Kantorovich-Rubinstein Duality

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The Wasserstein GAN [Arjovsky et al., 2017] seeks to minimize the objective

$$\underset{\theta}{\arg\min} W(p, p_{\theta}) = \underset{\theta}{\arg\min} \inf_{\pi \in \Pi(p,q)} \mathop{\mathbb{E}}_{(x,y) \sim \pi} \left[\|x - y\|_2 \right].$$

In this form, the inner estimation of the Wasserstein distance $W(p, p_{\theta})$ is intractable. But using a delicate duality argument, we are able to reformulate the Wasserstein distance as the solution to a maximization over 1-Lipschitz functions. This turns the Wasserstein GAN optimization problem into a saddle-point problem, analogous to the f-GAN. The following proof is loosely based on Basso [2015]; here we take a more concrete approach and fill in the details of the argument.

Theorem. (Kantorovich-Rubinstein)

$$W(p,q) = \inf_{\pi \in \Pi(p,q)} \mathop{\mathbb{E}}_{(x,y) \sim \pi} \left[\|x - y\|_2 \right] = \sup_{\|h\|_L \le 1} \left[\mathop{\mathbb{E}}_{x \sim p} \left[h(x) \right] - \mathop{\mathbb{E}}_{y \sim q} \left[h(x) \right] \right].$$

Proof. Introduce Lagrange multipliers $f, g : \mathcal{X} \to \mathbb{R}$ (bounded, measurable):

$$\begin{split} L(\pi, f, g) &= \int_{\mathcal{X} \times \mathcal{X}} \|x - y\|^2 \pi(x, y) \, dy \, dx + \int_{\mathcal{X}} \left(p(x) - \int_{\mathcal{X}} \pi(x, y) \, dy \right) f(x) \, dx \\ &+ \int_{\mathcal{X}} \left(q(y) - \int_{\mathcal{X}} \pi(x, y) \, dx \right) g(y) \, dy. \end{split}$$

Collecting terms algebraically, we can rewrite the Lagrangian as

$$L(\pi, f, g) = \mathop{\mathbb{E}}_{x \sim p} [f(x)] + \mathop{\mathbb{E}}_{y \sim q} [g(y)] + \int_{\mathcal{X} \times \mathcal{X}} \left(\|x - y\|_2 - f(x) - g(y) \right) \pi(x, y) \, dy \, dx.$$

And we appeal to strong duality to write

$$W(p, p_g) = \inf_{\pi} \sup_{f,g} L(\pi, f, g) = \sup_{f,g} \inf_{\pi} L(\pi, f, g).$$

Note that if $||x - y||_2 < f(x) + g(y)$ for some $x, y \in \mathcal{X}$ then we can concentrate mass of π at (x, y) and send $L(\pi, f, g)$ to $-\infty$. Therefore, for all x, y, we must have

$$f(x) + g(y) \le ||x - y||_2.$$

And with this constraint, the best we can do by minimizing over π is to set $\pi = 0$:

$$\sup_{f,g} \inf_{\pi} L(\pi, f, g) = \sup_{\substack{f,g \\ f(x) + g(y) \le \|x - y\|_2}} \left| \mathop{\mathbb{E}}_{x \sim p} \left[f(x) \right] + \mathop{\mathbb{E}}_{y \sim q} \left[g(y) \right] \right| = W(p,q).$$

We now perform an amazing sleight-of-hand. First, observe that optimizing over the class of 1-Lipschitz functions give us a lower bound on the Wasserstein distance; if h is 1-Lipschitz then

$$\mathbb{E}_{x \sim p} [h(x)] - \mathbb{E}_{y \sim q} [h(y)] = \int_{\mathcal{X} \times \mathcal{X}} (h(x) - h(y)) \, \pi(x, y) \, dx \, dy$$
$$\leq \int_{\mathcal{X} \times \mathcal{X}} \|x - y\|_2 \, \pi(x, y) \, dx \, dy \leq W(p, q).$$

It follows that

$$\sup_{\|h\|_{L} \le 1} \left[\mathbb{E}_{x \sim p} \left[h(x) \right] - \mathbb{E}_{y \sim q} \left[h(y) \right] \right] \le W(p,q).$$

Next we will show that the upper bound is attained.

Consider the function κ defined by

$$x \mapsto \inf_{u} \left[\|x - u\|_2 - g(u) \right].$$

Because g is bounded, the infimum is finite and this function is well-defined. Claim: κ is 1-Lipschitz. Given $x, y \in \mathcal{X}$, for any $u \in \mathcal{X}$ the triangle inequality give us

$$\kappa(x) \le ||x - u||_2 - g(y) \le ||x - y||_2 + ||y - u||_2 - g(u).$$

This holds for any u and therefore

$$\kappa(x) \le \|x - y\|_2 + \inf_u \left[\|x - u\|_2 - g(u) \right] = \|x - y\|_2 + \kappa(y).$$

I.e. $\kappa(x) - \kappa(y) \le ||x - y||_2$; exchanging x and y gives us $\kappa(y) - \kappa(x) \le ||x - y||_2$ and consequently κ is 1-Lipschitz:

$$|\kappa(x) - \kappa(y)| \le ||x - y||_2.$$

For any pair f, g that satisfies $f(x) + g(y) \le ||x - y||_2$,

$$f(x) \le \kappa(x) \le ||x - x||_2 - g(x) = -g(x).$$

From these facts, we have

$$\mathop{\mathbb{E}}_{x \sim p} \left[f(x) \right] + \mathop{\mathbb{E}}_{y \sim q} \left[g(y) \right] \le \mathop{\mathbb{E}}_{x \sim p} \left[\kappa(x) \right] - \mathop{\mathbb{E}}_{y \sim q} \left[\kappa(y) \right]$$

And we conclude that

$$W(p,q) = \sup_{\substack{f,g\\f(x)+g(y) \le \|x-y\|_2}} \left[\mathbb{E}_{x \sim p} \left[f(x) \right] + \mathbb{E}_{y \sim q} \left[g(y) \right] \right]$$
$$\leq \sup_{\|h\|_L \le 1} \left[\mathbb{E}_{x \sim p} \left[h(x) \right] - \mathbb{E}_{y \sim q} \left[h(y) \right] \right] \le W(p,q).$$

References

Martin Arjovsky, Soumith Chintala, and Léon Bottou. Wasserstein gan. International Conference on Machine Learning, 2017. (document)

Giuliano Basso. A hitchhikers guide to wasserstein distances, 2015. (document)