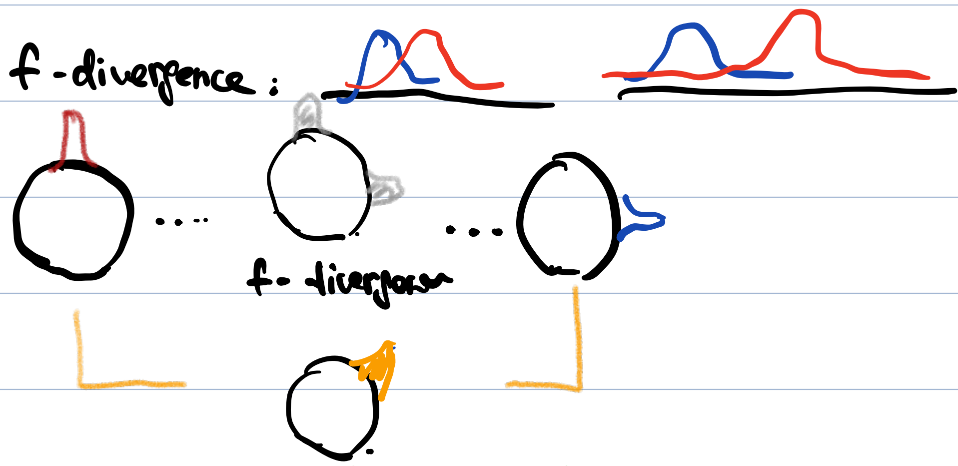
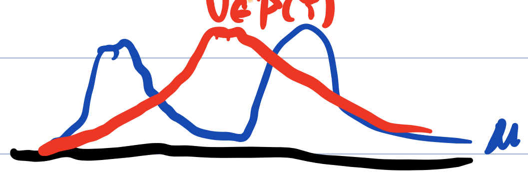
Introduction to Optimal Transport. (and Particle Systems)

Motivation. f-divergence:



Optimal Transport (Earth Moving distance, Wasserstein Distance)

Monge $\mu \in P(X)$



$\nu \in P(Y)$.

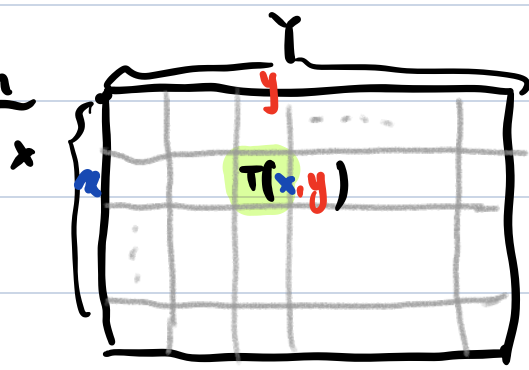
measurable map: $T: X \to Y$

① $\nu(A) = \mu(T^{-1}(A))$

② minimize. $\int_X \underline{c(x, T(x))}\, d\mu(x)$.

$c(x,y)$ is a cost function.

Kantorovich's Problem



$T(x,y)$: how many products I transport from x to y

$$\min_{T \geq 0} \sum_{x,y} T(x,y)\, c(x,y) \longrightarrow \min_{T \geq 0} \int T(x,y)\, c(x,y)\, dx\, dy$$

s.t. $\sum_y T(x,y) = \mu(x)$

$\sum_x T(x,y) = \nu(y)$

s.t. $\int_y T(x,y)\, dy = \mu(x) \quad \forall x$

$\underbrace{\int_x T(x,y)\, dx = \nu(y)}_{\text{coupling}} \quad \forall y$

$\sum_x \varphi(x) \left[\sum_y T(x,y) - \mu(x) \right]$

Optimal Transport as IPM (Kantorovich Duality)

$$\min_{T\geq 0}\sup_{\varphi,\psi}\Big[\int T(x,y)c(x,y)\,dx\,dy + \int_{X\times Y}\varphi(x)T(x,y)\,dx\,dy - \boxed{\int_X \varphi(x)\mu(x)\,dx} + \int_{X\times Y}\psi(y)T(x,y)\,dx\,dy - \boxed{\int_Y \psi(x)\nu(y)\,dy}\Big]$$

$$= \sup_{\varphi,\psi}\min_{T\geq 0}\int_{X\times Y} T(x,y)\big[c(x,y)+\varphi(x)+\psi(y)\big]\,dx\,dy. - \boxed{\int_X \varphi(x)\mu(x)\,dx} - \boxed{\int_Y \psi(y)\nu(y)\,dy}]$$

$$= \sup_{\varphi(x)+\psi(y)+c(x,y)\geq 0}\int_X -\varphi(x)\mu(x)\,dx - \int_Y \psi(y)\nu(y).$$

$$\Leftrightarrow \min_{\underline{\varphi}(x)-\underline{\psi}(y)\geq c(x,y)}\int_X \varphi(x)\mu(x)\,dx - \int_Y \psi(y)\nu(y)\,dy$$

shadow price

(proof provide at Appendix)

◆ if $c(x,y) = \|x-y\|$.

Optimal Transport cost

$$= \sup_{\underbrace{\varphi(x)-\varphi(y)\leq \|x-y\|}_{\text{the shadow price is Lipschitz.}}}\overbrace{\int_X \varphi\,\mu(x)\,dx - \int_Y \varphi\,\mu(y)\,dy}^{\text{IPM.}}$$

[hw for these week]

Optimal Transport Distance between empirical and population can be bounded by the covering number of Lipschitz function

$\Rightarrow W(\hat{\mathbb{P}}_n, \mathbb{P}_n) \propto n^{-1/d}$ "curse of dimensionality"

Shadow price has too much free dim.

§ Gradient flow is Wasserstein Space. $\boxed{\text{advance Things}}$.

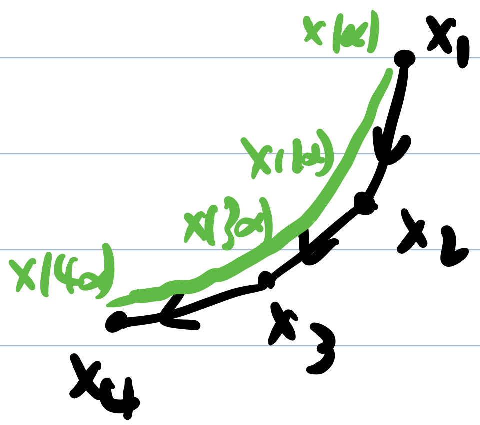
What is Gradient flow:

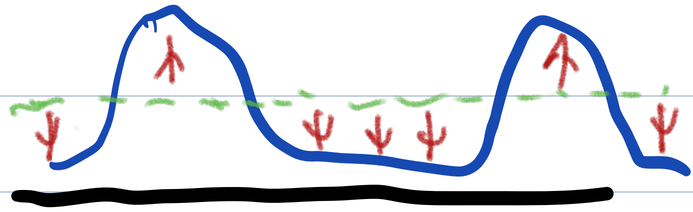
Gradient descent. $x_{t+1} = x_t - \alpha \nabla f(x_t)$

$$\Rightarrow \frac{x_{t+1} - x_t}{\alpha} = -\nabla f(x_t)$$

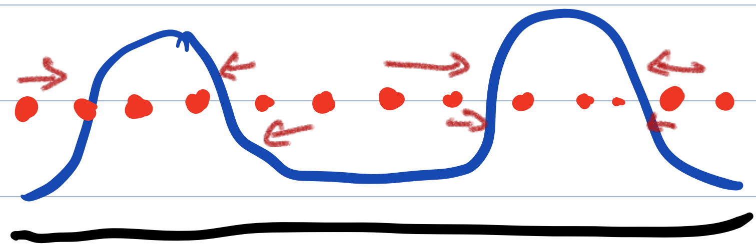
$x_t \approx x(\alpha t)$ $\qquad \dfrac{x(\alpha(t+1)) - x(\alpha t)}{\alpha} \approx \left.\dfrac{dx}{dt}\right|_{\alpha t}$

Gradient flow: $\dfrac{dx(t)}{dt} = -\nabla f(x(t))$



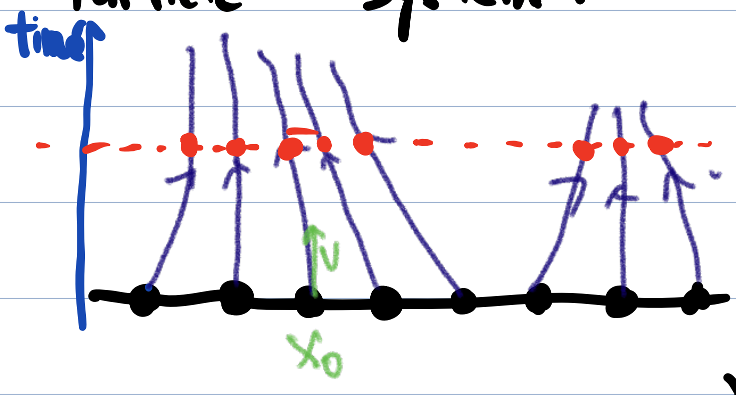


① ↑ ↓ consider in f-diver / as a vector



② Transporting the particles.

Particle. System.



assume every particle moves

$$\begin{cases} x(0) = x_0 \\ \frac{dx}{dt} = \vec{v}_t(x) \end{cases}$$

x is the position, v is the speed

Question! How does the density move?

$$\partial_t \rho_t = -\nabla \cdot (\vec{v}_t \rho_t)$$

⇑

$$\nabla \cdot \begin{pmatrix} \vec{v}_x \\ \vec{v}_y \end{pmatrix} = \frac{d\vec{v}_x}{dx} + \frac{d\vec{v}_y}{dy}$$

★ Introduce a test function. ψ

then we keep track of $\int_x \psi(x)\,\rho_t(x)\,dx = \mathbb{E}_{\rho_t}\psi$

$$\frac{d}{dt}\int_x \rho_t(x)\,\psi(x)\,dx$$

write down in particle side!!

$$\frac{d}{dt}\int \psi[X(t)]\,\rho_0(x)\,dx$$

we first sample $X(0) \sim \rho_0(x)$

run $\frac{dX(t)}{d(t)} = \vec{v}_t(X(t))$ till times

$$\| $$

$$\int_x \frac{d}{dt}\rho_t(x)\,\psi(x)\,dx$$

$$= \int \nabla\psi(X(t))\,V_t(X_t)\,\rho_0(x_0)\,dx.$$

chain rule: $\frac{d}{dt}\psi(X(t)) = \nabla\psi(X(t))\underbrace{\frac{dx}{dt}}_{= V_x.}$

$$= -\int \psi\,\nabla\cdot(v\rho)$$

Thus $\frac{d}{dt}\rho_t = -\nabla\cdot(v\rho)$.

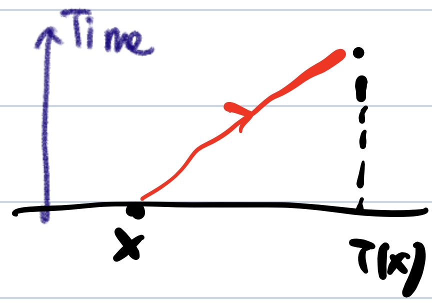
Benamou - Brenier. If $c(x,y) = \|x-y\|^2$, then optimal transport can be charatenize as

$$\min. \int_0^1\int_x |V_t(x)|^2\rho_t(x)\,dx\,dt.$$

$$\text{s.t.}\quad \partial_t\rho_t + \nabla\cdot(V_t\rho_t) = 0.$$

$$\rho(\cdot,0) = \mu,\qquad \rho(\cdot,1) = \nu$$

$$X(t,x) = x + t(T(x) - x),$$



Gradient Descent in Wasserstein Space.

$F(\rho)$ is a function of distribution ρ.

$\frac{dF(\rho)}{d\rho}$ is a function f, actually satisfies.

$$F(\rho + \varepsilon \rho_0) = F(\rho) + \varepsilon \int f \cdot \rho + o(\varepsilon)$$

$\frac{d\rho}{dt} = -\frac{dF(\rho)}{d\rho}$ (If I run the gradient in vector space - not exactly Fisher - Rao Flow)

Wasserstein Gradient Descent:

Particles, $x(t)$.

$$\frac{dx}{dt} = -\nabla\left(\frac{dF(\rho)}{d\rho}\right).$$

If $F(\rho) = \int \psi(x)\,\rho(x)$ is a linear function of ρ

$$\frac{dF(\rho)}{d\rho} = \psi$$

$$\Rightarrow \frac{dx}{dt} = -\nabla \psi$$

$$\min_{\varphi(x)-\psi(y)\geq c(x,y)} \int \varphi(x)\mu(x)\,dx - \int \psi(y)\nu(y)\,dy$$

Case 1. $c(x,y) = \|x-y\|$

[Appendix] Duality of Optimal Transport when $c(x,y)=\|x-y\|$

If g is 1-Lipschitz: then

$$\underbrace{\inf_x \{\|x-y\| - g(x)\}}_{\text{must}} = \underbrace{-g(y)}_{\text{be}}$$

must be 1-lipschitz.

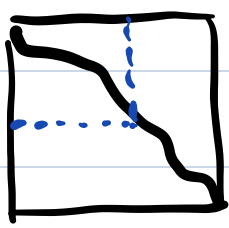
if φ is the shadow price for x, then the shadow price for y is $\psi(y) = \inf_x \{\|x-y\| - \varphi(x)\}$

Duality of W_1: $\sup_{\|f\|_{lip}\leq 1} \int f(x)\mu(x)\,dx - \int f(x)\nu(y)\,dy$

Case 2. $c(x,y) = \|x-y\|^2$

$$\Rightarrow \inf_x \{\|x-y\|_2^2 - g(x)\} = g^*(y)$$

★ Duality of W_2: $\sup_f \int f(x)\mu(x)\,dx - \int f^*(x)\nu(y)\,dy$.



Thm: $T: X \to Y$, $T = \nabla f$.

$$\nabla f^* = (\nabla f)^{-1}$$

$T^{-1}: Y \to X$

Provide $X(t)$ moves along

$$\frac{dX(t)}{dt} = -\nabla\left(\frac{dF(\rho)}{d\rho}\right)$$

is the fastest direction to transport the particles to minimize the objective function F.

If $\frac{dx(t)}{dt} = v(x(t))$, Then the density ρ will change according to

$$\partial_t \rho_t = -\nabla\cdot(\rho_t v_t)$$

Then

$$\partial_t F(\rho_t) = \int \frac{dF(\rho)}{d\rho}\,\partial_t \rho_t = \int \frac{dF(\rho)}{d\rho}\left(-\nabla\cdot(\rho_t \cdot v_t)\right)$$

Integral by parts
$$\int \left[\nabla\left(\frac{dF(\rho)}{d\rho}\right)\right] \rho_t v_t$$

$$= \int \left\langle \nabla\left(\frac{dF(\rho)}{d\rho}\right), v_t \right\rangle \rho_t .$$

$v_t = -\nabla\left(\frac{dF(\rho)}{d\rho}\right)$ is the best direction to move the particles!!!