Wasserstein GAN

Martin Arjovsky[1], Soumith Chintala[2], and Léon Bottou[1,2]

[1]Courant Institute of Mathematical Sciences
[2]Facebook AI Research

Improved Training of Wasserstein GANs

Ishaan Gulrajani[1], Faruk Ahmed[1], Martin Arjovsky[2], Vincent Dumoulin[1], Aaron Courville[1,3]
[1] Montreal Institute for Learning Algorithms
[2] Courant Institute of Mathematical Sciences
[3] CIFAR Fellow
igul222@gmail.com
{faruk.ahmed,vincent.dumoulin,aaron.courville}@umontreal.ca
ma4371@nyu.edu

Nishant Gurnani

Kreutz-Delgado Group

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

Outline

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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 $\mathbb{P}_r$.

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1. Directly learn the probability density function $\mathbb{P}_\theta$ and then optimize through maximum likelihood estimation

2. Learn a function that transforms an existing distribution Z into $\mathbb{P}_\theta$. Here, g_θ is some differentiable function, Z is a common distribution (usually uniform or Gaussian), and $\mathbb{P}_\theta = g_\theta(Z)$

Maximum Likelihood approach is problematic

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

$$KL(\mathbb{P}||\mathbb{Q}) = \int_x \mathbb{P}(x) \log \frac{\mathbb{P}(x)}{\mathbb{Q}(x)} dx$$

and given function $\mathbb{P}_\theta$, 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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- This unfortunately introduces some error, and empirically people have needed to add a lot of random noise to make models train

Transforming an existing distribution

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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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Kullback-Leibler (KL) divergence

$$KL(\mathbb{P}_r || \mathbb{P}_\theta) = \int_x \mathbb{P}_r(x) \log \frac{\mathbb{P}_r(x)}{\mathbb{P}_\theta(x)} d\mu(x)$$

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

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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 $\mathbb{P}_\theta$

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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 $\mathbb{P}_\theta$. For scoring, the effort spent is

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

Learning Parallel Lines Example

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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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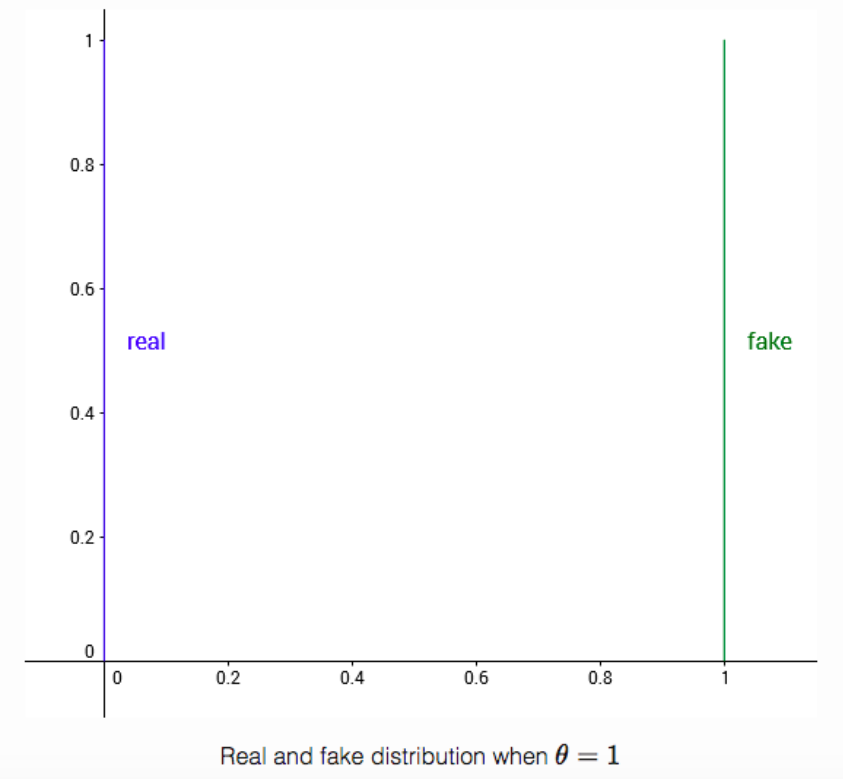

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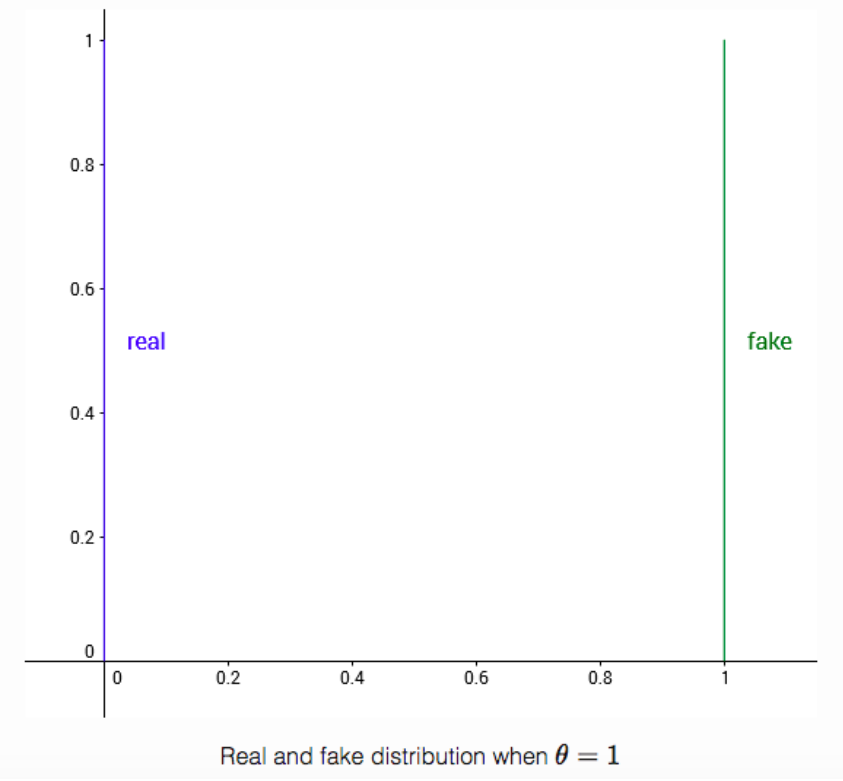

Real and fake distribution when $\theta = 1$

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.

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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 $\mathbb{P}_\theta$ 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*
   - $W(\mathbb{P}_n, \mathbb{P}) \to 0$
   - $\mathbb{P}_n \xrightarrow{D} \mathbb{P}$ *where* $\xrightarrow{D}$ *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 generator is trained to fool the discriminator.

Generative Adversarial Networks

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

$$\min_G \max_D \mathbb{E}_{x \sim \mathbb{P}_r}[\log(D(x))] + \mathbb{E}_{\widetilde{x} \sim \mathbb{P}_g}[\log(1 - D(\widetilde{x})]$$

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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- If the discriminator is trained to optimality before each generator parameter update, minimizing the value function amounts to minimizing the Jensen-Shannon divergence between the data and model distributions on x
- 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

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

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

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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$$\max_{w \in W} \mathbb{E}_{x \sim \mathbb{P}_r}[f_w(x)] - \mathbb{E}_{x \sim \mathbb{P}_\theta}[f_w(x)] \leq \sup_{||f||_L \leq K} \mathbb{E}_{x \sim \mathbb{P}_r}[f(x)] - \mathbb{E}_{x \sim \mathbb{P}_\theta}[f(x)]$$

$$= K \cdot W(\mathbb{P}_r, \mathbb{P}_\theta)$$

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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.

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

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Important Detail

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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.

Wasserstein GAN Algorithm

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

Comparison with Standard GANs

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- 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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- Although GANs are formulated as a min max problem, in practice we never train D to convergence
- 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

Properties of optimal WGAN critic

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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?

Properties of optimal WGAN critic

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If the optimal critic under the Kantorovich-Rubinstein dual D^* is differentiable, and x is a point from our generator distribution $\mathbb{P}_\theta$, 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, $\nabla D^*(x_t) = \frac{y - x_t}{||y - x_t||}$.

This implies that the optimal WGAN critic has gradients with norm 1 almost everywhere under $\mathbb{P}_r$ and $\mathbb{P}_\theta$

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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:

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

WGAN with gradient penalty

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

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.

while θ has not converged **do**
  for $t = 1, ..., n_{\text{critic}}$ **do**
    for $i = 1, ..., m$ **do**
      Sample real data $\boldsymbol{x} \sim \mathbb{P}_r$, latent variable $\boldsymbol{z} \sim p(\boldsymbol{z})$, a random number $\epsilon \sim U[0, 1]$.
      $\tilde{\boldsymbol{x}} \leftarrow G_\theta(\boldsymbol{z})$
      $\hat{\boldsymbol{x}} \leftarrow \epsilon \boldsymbol{x} + (1 - \epsilon)\tilde{\boldsymbol{x}}$
      $L^{(i)} \leftarrow D_w(\tilde{\boldsymbol{x}}) - D_w(\boldsymbol{x}) + \lambda(\|\nabla_{\hat{\boldsymbol{x}}} D_w(\hat{\boldsymbol{x}})\|_2 - 1)^2$
    end for
    $w \leftarrow \text{Adam}(\nabla_w \frac{1}{m} \sum_{i=1}^{m} L^{(i)}, w, \alpha, \beta_1, \beta_2)$
  end for
  Sample a batch of latent variables $\{\boldsymbol{z}^{(i)}\}_{i=1}^{m} \sim p(\boldsymbol{z})$.
  $\theta \leftarrow \text{Adam}(\nabla_\theta \frac{1}{m} \sum_{i=1}^{m} -D_w(G_\theta(\boldsymbol{z})), \theta, \alpha, \beta_1, \beta_2)$
end while