The Metric side of Optimal Transport

Jonas Müller

Outline

1. A metric for probabilites?
    - The Wasserstein distance
    - Dudley Lemma
    - Wasserstein for normal distributions
2. Lifting completeness from X to $\mathcal{P}_p(X)$
    - Iterated Dudley Lemma
3. Some things in case time permits
    - Comparing L^2 and Wasserstein distance
    - Duality for the Wasserstein 1 Metric
    - Wasserstein ∞ metric

The Wasserstein distance for finite p

As a reminder, we have for any $p \in [1, \infty[$

$$\mathcal{P}_p(X) := \left\{ \mu \in \mathcal{P}(X) \mid \int_X d^p(x, x_0)\, \mathrm{d}\mu(x) < \infty \right\}$$

and the following will be a metric on this space.

Definition

For any $p \in [1, \infty[$ and $\nu, \mu \in \mathcal{P}_p(X)$

$$W_p^p(\mu, \nu) := \min \left\{ \int_{X \times X} d^p(x, y) \mathrm{d}\pi(x, y) \mid \pi \in \Gamma(\mu, \nu) \right\}.$$

Theorem

$(\mathcal{P}_p(X), W_p)$ *is a metric space!*

Proof of Theorem

We assume $p = 2$, which makes it less messy, the other cases are similar.

1. $W_2(\mu, \nu) < \infty$ always
2. $\mu = \nu \Leftrightarrow W_2(\mu, \nu) = 0$
3. $W_2(\mu, \nu) = W_2(\nu, \mu)$
4. Dudley Lemma for triangle inequality
5. $W_2(\mu_1, \mu_3) \leq W_2(\mu_1, \mu_2) + W_2(\mu_2, \mu_3)$.

Reminder

Let $T : X \to Y$ be a measurable function and let μ, ν be measures on X, Y, then we have the Change of Variables Formula:

$$\int_Y f(y)\, d(T_\# \mu)(y) = \int_X f(T(x))\, d\mu(x).$$

Additionally, for any metric d on X it holds for any $x_0 \in X$ that

$$d^2(x, y) \leq (d(x, x_0) + d(x_0, y))^2 \leq 2(d^2(x, x_0) + d^2(x_0, y))$$

because $2ab \leq a^2 + b^2$ always.

The Dudley Lemma

In the Literature this is often called Gluing Lemma!

Lemma

Let $(X_1, \mu_1), (X_2, \mu_2), (X_3, \mu_3)$ *be Polish and* $\pi^{1,2} \in \Gamma(\mu_1, \mu_2)$ *and* $\pi^{2,3} \in \Gamma(\mu_2, \mu_3)$. *Then there exists some* $\pi \in \mathcal{P}(X_1 \times X_2 \times X_3)$ *such that*

$$p^{1,2}_{\#}(\pi) = \pi^{1,2} \quad \text{and} \quad p^{2,3}_{\#}(\pi) = \pi^{2,3}$$

where $p^{1,2}(x_1, x_2, x_3) = (x_1, x_2)$ *and* $p^{2,3}(x_1, x_2, x_3) = (x_2, x_3)$.

Proof is essentially just taking the product measures of the Disintegration's of $\pi^{2,3}$ and $\pi^{1,2}$ and "Gluing" them together with μ_2.

Triangle inequality

Let $\mu_1, \mu_2, \mu_3 \in \mathcal{P}_2(X)$, $\pi^{1,2} \in \Gamma_o(\mu_1, \mu_2)$ and $\pi^{2,3} \in \Gamma_o(\mu_2, \mu_3)$ and π is the measure we get from gluing $\pi^{1,2}$ with $\pi^{2,3}$. Let $p^{1,3}_{\#}(\pi) = \pi^{1,3} \in \Gamma(\mu_1, \mu_3)$.

$$W_2(\mu_1, \mu_3) \leq \left(\int_{X \times X} d^2(x_1, x_3) \mathrm{d}\pi^{1,3}(x_1, x_3) \right)^{1/2}$$

.

Triangle inequality

Let $\mu_1, \mu_2, \mu_3 \in \mathcal{P}_2(X)$, $\pi^{1,2} \in \Gamma_o(\mu_1, \mu_2)$ and $\pi^{2,3} \in \Gamma_o(\mu_2, \mu_3)$ and π is the measure we get from gluing $\pi^{1,2}$ with $\pi^{2,3}$. Let $p^{1,3}_{\#}(\pi) = \pi^{1,3} \in \Gamma(\mu_1, \mu_3)$.

$$W_2(\mu_1, \mu_3) \leq \left(\int_{X \times X} d^2(x_1, x_3) \mathrm{d}\pi^{1,3}(x_1, x_3) \right)^{1/2}$$

$$\overset{!}{=} \left(\int_{X \times X \times X} d^2(x_1, x_3) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2}$$

.

Triangle inequality

Let $\mu_1, \mu_2, \mu_3 \in \mathcal{P}_2(X)$, $\pi^{1,2} \in \Gamma_o(\mu_1, \mu_2)$ and $\pi^{2,3} \in \Gamma_o(\mu_2, \mu_3)$ and π is the measure we get from gluing $\pi^{1,2}$ with $\pi^{2,3}$. Let $p^{1,3}_{\#}(\pi) = \pi^{1,3} \in \Gamma(\mu_1, \mu_3)$.

$$W_2(\mu_1, \mu_3) \leq \left(\int_{X \times X} d^2(x_1, x_3) \mathrm{d}\pi^{1,3}(x_1, x_3) \right)^{1/2}$$

$$\overset{!}{=} \left(\int_{X \times X \times X} d^2(x_1, x_3) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2}$$

$$\leq \left(\int_{X \times X \times X} [d(x_1, x_2) + d(x_2, x_3)]^2 \, \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2}$$

.

Triangle inequality

Let $\mu_1, \mu_2, \mu_3 \in \mathcal{P}_2(X)$, $\pi^{1,2} \in \Gamma_o(\mu_1, \mu_2)$ and $\pi^{2,3} \in \Gamma_o(\mu_2, \mu_3)$ and π is the measure we get from gluing $\pi^{1,2}$ with $\pi^{2,3}$. Let $p^{1,3}_{\#}(\pi) = \pi^{1,3} \in \Gamma(\mu_1, \mu_3)$.

$$
\begin{aligned}
W_2(\mu_1, \mu_3) &\leq \left(\int_{X \times X} d^2(x_1, x_3) \mathrm{d}\pi^{1,3}(x_1, x_3) \right)^{1/2} \\
&\overset{!}{=} \left(\int_{X \times X \times X} d^2(x_1, x_3) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} \\
&\leq \left(\int_{X \times X \times X} \left[d(x_1, x_2) + d(x_2, x_3) \right]^2 \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} \\
&\overset{*}{\leq} \left(\int_{X \times X \times X} d^2(x_1, x_2) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} + \left(\int_{X \times X \times X} d^2(x_2, x_3) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2}
\end{aligned}
$$

.

Triangle inequality

Let $\mu_1, \mu_2, \mu_3 \in \mathcal{P}_2(X)$, $\pi^{1,2} \in \Gamma_o(\mu_1, \mu_2)$ and $\pi^{2,3} \in \Gamma_o(\mu_2, \mu_3)$ and π is the measure we get from gluing $\pi^{1,2}$ with $\pi^{2,3}$. Let $p_\#^{1,3}(\pi) = \pi^{1,3} \in \Gamma(\mu_1, \mu_3)$.

$$
\begin{aligned}
W_2(\mu_1, \mu_3) &\leq \left(\int_{X \times X} d^2(x_1, x_3) \mathrm{d}\pi^{1,3}(x_1, x_3) \right)^{1/2} \\
&\overset{!}{=} \left(\int_{X \times X \times X} d^2(x_1, x_3) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} \\
&\leq \left(\int_{X \times X \times X} \left[d(x_1, x_2) + d(x_2, x_3) \right]^2 \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} \\
&\overset{*}{\leq} \left(\int_{X \times X \times X} d^2(x_1, x_2) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} + \left(\int_{X \times X \times X} d^2(x_2, x_3) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} \\
&\overset{!}{=} \left(\int_{X \times X} d^2(x_1, x_2) \mathrm{d}\pi^{1,2}(x_1, x_2) \right)^{1/2} + \left(\int_{X \times X} d^2(x_2, x_3) \mathrm{d}\pi^{2,3}(x_2, x_3) \right)^{1/2}
\end{aligned}
$$

.

Triangle inequality

Let $\mu_1, \mu_2, \mu_3 \in \mathcal{P}_2(X)$, $\pi^{1,2} \in \Gamma_o(\mu_1, \mu_2)$ and $\pi^{2,3} \in \Gamma_o(\mu_2, \mu_3)$ and π is the measure we get from gluing $\pi^{1,2}$ with $\pi^{2,3}$. Let $p_{\#}^{1,3}(\pi) = \pi^{1,3} \in \Gamma(\mu_1, \mu_3)$.

$$
\begin{aligned}
W_2(\mu_1, \mu_3) &\leq \left(\int_{X \times X} d^2(x_1, x_3) \mathrm{d}\pi^{1,3}(x_1, x_3) \right)^{1/2} \\
&\overset{!}{=} \left(\int_{X \times X \times X} d^2(x_1, x_3) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} \\
&\leq \left(\int_{X \times X \times X} \left[d(x_1, x_2) + d(x_2, x_3) \right]^2 \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} \\
&\overset{*}{\leq} \left(\int_{X \times X \times X} d^2(x_1, x_2) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} + \left(\int_{X \times X \times X} d^2(x_2, x_3) \mathrm{d}\pi(x_1, x_2, x_3) \right)^{1/2} \\
&\overset{!}{=} \left(\int_{X \times X} d^2(x_1, x_2) \mathrm{d}\pi^{1,2}(x_1, x_2) \right)^{1/2} + \left(\int_{X \times X} d^2(x_2, x_3) \mathrm{d}\pi^{2,3}(x_2, x_3) \right)^{1/2} \\
&= W_2(\mu_1, \mu_2) + W_2(\mu_2, \mu_3).
\end{aligned}
$$

Wasserstein distance for normal distributions

For any $\mu_X, \mu_Y \in \mathcal{P}_2(\mathbb{R}^d)$ with $\mathcal{L}(X) = \mu_X$ and $\mathcal{L}(Y) = \mu_Y$ where X and Y are normally distributed, the Wasserstein distance can be calculated as follows

$$W_2^2(\mu_x, \mu_Y) = \|m_X - m_Y\|^2 + \operatorname{tr}\left(\Sigma_X - 2 \cdot \left(\Sigma_Y^{1/2} \Sigma_X \Sigma_Y^{1/2}\right)^{1/2} + \Sigma_Y\right)$$

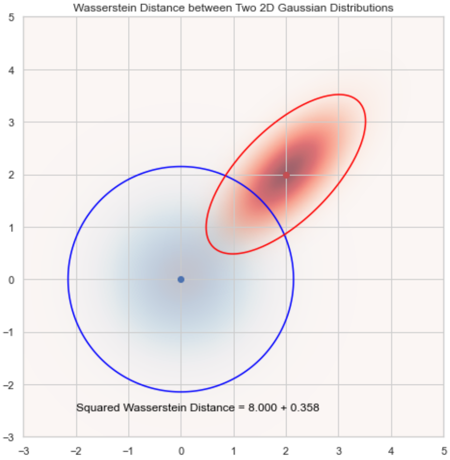
If Σ_X and Σ_Y commute, this simplifies to

$$W_2^2(\mu_x, \mu_Y) = \|m_X - m_Y\|^2 + \sum_{i=1}^{d} \left(\sqrt{\lambda_i^X} - \sqrt{\lambda_i^Y}\right)^2$$

where λ_i^X and λ_i^Y are the Eigenvalues of Σ_X and Σ_Y respectively.

Normally distributed examples

Assume $\Sigma_X = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\Sigma_Y = \begin{pmatrix} \frac{1}{2} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{2} \end{pmatrix}$ with $m_X = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and $m_Y = \begin{pmatrix} 2 \\ 2 \end{pmatrix}$.



Lifting completeness from X to $\mathcal{P}_p(X)$

We remind ourselves of the metric version of the L^p spaces.

$$L^p(\Omega, \mathcal{F}, P, X) := \left\{ f : \Omega \to X \mid f \text{ measurable }, \int_\Omega d^p(f, z_0) dP < \infty \right\}$$

with

$$d^p_{L^p}(f, g) := \int_\Omega d^p(f, g) dP$$

These are not necessarily vector spaces, but one can show that this more general notion of L^p space is still complete if (X, d) is.
This completeness is important for the following Theorem.

Theorem

Let (X, d) be a complete metric space, then $(\mathcal{P}_p(X), W_p)$ is complete.

Iterated Dudley Lemma

We want to represent a sequence of measures (μ_n) as the marginals of some measure in an infinite product space.

For that we need the iterated Dudley Lemma. Note that we also allow $N = \infty$ in this Lemma, in that case, the $\leq$ become $<$.

Lemma

Let $N \geq 3$ and for any $n \leq N$ (X_n, d_n) Polish, $\mu_n \in \mathcal{P}(X_n)$ and $\theta_n \in \Gamma(\mu_{n-1}, \mu_n)$. Then there exists $\pi_n \in \mathcal{P}(X_1 \times \ldots \times X_n)$ for any $n \leq N$ such that.

1. $p_{\#}^{1,\ldots,n-1}\pi_n = \pi_{n-1}$ *for* $2 \leq n \leq N$
2. $p_{\#}^{i}\pi_n = \mu_i$ *for* $1 \leq i \leq n \leq N$
3. $p_{\#}^{i-1,i}\pi_n = \theta_i$ *for* $2 \leq i \leq n \leq N$

Proof is just applying the Dudley Lemma iteratively (hence the name :).

Proof of completeness

We again consider $p = 2$. Assume $(\mu_n) \subseteq \mathcal{P}_2(X)$ is Cauchy.

1. Applying Iterated Dudley on (X, μ_n) to get $(\pi_n)_{n\in\mathbb{N}}$
2. Get π_∞ on $\mathbb{X} = \prod_{i=1}^{\infty} X$ with $p_\#^{(1,\ldots,n)}(\pi_\infty) = \pi_n$ by Ionescu-Tulcea.
3. Show that the projections (p_n) are Cauchy in $L^2(\mathbb{X}, \mathcal{B}_\infty, \pi_\infty, X)$
4. Use that $L^2(\mathbb{X}, \mathcal{B}_\infty, \pi_\infty, X)$ is complete to get $p_n \to p_\infty$
5. Define $\mu_\infty = (p_\infty)_\#(\pi_\infty)$ and prove $\mu_n \xrightarrow{W_2} \mu_\infty$.

Reminder

If $\sum_{k=1}^{\infty} d(x_n, x_{n+1}) < \infty$ *then* (x_n) *is Cauchy.*

Also earlier in the Book, we had

$$S_\#(P) = \mu \quad \text{and} \quad T_\#(P) = \nu \Rightarrow (S, T)_\#(P) \in \Gamma(\mu, \nu).$$

Comparing L^2 norm and Wasserstein distance

Let $\nu \ll \lambda^n$ with Radon Nikodym derivative f such that $\mathrm{supp}(f) \subseteq \overline{B_1}$.

Additionally, let $\mu_h \ll \lambda^n$ such that $f_h(x) = f(x+h)$. Then we have

$$\|f_h - f\|^2_{L^2(\mathbb{R}^n)} = 2\|f\|^2_{L^2(\mathbb{R}^n)}$$

but on the other hand

$$W_2(\mu_h, \mu) = \|h\|_2$$

which for large $\|h\|$ implies

$$W_2(\mu_h, \mu) \gg \|f_h - f\|_{L^2(\mathbb{R}^n)}.$$

In case of small $\|h\|$ we can also find $W_2(\mu_h, \mu) \ll \|f_h - f\|_{L^2(\mathbb{R}^n)}$.

Duality for the Wasserstein Distance

By the Kantorovich-Rubinstein Duality we have

$$\begin{aligned} W_1(\mu,\nu) &= \sup_{(\phi,\psi)\in I_c} \left\{ \int_X \phi d\mu + \int_X \psi d\nu \right\} \\ &= \sup_{\|\phi\|_{Lip}\leq 1} \left\{ \int_X \phi d\mu + \int_X \phi^c d\nu \right\} \\ &= \sup_{\|\phi\|_{Lip}\leq 1} \left\{ \int_X \phi d\mu - \int_X \phi d\nu \right\} \end{aligned}$$

where the first equality holds for any W_p distance, the latter need that $c = d$.

Wasserstein distance for $p = \infty$

If we restrict ourselves to $\mathcal{P}_\infty(X)$, the space of probability measures with bounded support. We can also define W_∞ as the limit of W_p.

$$\lim_{p\to\infty} W_p(\mu,\nu) = W_\infty(\mu,\nu) = \inf\{\|d(x,y)\|_{L^\infty}(\pi) \mid \pi \in \Gamma(\mu,\nu)\}$$
$$= \inf_{\pi\in\Gamma(\mu,\nu)} \inf\{C \geq 0 \mid |d(x,y)| \leq C \text{ for } \pi \text{ almost all } (x,y)\}$$

and we have

$$(\mathcal{P}_\infty(X), W_\infty) \text{ is a metric space}$$