Wasserstein-Distance

This is an brief introduction to Wasserstein-Distance, including its formulation, computation and application.

Tutorials

1. Optimal Transport for Applied Mathematicians
2. Optimal Transport for Data Analysis
3. A user's guide to optimal transport

Introduction

We will start from some some intuitive examples.

Existing metrics

1. metrics
   1. KL divergence: $D_{\mathrm{KL}}(P\|Q)=-\sum_i P(i)\ln\frac{Q(i)}{P(i)}$
   2. JS divergence: $D_{\mathrm{JS}}(P,Q)=\frac{1}{2}\left(D_{\mathrm{KL}}\left(P\|\frac{P+Q}{2}\right)+D_{\mathrm{KL}}\left(Q\|\frac{P+Q}{2}\right)\right)$

3. F divergence: $D_f(p\|q)=\int q(x) f\left(\frac{p(x)}{q(x)}\right) dx$, where f is a convex function.
2. Issues
    1. can not evaluate 2 distributions with different support set.
        1. example: $\{p(x)|x\in[0,1]\}$ and $\{q(y)|y\in[2,3]\}$
    2. use KL/JS divergence as loss function -> gradient vanishing!
    3. need well-defined distance metric

Transportation problem

	D_1	D_2	$\cdots$	D_n	Supply
O_1	c_{11}	c_{12}	$\cdots$	c_{1n}	a_1
O_2	c_{21}	c_{22}	$\cdots$	c_{2n}	a_2
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
O_m	c_{m1}	c_{m2}	$\cdots$	c_{mn}	a_m
Demand	b_1	b_2	$\cdots$	b_n	

1. Problem:
    1. origin: $\{O_1,...,O_m\}$, destination: $\{D_1,...,D_n\}$
    2. supply: $\{a_1,...,a_m\}$, demand: $\{b_1,...,b_n\}$
    3. transport supply goods in origin locations to satisfy demand in destinations
    4. transport plan/matrix: x_{ij}
    5. transport cost: c_{ij}
2. Formulation
    1. Primal formation
       Minimize $\sum_{i=1}^m \sum_{j=1}^n c_{ij} x_{ij}$
       Subject to:

$$\begin{aligned}&\textstyle\sum_{j=1}^n x_{ij}=a_i \quad \text{for } i=1,2,\ldots,m\\ &\textstyle\sum_{i=1}^m x_{ij}=b_j \quad \text{for } j=1,2,\ldots,n\\ &x_{ij}\geq 0 \quad \text{for } i=1,2,\ldots,m \text{ and } j=1,2,\ldots,n\end{aligned}$$

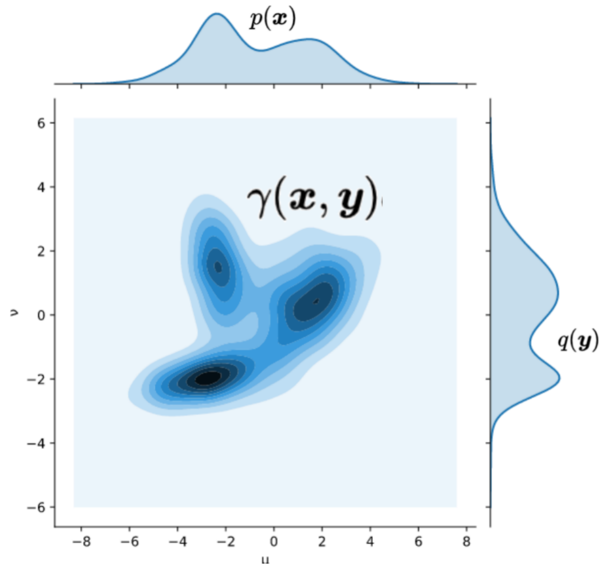
    2. Dual formulation
       Maximize $\sum_{i=1}^m a_i f_i+\sum_{i=1}^n b_i g_i$
       Subject to:

$$f_i+g_j\leq c_{ij} \quad \text{for } i=1,2,\ldots,m,\ \text{for } j=1,2,\ldots,n$$

Formulation

Wasserstein distance (Kantorovich formulation)

1. view it as a continuous version of transportation problem



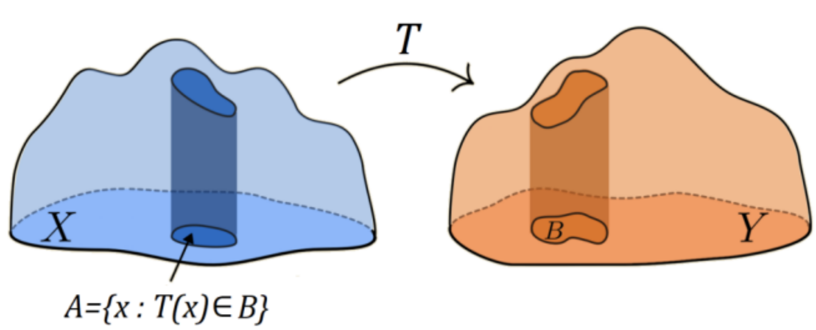
Minimize $\mathcal{W}[p, q] = \inf_{\gamma \in \Pi[p,q]} \iint \gamma(x, y) c(x, y) dx dy$
Subject to:

$$\int \gamma(x, y) dy = p(x)$$
$$\int \gamma(x, y) dx = q(y)$$

2. cost function $c(x, y)$:
   1. any norm, $\|x - y\|_1, \ \|x - y\|_2, \ \|x - y\|_2^2$
3. joint distribution $\gamma(x, y)$:
   1. with marginal distribution $\gamma(x) = p(x), \gamma(y) = q(y)$

Optimal transport and Wasserstein distance

1. Optimal transport (Monge formulation)



$$C_M(T) = \int_\Omega c(x, T(x))p(x)\mathrm{d}$$
$$q = T(p)$$

1. transport map: $q(y) = T(p(x))$
    1. non-linear constraint

Several dual formulations

Kantorovich-Rubinstein Duality

$$\mathcal{W}[p,q] = \max_{f,g}\left\{\int [p(x)f(x) + q(x)g(x)]dx \mid f(x) + g(y) \leq c(x,y)\right\}$$

1. primal-dual optimality condition
1. $f(x) + g(y) = c(x,y)$
2. Proof:
1. forward: if primal and dual reach optimality, then

$$\begin{align} & \underbrace{\iint \gamma(x,y)c(x,y)dxdy}_{\text{primal formulation}} \tag{1} \\ = & \underbrace{\int [p(x)f(x) + q(x)g(x)]dx}_{\text{primal=dual when reaching optimality}} \tag{2} \\ = & \underbrace{\iint [f(x) + g(y)]\gamma(x,y)dxdy}_{\text{marginal distribution}} \tag{3} \\ & \to f(x) + g(y) = c(x,y) \tag{4} \end{align}$$

2. backward: if $f(x) + g(y) = c(x,y)$ holds, then:

$$
\begin{aligned}
&\underbrace{\int [p(x)f(x)+q(x)g(x)]dx}_{\text{dual formulation}} && (5)\\
=&\underbrace{\iint [f(x)+g(y)]\gamma(x,y)dxdy}_{\text{marginal distribution}} && (6)\\
=&\underbrace{\iint \gamma(x,y)c(x,y)dxdy}_{f(x)+g(y)=c(x,y)} && (7)\\
&\rightarrow \text{primal} = \text{dual when reaching optimality} && (8)
\end{aligned}
$$

Lipschitz constrained formulation

$$
\mathcal{W}[p,q] = \max_f \left\{ \int [p(x)f(\boldsymbol{x}) - q(\boldsymbol{x})f(\boldsymbol{x})]dx \mid \|f\|_L \leq 1 \right\}
$$

1. consider the optimality condition when $x = y$
1. $f(y)+g(y)=c(y,y)=0 \rightarrow g(y)=-f(y)$
2. take $g(y)=-f(y)$ into the $\mathcal{W}[p,q]$
1. objective function: $\max_f \left\{ \int [p(x)f(\boldsymbol{x}) - q(\boldsymbol{x})f(\boldsymbol{x})]dx \right\}$
2. constraints: $\|f\|_L \leq 1$
1. $f(x)-f(y) \leq c(x,y)$ and $f(y)-f(x) \leq c(y,x)$
2. $\|f\|_L = \frac{|f(x)-f(y)|}{c(x,y)} \leq 1$

Unconstrained formulation

$$
\mathcal{W}[p,q] = \max_f \int f(x)dp(x) + \int \min_x [c(x,y)-f(x)]dq(y)
$$

1. C-transform:
For $f \in C(\Omega)$ define its c-transform $f^c \in C(\Omega)$ by

$$
f^c(y) = \inf\{c(x,y) - f(x) \mid x \in \Omega\}
$$

and its $\bar{c}$-transform $g^{\bar{c}} \in C(\Omega)$ by

$$
g^{\bar{c}}(x) = \inf\{c(x,y) - g(y) \mid y \in \Omega\}
$$

1. $f^{c\hat{c}}(x) \geq f(x)$, "$=$" holds when f is concave

2. Consider $g(y)$ is the C-transform of $f(x)$
1. $f^c(y) = \inf_x \{c(x,y) - f(x)\}$
2. Proof of such a transform will not affect the optimality
1. prove $f(x)$ and $f^c(y)$ satisfy the constraint

$$\begin{aligned} & f(x) + \inf\{c(x,y) - f(x)\} && (9) \\ \leq & f(x) + c(x,y) - f(x) && (10) \\ = & c(x,y) && (11) \end{aligned}$$

The constraint is always be satisfied under C-transform
2. prove $f(x)$ and $f^c(y)$ reach optimality condition

$$\begin{aligned} & f(x) = g^c(x) && (12) \\ \rightarrow & f^c(y) = g^{c\hat{c}}(y) \geq g(y) && (13) \\ \rightarrow & f(x) + f^c(y) \geq f(x) + g(y) && (14) \end{aligned}$$

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when $f(x)+g(y)=c(x,y)$, $c(x,y)\leq f(x)+f^{c}(y)\geq c(x,y)$
Therefore $f(x)+f^{c}(y)=c(x,y)$ and reaches optimality.
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Quadratic cost function

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1. quadratic cost function: $c(x,y)=\frac{1}{2}\|x-y\|^2$
2. The C-transform can be simplified as:
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$$\begin{aligned} f(x) &= \inf_y \left\{ \frac{1}{2}\|x-y\|^2 - g(y) \right\} \\ &= \frac{1}{2}\|x\|^2 + \inf_y \left\{ -\langle x, y\rangle + \frac{1}{2}\|y\|^2 - g(y) \right\} \\ &= \frac{1}{2}\|x\|^2 - \underbrace{\sup_y \left\{ \langle x, y\rangle - \left[\frac{1}{2}\|y\|^2 - g(y) \right] \right\}}_{:=\phi(x):\text{convex}} \end{aligned}$$

1. $\phi(x)$ is the convex conjugate of $\frac{1}{2}\|y\|^2 - g(y)$
1. Brenier theorem:
1. Under quadratic case, optimal transport map $T(x)$ is equivalent with transport plan $\gamma(x,y)$

$$T(x) = x - \nabla f(x) = x - (x - \nabla\phi(x)) = \nabla\phi(x)$$

Convex formulation

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1. under quadratic case:
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$$
\begin{aligned}
&f(x)+g(y) \leq \tfrac{1}{2}\|x-y\|_2^2 \Longleftrightarrow \\
&\left[\tfrac{1}{2}\|x\|_2^2-f(x)\right]+\left[\tfrac{1}{2}\|y\|_2^2-g(y)\right] \geq \langle x, y\rangle
\end{aligned}
$$

2. define:
1. $f'(x)=\frac{1}{2}\|x\|_2^2-f(x)$
2. $g'(y)=\frac{1}{2}\|y\|_2^2-g(y)$
3. The objective function becomes:

$$
\begin{aligned}
&\mathcal{W}[p, q]=C_{p, q}-\min_{f', g'}\left\{\mathbb{E}_p\left[f'(x)\right]+\mathbb{E}_q\left[g'(y)\right] \mid f'(x)+g'(y) \geq\langle x, y\rangle\right\} \\
&C_{p, q}=\tfrac{1}{2} \mathbb{E}_p\left[\|X\|_2^2\right]+\mathbb{E}_q\left[\|Y\|_2^2\right]
\end{aligned}
$$

4. apply the conjugate transformation
1. $g'(y)=f^{'*}(y)=\sup_x\left\{\langle x, y\rangle-\underbrace{\left[\frac{1}{2}\|x\|^2-f(x)\right]}_{f'(x)}\right\}$
5. unconstrained optimization

$$
\mathcal{W}[p, q]=C_{p, q}-\min_{f', g'}\left\{\mathbb{E}_p\left[f'(x)\right]+\mathbb{E}_q\left[f^{'*}(y)\right]\right\}
$$

1. similar proof as C-transform
1. constraint:
1. $f'(x)+f^{'*}(y) \geq\langle x, y\rangle$
2. optimality
1. $f^{**} \leq f$, "$=$" holds when f is convex
2. f' and g' are convex
1. According to the Brenier theorem, when reach optimality
1. $\nabla g'(y)=T(y)$ is the optimal transport map
2. $f^{'*}(y)=\sup_x\left\{\langle x, y\rangle-\left[\frac{1}{2}\|x\|^2-f(x)\right]\right\}=\langle T(y), y\rangle-\left[\frac{1}{2}\|T(y)\|^2-f(T(y))\right]$
2. convex formulation:

$$
\mathcal{W}[p, q]=C_{p, q}-\min_{f' \in \mathrm{cvx}} \max_{g' \in \mathrm{cvx}}\left\{\mathbb{E}_p\left[f'(x)\right]+\mathbb{E}_q\left[f^{'*}(y)\right]\right\}
$$

Computation

Application