THE QUADRATIC CASE $c(x,y)=\frac{|x-y|^2}{2}$ IN $\mathbb{R}^d$

We need now to establish the two big results of the subject: the KANTOROVICH Duality Theorem, and the BRENIER Theorem which pertains to the original MONGE Problem.

The former holds in great generality, for general Polish spaces and lower-semi-continuous cost functions; the latter is very specific to Euclidean spaces and to quadratic costs. For economy and unity of exposition, we shall prove both results in the case

$$X = Y = \mathbb{R}^d, \qquad c(x,y) = \frac{1}{2}|x-y|^2 .$$

Very similar convex duality methodologies, as those deployed here to establish the KANTOROVICH Duality in this special case, can also be used to establish this result in its full generality.

Now, the cost function $c(\cdot,\cdot)$ above is nonnegative and continuous; thus, we know that a minimizer $\bar{\pi} \in \Pi(\mu,\nu)$ exists for the KANTOROVICH Problem. We have also

$$I(\pi) \triangleq \int_X\int_Y \frac{1}{2}|x-y|^2 \pi(dx,dy) = \underbrace{\frac{1}{2}\left(\int_{\mathbb{R}^d}|x|^2\mu(dx)+\int_{\mathbb{R}^d}|y|^2\nu(dy)\right)}_{\text{assumed finite: } <\infty} + \underbrace{\int_X\int_Y (-x\cdot y)\,\pi(dx,dy)}_{\tilde{I}(\pi)}$$

and so minimizing $I(\pi)$ over $\Pi(\mu,\nu)$ amounts to minimizing

$$\tilde{I}(\pi) \triangleq \int_X\int_Y \tilde{c}(x,y)\,\pi(dx,dy), \quad \tilde{c}(x,y) \triangleq -\langle x,y\rangle \equiv -x.y.$$

For this new cost function $\tilde{c}(\cdot,\cdot)$, the requirement of cyclical monotonicity becomes

$$\sum_{i=1}^{N} \langle y_i, x_{i+1}-x_i\rangle \leq 0 .$$

And we shall say that a set $S \subset \mathbb{R}^d \times \mathbb{R}^d$ is <u>cyclically monotone</u>, if the above inequality holds for any points $(x_1,y_1),\ldots,(x_N,y_N)$ in S.

We have the following fundamental result.

<u>THEOREM</u> (ROCKAFELLAR): A set $S \subset \mathbb{R}^d \times \mathbb{R}^d$ is cyclically monotone if, and only if, there exists a convex function $\varphi : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ with

$$S \subseteq \partial\varphi \triangleq \bigcup_{x\in\mathbb{R}^d} \left(\{x\} \times \partial\varphi(x)\right), \text{ where}$$

$$\partial\varphi(x) \triangleq \{y \in \mathbb{R}^d : (\forall z \in \mathbb{R}^d)\ \varphi(z) \geq \varphi(x) + \langle y, z-x\rangle\}$$

is the subdifferential of φ at $x \in \mathbb{R}^d$.

<u>Remark</u>: If a convex function $\varphi : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ is differentiable at some $\bar{x} \in \mathbb{R}^d$, then
$$\partial\varphi(\bar{x}) = \{\nabla\varphi(\bar{x})\}.$$

<u>Definition</u>: <u>LEGENDRE Transform</u>.

For a given convex function $\varphi : \mathbb{R}^d \to \mathbb{R}\cup\{+\infty\}$ (with $\varphi \not\equiv +\infty$), we define its LEGENDRE Transform $\varphi^* : \mathbb{R}^d \to \mathbb{R}\cup\{+\infty\}$
$$\varphi^*(y) \triangleq \sup_{x \in \mathbb{R}^d} \left(x.y - \varphi(x) \right), \quad y \in \mathbb{R}^d.$$

We have then:
$$\varphi(x) + \varphi^*(y) \geq x.y, \quad \forall\, (x,y) \in \mathbb{R}^d \times \mathbb{R}^d$$
$$\varphi(x) + \varphi^*(y) = x.y \iff y \in \partial\varphi(x).$$

Let us return to the KANTOROVICH Problem of minimizing
$$I(\pi) = \iint_{XY} c(x,y)\,\pi(dx,dy), \quad c(x,y) = \frac{1}{2}|x-y|^2$$
or equivalently
$$\tilde{I}(\pi) = \iint_{XY} \tilde{c}(x,y)\,\pi(dx,dy), \quad \tilde{c}(x,y) = -\,x.y$$
over $\Pi(\mu,\nu)$. Clearly there problems have finite value:
$$\inf_{\pi \in \Pi(\mu,\nu)} I(\pi) \leq \iint_{XY} \frac{|x-y|^2}{2}\,\mu(dx)\nu(dy) \leq \int_{\mathbb{R}^d} |x|^2 \mu(dx) + \int_{\mathbb{R}^d} |y|^2 \nu(dy) < \infty.$$

THEOREM: KANTOROVICH Duality in the Quadratic Case.

Consider two probability measures μ, ν on $\mathcal{B}(\mathbb{R}^d)$ with finite second moments:

$$\int_{\mathbb{R}^d} |x|^2 \mu(dx) + \int_{\mathbb{R}^d} |y|^2 \nu(dy) < \infty.$$

Then, for any measure $\pi \in \Pi(\mu,\nu)$, and any measurable functions φ, ψ from $\mathbb{R}^d$ into $\mathbb{R} \cup \{+\infty\}$, we have

PRIMAL
$$\max_{\pi \in \Pi(\mu,\nu)} \int_X \int_Y (x \cdot y)\, \pi(dx, dy)$$

DUAL
$$= \min_{\varphi(x) + \psi(y) \geq x \cdot y} \left(\int_X \varphi(x)\mu(dx) + \int_Y \psi(y)\nu(dy) \right)$$

STRONG DUAL
$$= \min_{\varphi(\cdot) \text{ Convex}} \left(\int_X \varphi(x)\mu(dx) + \int_Y \varphi^*(y)\nu(dy) \right).$$

<u>Proof</u>: Consider measurable functions $\varphi(\cdot)$, $\psi(\cdot)$ with $\varphi(x)+\psi(y) \geq x \cdot y$, $\forall\, (x,y) \in (\mathbb{R}^d)^2$, and integrate w.r.t. the measure $\pi \in \Pi(\mu,\nu)$:

$$\int_X \int_Y x \cdot y \,\pi(dx,dy) \leq \int_X \int_Y \varphi(x)\,\pi(dx,dy) + \int_X \int_Y \psi(y)\,\pi(dx,dy)$$

$$= \int_{\mathbb{R}^d} \varphi(x)\,\mu(dx) + \int_{\mathbb{R}^d} \psi(y)\,\nu(dy).$$

(<u>Exercise</u>: Justify the use of FUBINI–TONELLI, that yields this last equality.) Thus,

$$\sup_{\pi \in \Pi(\mu,\nu)} \int_X \int_Y x \cdot y\,\pi(dx,dy) \leq \inf_{\varphi(x)+\psi(y) \geq x \cdot y} \left(\int_{\mathbb{R}^d} \varphi(x)\,\mu(dx) + \int_{\mathbb{R}^d} \psi(y)\,\nu(dy) \right)$$

$$\leq \inf_{\varphi(\cdot)\text{ convex}} \left(\int_X \varphi\, d\mu + \int_Y \varphi^*\, d\nu \right).$$

• Now, suppose that $\bar{\pi} \in \Pi(\mu,\nu)$ is optimal for the KANTOROVICH problem (we have argued already that such an optimal $\bar{\pi}$ exists). Then its support is <u>cyclically monotone</u>, as we have argued already; and by the ROCKAFELLAR Theorem, there exists a convex $\varphi : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ with $\mathrm{supp}(\bar{\pi}) \subset \partial\varphi$; to wit, $y \in \partial\varphi(x)$ for every $(x,y) \in \mathrm{supp}(\bar{\pi})$. But this is equivalent to

$$\varphi(x) + \varphi^*(y) = x \cdot y, \quad \bar{\pi}\text{-a.e.}$$

and gives
$$\int_X\int_Y x.y\ \bar{\pi}(dx,dy) = \int_X \varphi\, d\mu + \int_Y \varphi^*\, d\nu ,$$

i.e., renders the last displayed inequality an equality. $\square$

<u>Remark:</u> The last part of the argument uses the optimality of $\bar{\pi}$ only in order to deduce $\mathrm{supp}(\bar{\pi}) \subset \partial\varphi$; then goes on to show that this property implies the identity at the top of the page. But note

$$\int_X \varphi\, d\mu + \int_Y \varphi^*\, d\nu \geqslant \int_X\int_Y x.y\ \pi(dx,dy) , \quad \forall\ \pi \in \Pi(\mu,\nu)$$

from the first display of the previous page, so in fact <u>$\mathrm{supp}(\bar{\pi}) \subset \partial\varphi$</u> implies

$$\int_X\int_Y x.y\ \bar{\pi}(dx,dy) \geqslant \int_X\int_Y x.y\ \pi(dx,dy), \ \forall\ \pi \in \Pi(\mu,\nu),$$

i.e., the <u>optimality of $\bar{\pi}$</u>. Thus, we have proved also the following result.

<u>PROPOSITION:</u> For the KANTOROVICH Problem with cost $c(x,y) = |x-y|^2$, the following are equivalent:

- $\bar{\pi}$ is optimal;
- $\mathrm{supp}(\bar{\pi})$ is cyclically monotone;
- $\mathrm{supp}(\bar{\pi}) \in \partial\varphi$ for some convex $\varphi : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$.

Here are a couple of straightforward, but important to keep in mind, remarks.

<u>Remark:</u> Suppose we are trying to show that a certain transport map $T: X \to Y$ from μ to ν, is optimal in the MONGE problem with $c(x,y) = |x-y|^2$ and $X = Y = \mathbb{R}^d$.

On account of the Proposition this will be the case if, and only if, $\operatorname{supp}(\pi) \in \partial\varphi$ for some convex $\varphi : \mathbb{R}^d \to \mathbb{R} \cup \{\infty\}$, where

$$\pi = (Id \times T)\# \mu .$$

But this is equivalent to requiring

(*) $$T(x) \in \partial\varphi(x), \quad \mu\text{-a.e. } x \in X.$$

<u>Remark:</u> In particular, given a measure $\mu \in \mathcal{P}(\mathbb{R}^d)$ and a convex function $\varphi : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ which is differentiable μ-a.e., the map $T = \nabla\varphi$ is well-defined μ-a.e. and we can consider the measure $\nu \triangleq (\nabla\varphi)\#\mu \in \mathcal{P}(\mathbb{R}^d)$. Now $\partial\varphi(x) = \{\nabla\varphi(x)\}$ holds at every $x \in \mathbb{R}^d$ where φ is differentiable, (*) is satisfied trivially, and

$\nabla\varphi$ is an optimal transport map from μ onto

$$\nu = (\nabla\varphi)\#\mu .$$

PROOF OF THE BRENIER THEOREM: We know that an optimal transport plan $\bar{\pi} \in \Pi(\mu, \nu)$ exists in the KANTOROVICH Problem (because $c(x,y) = |x-y|^2$ is continuous and nonnegative); and that $\underline{\mathrm{supp}(\bar{\pi}) \subset \partial\varphi}$ for some convex $\varphi : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, as well as that

$$\varphi(x) + \varphi^*(y) = x \cdot y \quad \text{on } \partial\varphi \supset \mathrm{supp}(\bar{\pi}).$$

In particular $(\varphi(x), \varphi^*(y)) \in \mathbb{R}^2$ for $\bar{\pi}$-a.e. (x,y), thus $\varphi(x) \in \mathbb{R}$ for μ-a.e. x. But convex functions are differentiable λ-a.e. on the region where they are finite (by the ALEXANDROV Theorem), so

$$\varphi \text{ is differentiable } \mu\text{-a.e.}$$

In other words, there exists a set $A \in \mathcal{B}(\mathbb{R}^d)$ with $\mu(A) = 0$ and φ differentiable everywhere in $\mathbb{R}^d \setminus A$.

- Now fix $\bar{x} \in \mathbb{R}^d \setminus A$, $\bar{y} \in \mathbb{R}^d$ such that $(\bar{x}, \bar{y}) \in \mathrm{supp}(\bar{\pi}) \subset \partial\varphi$; i.e., $\bar{y} \in \partial\varphi(\bar{x})$. Because φ is differentiable at $\bar{x}$, we get $\bar{y} = \nabla\varphi(\bar{x})$.

Therefore,

$$\mathrm{supp}(\bar{\pi}) \cap \left((\mathbb{R}^d \setminus A) \times \mathbb{R}^d \right) \subset \mathrm{graph}\,(\nabla\varphi)$$

and since $\bar{\pi}(A \times \mathbb{R}^d) = \mu(A) = 0$ we deduce that the set

$$\{(x,y) : y = \nabla\varphi(x)\} \quad \text{has full } \bar{\pi}\text{-measure.}$$

Therefore, for every $F: X \times Y \to \mathbb{R}$ bounded and continuous, we have

$$\iint_{XY} F(x,y)\,\bar{\pi}(dx,dy) = \iint_{XY} F(x,\nabla\varphi(x))\,\pi(dx,dy)$$

$$= \int_X F(x,\nabla\varphi(x))\,\mu(dx) = \iint_{XY} F(x,y)\cdot\left[(Id \times \nabla\varphi)\#\mu\right](dx,dy),$$

i.e., $\bar{\pi} = (Id \times \nabla\varphi)\#\mu$.

$\square$

Proof of the ROCKAFELLAR Theorem:

1) Assume $S \subset \partial\varphi$ for some convex φ, and consider a string $(x_1, y_1), \dots, (x_N, y_N)$ in S. Then, for each $i = 1, \dots, N$ we have $(x_i, y_i) \in \partial\varphi$; to wit,

$$\varphi(z) \geq \varphi(x_i) + \langle y_i, z - x_i \rangle \quad , \quad \forall z \in \mathbb{R}^d.$$

In particular, $\qquad \varphi(x_{i+1}) \geq \varphi(x_i) + \langle y_i, x_{i+1} - x_i \rangle .$

Summing up over $i = 1, \dots, N$ with $x_{N+1} = x_1$, we obtain

$$\sum_{i=1}^{N} \langle y_i, x_{i+1} - x_i \rangle \leq 0 \quad , \quad \text{as claimed.}$$

2) Now assume cyclical monotonicity, fix $(x_0, y_0) \in S$, and note that if φ is convex and $S \subset \partial\varphi$, $\varphi(x_0) = 0$ we have, by induction on $N \in \mathbb{N}$,

$$\varphi(x) \geq \langle y_N, x - x_N \rangle + \sum_{i=0}^{N-1} \langle y_i, x_{i+1} - x_i \rangle \quad , \forall x \in S$$

for any string $(x_1, y_1), \dots, (x_N, y_N)$ in S. We select then the smallest such function

$$\varphi(x) \triangleq \sup_{\substack{N \in \mathbb{N} \\ (x_i, y_i)_{i=1}^N \subset S}} \left(\langle y_N, x - x_N \rangle + \sum_{i=0}^{N-1} \langle y_i, x_{i+1} - x_i \rangle \right).$$

A few observations are in order:

- This function is convex, as the supremum of affine ones.
- With $N=1$, $(x_1,y_1)=(x_0,y_0)$ we get $\varphi(x)\geqslant\langle y_0, x-x_0\rangle$, in particular $\varphi(x_0)\geqslant 0$.
- Cyclical monotonicity implies

$$\langle y_N, x_0-x_N\rangle+\sum_{i=0}^{N-1}\langle y_i, x_{i+1}-x_i\rangle=\sum_{i=1}^{N}\langle y_i, x_{i+1}-x_i\rangle\leq 0.$$

In other words, $\varphi(x_0)\leq 0$, so in fact $\varphi(x_0)=0$; in particular, $\varphi\not\equiv\infty$.

Now we need to show $S\subset\partial\varphi$, for this function. Take $(\bar{x},\bar{y})\in S$, $\alpha<\varphi(\bar{x})$; then the definition of φ implies the existence of $N\in\mathbb{N}$ and of a string $(x_1,y_1),\dots,(x_N,y_N)$ of points in S with

$$\langle y_N, \bar{x}-x_N\rangle+\dots+\langle y_0, x_1-x_0\rangle\geqslant\alpha.$$

We extend this string to (x_i,y_i), $i=1,\dots,N,\underline{\underline{N+1}}$ by taking $x_{N+1}=\bar{x}$, $y_{N+1}=\bar{y}$; this new string is admissible in the definition of φ, so for any $z\in\mathbb{R}^d$ we have

$$\varphi(z) \geq \langle \underbrace{y_{N+1}}_{\bar{y}}, z - \underbrace{x_{N+1}}_{\bar{x}} \rangle + \langle y_N, \underbrace{x_{N+1}}_{\bar{x}} - x_N \rangle + \dots + \langle y_0, x_1 - x_0 \rangle$$

$$\geq \langle \bar{y}, z - \bar{x} \rangle + \alpha .$$

Letting $\alpha \uparrow \varphi(\bar{x})$, we obtain

$$\varphi(z) \geq \langle \bar{y}, z - \bar{x} \rangle + \varphi(\bar{x}), \quad \forall z \in \mathbb{R}$$

and this shows $\bar{y} \in \partial\varphi(\bar{x})$; i.e., $S \subset \partial\varphi$. $\square$

THE BENAMOU – BRENIER FORMULA

Consider a probability measure $\mu_0(\cdot) = \int_\cdot \rho_0(x)\lambda(dx)$ on $\mathcal{B}(\mathbb{R}^d)$ with density function $\rho_0(\cdot)$ which satisfies $\int_{\mathbb{R}^d} |x|^2 \rho_0(x)\,dx < \infty$; i.e., $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$.

Consider also a smooth, bounded vector field $v : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ along with its FLOW

$$\left\{ \begin{array}{c} \frac{d}{dt} X(t,x) = v(t, X(t,x)) \\ X(0,x) = x \end{array} \right\},$$

as well as the induced probability measures

$$\mu_t := X(t,\cdot) \# \mu_0 = \int_\cdot \rho_t(x)\lambda(dx).$$

Because $v(\cdot,t)$ is bounded, $|X(t,x) - x| \le C \cdot t$, therefore

$$\int_{\mathbb{R}^d} |x|^2 \mu_t(dx) = \int_{\mathbb{R}^d} |x|^2 \rho_t(x)\,dx = \int_{\mathbb{R}^d} |X(t,x)|^2 \underbrace{\rho_0(x)\,dx}_{\mu_0(dx)} \le 2\int_{\mathbb{R}^d} (|x|^2 + C^2t^2)\rho_0(x)\,dx < \infty,$$

i.e., $\mu_t \in \mathcal{P}_2(\mathbb{R}^d)$. In other words, $(\mu_t)_{0 \le t \le T}$ is a curve in $\mathcal{P}_2(\mathbb{R}^d)$.

LEMMA: The family of probability density functions $(\rho_t)_{0 \le t \le T}$ satisfies the continuity equation of EULER

$$\partial_t \rho_t + \operatorname{div}(v_t \rho_t) = 0$$

of fluid mechanics, in the distributional sense.

Here we interpret $v_t(\cdot) \equiv v(t,\cdot)$ as a velocity field, and $\rho_t(\cdot) = \rho(t,\cdot)$ as the density of the fluid.

<u>Proof:</u> For every function ψ in $C_c^\infty(\mathbb{R}^d)$, we have

$$\int_{\mathbb{R}^d} \partial_t \rho_t(x)\psi(x)\,dx = \frac{d}{dt}\int_{\mathbb{R}^d} \psi(x)\rho_t(x)\,dx = \frac{d}{dt}\int_{\mathbb{R}^d}\psi(x)\,\mu_t(dx) =$$

$$= \frac{d}{dt}\int_{\mathbb{R}^d}\psi(X(t,x))\,\mu_0(dx) = \int_{\mathbb{R}^d}\nabla\psi(X(t,x))\cdot\dot{X}(t,x)\,\mu_0(dx)$$

$$= \int_{\mathbb{R}^d}\nabla\psi(X(t,x))\cdot v(t,X(t,x))\,\mu_0(dx) = \int_{\mathbb{R}^d}\nabla\psi(\xi)\cdot v(t,\xi)\,\mu_t(d\xi)$$

$$= \int_{\mathbb{R}^d}\nabla\psi(\xi)\cdot v(t,\xi)\rho_t(\xi)\,d\xi = -\int_{\mathbb{R}^d}\psi(\xi)\,\mathrm{div}\big(v_t(\xi)\rho_t(\xi)\big)\,d\xi.$$

$\square$

Now, given a pair of functions (ρ_t, v_t), scalar and vector, respectively, solving the continuity equation, let us consider the ACTION FUNCTIONAL (Kinetic Energy)

$$A[\rho,v] \triangleq \int_0^1\int_{\mathbb{R}^d}|v_t(x)|^2\rho_t(x)\,dx\,dt.$$

(We take $T=1$.)

<u>THEOREM</u> (BENAMOU–BRENIER, 1998): Given two probability measures $\mu_0(\cdot)=\int_\cdot \rho_0^*\,d\lambda$, $\mu_1(\cdot)=\int_\cdot \rho_1^*\,d\lambda$ in $\mathcal{P}_2(\mathbb{R}^d)$, we have

$$W_2^2(\mu_0,\mu_1) = \inf\Big\{A[\rho,v] : \partial_t\rho_t + \mathrm{div}(\rho_t v_t) = 0,\ \rho_0=\rho_0^*,\ \rho_1=\rho_1^*\Big\}.$$

<u>Proof:</u> For any pair $(\rho_t, v_t)_{0\le t\le 1}$ as in the infimum right above, and with the notation used,

$$A[\rho,v] = \int_0^1\int_{\mathbb{R}^d}|v_t(x)|^2\rho_t(x)\,dx\,dt = \int_0^1\int_{\mathbb{R}^d}|v_t(x)|^2\mu_t(dx)\,dt = \int_0^1\int_{\mathbb{R}^d}|v_t(X(t,x))|^2\mu_0(dx)\,dt$$

$$= \int_{\mathbb{R}^d}\Big(\int_0^1|\dot{X}(t,x)|^2dt\Big)\underbrace{dx)}_{(\mu_0(}\ \geq \int_{\mathbb{R}^d}\Big|\int_0^1\dot{X}(t,x)\,dt\Big|^2\mu_0(dx) \qquad \text{(by Hölder)}$$

$$= \int_{\mathbb{R}^d} |X(1,x)-x|^2 \mu_0(dx) \geq W_2^2(\mu_0,\mu_1).$$

• To show equality, we summon from the BRENIER Theorem the map $T = \nabla\varphi$, gradient of a convex function $\varphi : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, that transports optimally the measure μ_0 to the measure μ_1 with quadratic cost, and take $X(t,x) \triangleq x + t\big(T(x)-x\big)$.

We define the probability measures $\mu_t \triangleq X(t,\cdot) \# \mu_0$, $0 \leq t < 1$ and let $(v_t)_{0\leq t<1}$ be such that
$$\dot{X}(t) = v_t \circ X(t), \quad 0 \leq t \leq 1$$
equivalently, $\dot{X}(t,x) = v(t, X(t,x))$. This amounts to selecting $v(t,\xi) = \dot{X}(t, X^{-1}(t,\xi))$ provided, as indeed can be shown, that the inverse $X^{-1}(t,\cdot)$ exists. Here the particular form $T = \nabla\varphi$ of the transport map, as gradient of a convex function, is used crucially. With these choices, $T(x) - x = \dot{X}(t,x) = v(t, X(t,x))$ and the two inequalities in the string that straddles the previous page and this one, become equalities.

$\square$