D} \mathbb{E}_{\mathbf{x} \sim \mathbb{P}_r}[\log(D(\mathbf{x}))] + \mathbb{E}_{\widetilde{\mathbf{x}} \sim \mathbb{P}_g}[\log(1 - D(\widetilde{\mathbf{x}}))]$$

where \mathbb{P}_r is the data distribution and \mathbb{P}_g is the model distribution implicitly defined by $\widetilde{x} = G(z)$, $z \sim p(z)$

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- ► This is expensive and often leads to vanishing gradients as the discriminator saturates
- In practice, this requirement is relaxed, and the generator and discriminator are update simultaneously

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Kantorivich-Rubinstein Duality

Unfortunately, computing the Wasserstein distance exactly is intractable.

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However, a result from the Kantorivich-Rubinstein Duality (Villani 2008) shows W is equivalent to

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

where the supremum is taken over all 1-Lipschitz functions

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Calculating this is still intractable, but now it's easier to approximate.

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$$egin{aligned} \max_{w \in \mathcal{W}} \mathbb{E}_{x \sim \mathbb{P}_r}[f_w(x)] - \mathbb{E}_{x \sim \mathbb{P}_{ heta}}[f_w(x)] &\leq \sup_{||f||_L \leq \mathcal{K}} \mathbb{E}_{x \sim \mathbb{P}_r}[f(x)] - \mathbb{E}_{x \sim \mathbb{P}_{ heta}}[f(x)] \\ &= \mathcal{K} \cdot \mathcal{W}(\mathbb{P}_r, \mathbb{P}_{ heta}) \end{aligned}$$

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$$egin{aligned} \max_{w \in W} \mathbb{E}_{x \sim \mathbb{P}_r}[f_w(x)] - \mathbb{E}_{x \sim \mathbb{P}_{ heta}}[f_w(x)] &\leq \sup_{||f||_L \leq K} \mathbb{E}_{x \sim \mathbb{P}_r}[f(x)] - \mathbb{E}_{x \sim \mathbb{P}_{ heta}}[f(x)] \\ &= K \cdot W(\mathbb{P}_r, \mathbb{P}_{ heta}) \end{aligned}$$

If $\{f_w\}_{w\in W}$ contains the true supremum among K-Lipschitz functions, this gives the distance exactly.

Note that if we replace the supremum over 1-Lipschitz functions with the supremum over K-Lipschitz functions, then the supremum is $K \cdot W(\mathbb{P}_r, \mathbb{P}_\theta)$ instead.

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In practice this won't be true!

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We can then backpropagate through $W(\mathbb{P}_r, g_{\theta}(Z))$ to get the gradient for θ .

$$\begin{split} \nabla_{\theta} W(\mathbb{P}_r, \mathbb{P}_{\theta}) &= \nabla_{\theta} (\mathbb{E}_{x \sim \mathbb{P}_r} [f_w(x)] - \mathbb{E}_{z \sim Z} [f_w(g_{\theta}(z))]) \\ &= -\mathbb{E}_{z \sim Z} [\nabla_{\theta} f_w(g_{\theta}(z))] \end{split}$$

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To guarantee this is true, the authors use weight clamping. The weights w are constrained to lie within [-c,c], by clipping w after every update to w.

Algorithm 1 WGAN, our proposed algorithm. All experiments in the paper used the default values $\alpha=0.00005,\,c=0.01,\,m=64,\,n_{\rm critic}=5.$

```
Require: \alpha, the learning rate. c, the clipping parameter. m, the batch size.
     n_{\text{critic}}, the number of iterations of the critic per generator iteration.
Require: : w_0, initial critic parameters. \theta_0, initial generator's parameters.
 1: while \theta 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.
 3:
               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]
 5:
               w \leftarrow w + \alpha \cdot \text{RMSProp}(w, q_w)
 6:
               w \leftarrow \text{clip}(w, -c, c)
 7:
          end for
 8:
          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)}))
10:
          \theta \leftarrow \theta - \alpha \cdot \text{RMSProp}(\theta, q_{\theta})
11:
12: end while
```

▶ In GANs, the discriminator maximizes

$$\frac{1}{m} \sum_{i=1}^{m} \log D(x^{(i)}) + \frac{1}{m} \sum_{i=1}^{m} \log(1 - D(g_{\theta}(z^{(i)})))$$

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where we constrain D(x) to always be a probability $p \in (0,1)$

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- Consequently, we're updating G against an objective that kind of aims towards the JS divergence, but doesn't go all the way
- ▶ In constrast, because the Wasserstein distance is differentiable nearly everywhere, we can (and should) train f_w to convergence before each generator update, to get as accurate an estimate of $W(\mathbb{P}_r, \mathbb{P}_\theta)$ as possible

Introduction

Different Distances

Standard GAN

Wasserstein GAN

Improved Wasserstein GAN

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To understand why weight clipping is problematic in WGAN critic we need to understand what are the properties of the optimal WGAN critic?

If the optimal critic under the Kantorovich-Rubinstein dual D^* is differentiable, and x is a point from our generator distribution \mathbb{P}_{θ} , then there is a point y sampled from the true distribution \mathbb{P}_r such that the gradient of D^* at all points $x_t = (1-t)x + ty$ lie on a straight line between x and y.

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In other words,
$$\nabla D^*(x_t) = \frac{y - x_t}{||y - x_t||}$$
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This implies that the optimal WGAN critic has gradients with norm 1 almost everywhere under \mathbb{P}_r and \mathbb{P}_{θ}

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A differentiable function is 1-Lipschitz if and only if it has gradients with norm less than or equal to 1 everywhere.

This implies we should directly constrain the gradient norm of our critic function with respect to its input.

Enforcing a soft version of this we get:

$$L = \underbrace{\mathbb{E}_{\tilde{\boldsymbol{x}} \sim \mathbb{P}_g} \left[D(\tilde{\boldsymbol{x}}) \right] - \mathbb{E}_{\boldsymbol{x} \sim \mathbb{P}_r} \left[D(\boldsymbol{x}) \right]}_{\text{Original critic loss}} + \underbrace{\lambda \mathop{\mathbb{E}}_{\hat{\boldsymbol{x}} \sim \mathbb{P}_{\hat{\boldsymbol{x}}}} \left[(\|\nabla_{\hat{\boldsymbol{x}}} D(\hat{\boldsymbol{x}})\|_2 - 1)^2 \right]}_{\text{Our gradient penalty}}$$

WGAN with gradient penalty

Algorithm 1 WGAN with gradient penalty. We use default values of $\lambda=10$, $n_{\rm critic}=5$, $\alpha=0.0001, \beta_1=0.5, \beta_2=0.9$.

Require: The gradient penalty coefficient λ , the number of critic iterations per generator iteration n_{critic} , the batch size m, Adam hyperparameters α , β_1 , β_2 .

Require: initial critic parameters w_0 , initial generator parameters θ_0 .

```
1: while \theta has not converged do
 2:
             for t = 1, ..., n_{\text{critic}} do
 3:
                    for i = 1, ..., m do
                           Sample real data x \sim \mathbb{P}_r, latent variable z \sim p(z), a random number \epsilon \sim U[0,1].
 4:
 5:
                           \tilde{\boldsymbol{x}} \leftarrow G_{\theta}(\boldsymbol{z})
                          \hat{\boldsymbol{x}} \leftarrow \epsilon \boldsymbol{x} + (1 - \epsilon)\tilde{\boldsymbol{x}}
 6:
                           L^{(i)} \leftarrow D_w(\tilde{x}) - D_w(x) + \lambda (\|\nabla_{\hat{x}} D_w(\hat{x})\|_2 - 1)^2
 7:
 8:
                    end for
                    w \leftarrow \operatorname{Adam}(\nabla_w \frac{1}{m} \sum_{i=1}^m L^{(i)}, w, \alpha, \beta_1, \beta_2)
 9:
10:
             end for
              Sample a batch of latent variables \{z^{(i)}\}_{i=1}^m \sim p(z).
11:
              \theta \leftarrow \text{Adam}(\nabla_{\theta} \frac{1}{m} \sum_{i=1}^{m} -D_{w}(G_{\theta}(z)), \theta, \alpha, \beta_{1}, \beta_{2})
12:
13: end while
```