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 for evaluating distance between distributions

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 $\quad \sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}x_{ij}$
       Subject to:

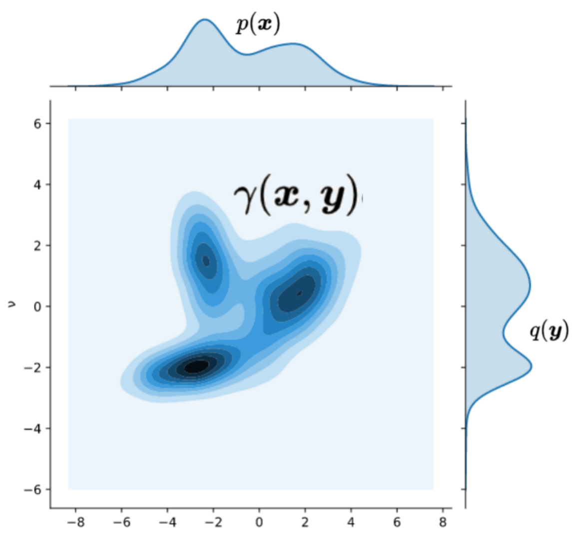
$$\begin{aligned}&\textstyle\sum_{j=1}^{n} x_{ij} = a_i \quad \text{for } i = 1, 2, \ldots, m\\ &\textstyle\sum_{i=1}^{m} x_{ij} = b_j \quad \text{for } j = 1, 2, \ldots, n\\ &x_{ij} \geq 0 \quad \text{for } i = 1, 2, \ldots, m \text{ and } j = 1, 2, \ldots, n\end{aligned}$$

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

1. Wasserstein distance (Kantorovich formulation)
    1. view it as a continuous version of transportation problem

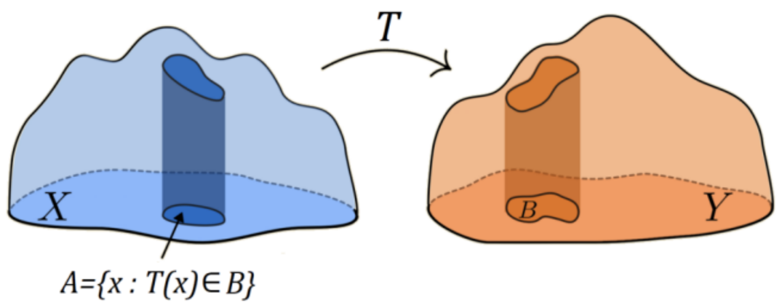


       Minimize $\mathcal{W}[p, q] = \inf_{\gamma\in\Pi[p,q]} \iint \gamma(x, y)c(x, y)dxdy$
       Subject to:

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

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 $\gamma(x)=p(x), \gamma(y)=q(y)$

2. 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

3. Several dual formulations
    1. Kantorovich-Rubinstein Duality

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

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

$$\underbrace{\iint \gamma(x,y)c(x,y)dxdy}_{\text{primal formulation}} \tag{1}$$

$$= \underbrace{\int [p(x)f(x) + q(x)g(x)]dx}_{\text{primal=dual when reaching optimality}} \tag{2}$$

$$= \underbrace{\iint [f(x) + g(y)]\gamma(x,y)dxdy}_{\text{marginal distribution}} \tag{3}$$

$$\to f(x) + g(y) = c(x,y) \tag{4}$$

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

$$\underbrace{\int [p(x)f(x) + q(x)g(x)]dx}_{\text{dual formulation}} \tag{5}$$

$$= \underbrace{\iint [f(x) + g(y)]\gamma(x,y)dxdy}_{\text{marginal distribution}} \tag{6}$$

$$= \underbrace{\iint \gamma(x,y)c(x,y)dxdy}_{f(x)+g(y)=c(x,y)} \tag{7}$$

$$\to \text{primal} = \text{dual when reaching optimality} \tag{8}$$

2. Lipschitz constrained formulation

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

1. consider the optimality condition when $x = y$
   1. $f(y) + g(y) = c(y,y) = 0 \to g(y) = -f(y)$
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: $\|f\|_L \le 1$
      1. $f(x) - f(y) \le c(x,y)$ and $f(y) - f(x) \le c(y,x)$
      2. $\|f\|_L = \frac{|f(x)-f(y)|}{c(x,y)} \le 1$

3. 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

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

         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.

4. Quadratic cost function
   1. quadratic cost function: $c(x,y) = \frac{1}{2}\|x-y\|^2$
   2. The C-transform can be simplified as:

$$
\begin{aligned}
f(x) &= \inf_y \left\{ \frac{1}{2}\|x-y\|^2 - g(y) \right\} \\
&= \frac{1}{2}\|x\|^2 + \inf_y \left\{ -\langle x, y\rangle + \frac{1}{2}\|y\|^2 - g(y) \right\} \\
&= \frac{1}{2}\|x\|^2 - \underbrace{\sup_y \left\{ \langle x, y\rangle - \left[\frac{1}{2}\|y\|^2 - g(y) \right] \right\}}_{:=\phi(x):\text{convex}}
\end{aligned}
$$

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

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

5. Convex formulation
    1. under quadratic case:

$$
\begin{aligned}
&f(x) + g(y) \le \tfrac{1}{2}\|x-y\|_2^2 \iff \\
&\left[\tfrac{1}{2}\|x\|_2^2 - f(x)\right] + \left[\tfrac{1}{2}\|y\|_2^2 - g(y)\right] \ge \langle x, y\rangle
\end{aligned}
$$

    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:

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

    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

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

        1. similar proof as C-transform
            1. constraint:
                1. $f'(x) + f^{'*}(y) \ge \langle x, y\rangle$

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

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

Computation

Application