On the relation between Kantorovich's and Shannon's optimization problems

Roman V. Belavkin

Faculty of Science and Technology Middlesex University, London NW4 4BT, UK

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Information and entropy

Optimal channel problem (OCP)

Dual formulation of OTP

Geometry of information divergence and optimization

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Kantorovich (aka Wassershtain) metric (Kantorovich, 1939, 1942; Vasershtein, 1969; Dobrushin, 1970) between *q*, *p*:

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#### Optimal transportation problems (OTPs)

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# Kantorovich's OTP

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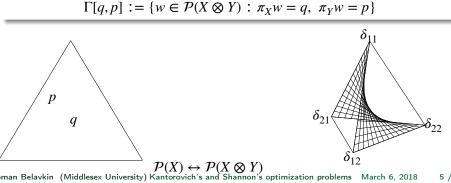
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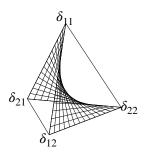
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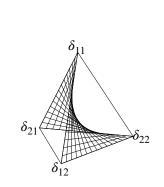
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• Linear operator (Markov morphism)  $T : \mathcal{P}(X) \to \mathcal{P}(Y)$ :

$$q \mapsto Tq = p = \int_X p(y \mid x) dq$$



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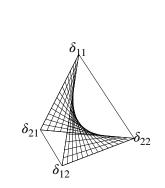
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•  $p(y \mid x)$  — Markov transition kernel



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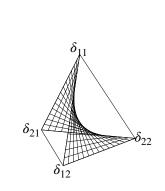
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- $p(y \mid x)$  Markov transition kernel
- T is determined by  $w \in \mathcal{P}(X \otimes Y)$ :

$$w = p(y \mid x) \otimes q$$



Monge OTP

Optimal Transportation Problem (Monge, 1781)

$$K_c[p,q] := \inf \left\{ \int_X c(x,f(x)) \, dq : f : p = q \circ f^{-1} \right\}$$

where  $p = q \circ f^{-1}$  is push-forward under measurable mapping  $f : X \to Y$ :

$$p(E) = q \circ f^{-1}(E) = q\{x : f(x) \in E\}$$

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#### Optimal Transport

•  $p(E \mid x)$  has the form:

$$\delta_{f(x)}(E) = \begin{cases} 1 & \text{if } f(x) \in E \\ 0 & \text{otherwise} \end{cases}$$

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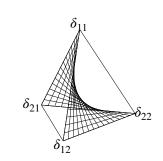
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•  $w_f \in \partial \mathcal{P}(X \otimes Y)$ :

$$w_f(X, Y \setminus f(X)) = 0$$



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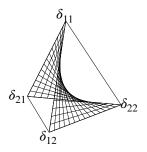
Geometry of information divergence and optimization

Shannon's Information and Entropy KL-divergence (Kullback & Leibler, 1951)

$$D_{KL}[p,q] = \int \left[\ln p - \ln q\right] dp$$

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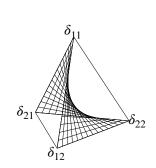
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Shannon's information (Shannon, 1948) For  $w \in \Gamma[q, p] \subset \mathcal{P}(X \otimes Y)$ :  $I_w\{x, y\} := D_{KL}[w, q \otimes p]$   $= H[q] - H[q(x \mid y)]$  $= H[p] - H[p(y \mid x]$ 



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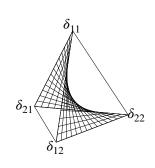
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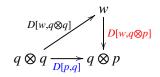
$$I_w\{x, y\} := D_{KL}[w, q \otimes p]$$
  
= H[q] - H[q(x | y)]  
= H[p] - H[p(y | x]

Entropy  $H[p] = -\int \ln p \, dp$ 

$$H[p] := I_w\{y, y\} = \sup_{w: \pi_Y w = p} I_w\{x, y\}$$



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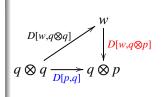


### Theorem (Shannon-Pythagorean)

•  $w \in \mathcal{P}(X \otimes Y), \ \pi_X w = q, \ \pi_Y w = p$ 

 $D_{KL}[w, q \otimes q] = D_{KL}[w, q \otimes p] + D_{KL}[p, q]$ 

(Belavkin, 2013a)

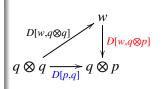


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#### Proof.

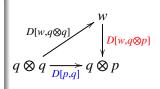
$$D[w, q \otimes q] = \underbrace{D[w, q \otimes p]}_{I_w\{x,y\}} + \underbrace{D[q \otimes p, q \otimes q]}_{D[p,q]} - \underbrace{\langle \ln q \otimes p - \ln q \otimes q, q \otimes p - w \rangle}_{0}$$
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 $\ln q \otimes p - \ln q \otimes q = \mathbf{1}_X \otimes (\ln p - \ln q)$ 

### Cross-Information (Belavkin, 2013a)

$$D_{KL}[w, q \otimes q] = \underbrace{-\langle \ln q, p \rangle}_{\text{Cross-entropy}} - \underbrace{\left(H[p] - D_{KL}[w, q \otimes p]\right)}_{\text{Cross-entropy}}$$
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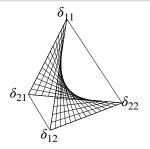
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$$R_c[q](\lambda) := \inf\left\{\int_{X \times Y} c(x, y) \, dw : \pi_X w = q, \ I_w\{x, y\} \le \lambda\right\}$$

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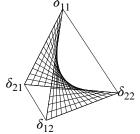


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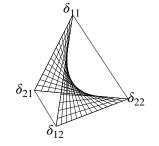
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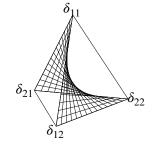
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### Value of Information (Stratonovich, 1965)

$$V(\lambda) := R_c[q](\mathbf{0}) - R_c[q](\lambda) = \sup\{\mathbb{E}_w\{u\} : I_w\{x, y\} \le \lambda\}$$

# Relation to Kantorovich OTP Optimal Channel Problem

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•  $K_c[q,p]$  has implicit constraint  $I_w\{x,y\} \le \lambda = \min\{H[q], H[p]\}\]$  and  $R_c[q](\lambda) \le K_c[q,p](\lambda)$ 

Inverse Optimal Values

Inverse of the OCP Value

$$R_c^{-1}[q](\boldsymbol{v}) := \inf \left\{ I_w\{x, y\} : \pi_X w = q, \int c \, dw \le \boldsymbol{v} \right\}$$

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• If  $v = K_c[q, p](\lambda)$ , then

$$R_c^{-1}[q](v) \le K_c^{-1}[q,p](v)$$

### Common Solution

#### Theorem

Let  $w_{OCP}$  and  $w_{OTP} \in \mathcal{P}(X \times Y)$  be optimal solutions to OCP and OTP problems with the same constraint  $I(x, y) \leq \lambda$ . Then  $R_c[q](\lambda) = K_c[p, q](\lambda)$  if and only if  $w_{OCP} = w_{OTP} \in \Gamma[p, q]$ .

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Proof.

•  $w_{OCP} \in \partial D^*[-\beta c, q \otimes p]$  of subdifferential of  $D^*$  at  $u = -\beta c$ :

$$D^*[u, q \otimes p] = \ln \int_{X \times Y} e^{u(x, y)} dq(x) dp(y)$$

•  $w_{OTP} \in \partial D^*[-\beta c, q \otimes p]$  implies

$$(1-t)w_{OCP} + tw_{OTP} \in \partial D^*[-\beta c, q \otimes p], \quad t \in [0,1]$$

# Common Solution

### Theorem

Let  $w_{OCP}$  and  $w_{OTP} \in \mathcal{P}(X \times Y)$  be optimal solutions to OCP and OTP problems with the same constraint  $I(x, y) \leq \lambda$ . Then  $R_c[q](\lambda) = K_c[p, q](\lambda)$  if and only if  $w_{OCP} = w_{OTP} \in \Gamma[p, q]$ .

Proof.

•  $w_{OCP} \in \partial D^*[-\beta c, q \otimes p]$  of subdifferential of  $D^*$  at  $u = -\beta c$ :

$$D^*[u, q \otimes p] = \ln \int_{X \times Y} e^{u(x, y)} dq(x) dp(y)$$

•  $w_{OTP} \in \partial D^*[-\beta c, q \otimes p]$  implies

$$(1-t)w_{OCP} + tw_{OTP} \in \partial D^*[-\beta c, q \otimes p], \quad t \in [0,1]$$

• and the KL-divergence  $D[w, q \otimes p]$ , the dual of  $D^*[u, q \otimes p]$ , not strictly convex.

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Optimal transportation problems (OTPs)

Information and entropy

Optimal channel problem (OCP)

Dual formulation of OTP

Geometry of information divergence and optimization

### Dual formulation

#### • Consider $f: X \to \mathbb{R}$ and $g: Y \to \mathbb{R}$ such that

 $f(x) - g(y) \leq c(x,y)$ 

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$$f(x) - g(y) \leq c(x,y)$$

• Define

$$J_c[p,q] := \sup \left\{ \mathbb{E}_p\{f\} - \mathbb{E}_q\{g\} : f(x) - g(y) \le c(x,y) \right\}$$

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• Clearly  

$$J_c[p,q] \le K_c[p,q]$$

• Can  $J_c[p,q]$  be related to  $D_{KL}[p,q]$ ?

### KL-divergence

$$D[p,q] = D[p,r] + D[r,q] - \int_X \ln \frac{dq(x)}{dr(x)} [dp(x) - dr(x)]$$
  
=  $D[p,r] - D[q,r] - \int_X \ln \frac{dq(x)}{dr(x)} [dp(x) - dq(x)]$ 

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• Let  $f(x) - g(y) \le c(x, y)$  satisfy also:

$$\beta f(x) = \nabla D[p, r] = \ln \frac{dp(x)}{dr(x)}, \qquad \beta \ge 0$$
$$\alpha g(x) = \nabla D[q, r] = \ln \frac{dq(x)}{dr(x)}, \qquad \alpha \ge 0$$

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• Thus  $dp(x) = e^{\beta f(x) - \kappa[\beta f]} dr(x)$ ,  $dq(x) = e^{\alpha g(x) - \kappa[\alpha g]} dr(x)$  and  $D[p, r] = \beta \mathbb{E}_p\{f\} - \kappa[\beta f]$ ,  $D[q, r] = \alpha \mathbb{E}_q\{g\} - \kappa[\alpha g]$ 

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• Thus  $dp(x) = e^{\beta f(x) - \kappa[\beta f]} dr(x)$ ,  $dq(x) = e^{\alpha g(x) - \kappa[\alpha g]} dr(x)$  and  $D[p, r] = \beta \mathbb{E}_p\{f\} - \kappa[\beta f], \quad D[q, r] = \alpha \mathbb{E}_q\{g\} - \kappa[\alpha g]$ 

• Therefore

$$D[p,q] = \beta \mathbb{E}_{p} \{f\} - \alpha \mathbb{E}_{q} \{g\} - (\kappa [\beta f] - \kappa [\alpha g]) - \alpha \int_{\alpha} g(x) [dp(x) - dq(x)]$$
  
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### KL-divergence (cont.)

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Let us denote

$$J_{c,\varepsilon}[p,q] := \frac{1}{\varepsilon} \left[ \beta \mathbb{E}_p \{f\} - \alpha \mathbb{E}_q \{g\} \right]$$

where  $\varepsilon = \inf \{ \epsilon \ge 0 : \beta f(x) - \alpha g(y) \le \epsilon c(x, y) \}.$ 

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$$D[p,q] \le \varepsilon K_c[p,q] - (\kappa[\beta f] - \kappa[\alpha g]) - \alpha \int g(x) \left[dp(x) - dq(x)\right]$$

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# Common solution for Dual OTP

#### Theorem

Let (f,g) be the solution to the dual OTP. If there exists a reference measure  $r \in \mathcal{P}(X)$  such that  $f = \nabla D[p,r]$  and  $g = \nabla D[q,r]$ , then

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Proof.

• 
$$f = \nabla D[p, r]$$
 and  $g = \nabla D[q, r]$  imply that  $\alpha = \beta = 1$ , and

$$p = \exp(f - \kappa[f]) r$$
,  $q = \exp(g - \kappa[g]) r$ 

• The result follows, because

$$\mathbb{E}_p\{f\} - \mathbb{E}_q\{g\} = J_c[p,q] = K_c[p,q]$$

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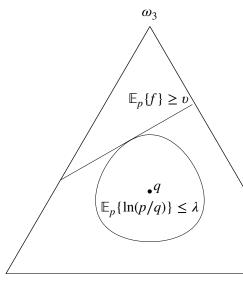
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### Problems on Conditional Extremum

•  $\mathbb{E}_{p}\{u\} = \langle u, p \rangle$  expected utility

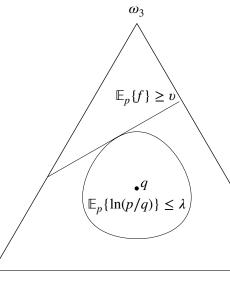


 $\omega_2$ 

# Problems on Conditional Extremum

- $\mathbb{E}_{p}\{u\} = \langle u, p \rangle$  expected utility
- $v_u(\lambda) = -R_{-u}[q](\lambda)$  utility of information  $\lambda$ :

$$v_u(\lambda) := \sup\{\langle u, p \rangle : F[p,q] \le \lambda\}$$



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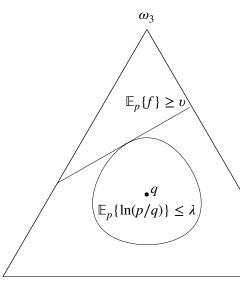
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 $\omega_2$ 

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•  $p(\beta)$  optimal solutions:

 $p(\beta) \in \partial F^*[\beta u, q], \quad F[p(\beta), q] = \lambda$ 

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 $\omega_{\gamma}$ 

 $\omega_3$ 

 $\mathbb{E}_p\{f\} \ge v$ 

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 $\mathbb{E}_p\{\ln(p/q)\} \le \lambda$ 

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||p-q|

 $p_{\ell}$ 

 $\mathbb{E}_n\{w\}$ 

### General Solution

• Lagrange function for  $v_u(\lambda) := \sup\{\langle u, p \rangle : F[p,q] \le \lambda\}$  $(\lambda_u(v) := \inf\{F[p,q] : \langle u, p \rangle \ge v\}):$ 

$$L(p, \beta^{-1}) = \langle u, p \rangle + \beta^{-1}(\lambda - F[p, q])$$
$$\left(L(p, \beta) = F[p, q] + \beta(v - \langle u, p \rangle)\right)$$

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• Necessary and sufficient conditions  $\partial L \ni 0$ :

$$\partial_p L(p, \beta^{-1}) = \{\beta u\} - \partial_p F[p, q] \ni 0$$
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$$\begin{split} L(p,\beta^{-1}) &= \langle u,p \rangle + \beta^{-1}(\lambda - F[p,q]) \\ \left( L(p,\beta) &= F[p,q] + \beta(v - \langle u,p \rangle) \right) \end{split}$$

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• Optimal solutions are subgradients of  $F^*[u, q] = \sup\{\langle u, p \rangle - F[p, q]\}$ :

$$p(\beta) \in \partial F^*[\beta u], \qquad F[p,q] = \lambda \quad (\langle u, p(\beta) \rangle = v)$$

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### Example: Exponential Solution

• For  $F[p,q] = D_{KL}[p,q]$ :

$$L(p,\beta^{-1}) = \langle u,p \rangle + \beta^{-1}(\lambda - \langle \ln(p/q),p \rangle + \langle 1,p-q \rangle)$$

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$$\nabla_p L(p, \beta^{-1}) = u - \beta^{-1} \ln(p/q) = 0$$
  
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• Optimal solutions are gradients of  $D^*_{KL}[u,q] = \ln \langle e^u,q \rangle$ :

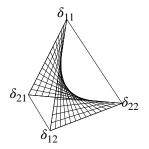
$$p(\beta) = e^{\beta u - \ln Z[\beta u]} q, \qquad D_{KL}[p(\beta), q] = \lambda$$

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## Solution to Shannon's OCP

• The solution for  $I_w\{x,y\} = D_{KL}[w,q \otimes p] \le \lambda$ :

$$w(\beta) = e^{\beta u - \ln Z[\beta u]} q \otimes p$$

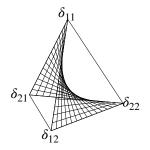


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•  $w \notin \partial \mathcal{P}(X \otimes Y)$ .

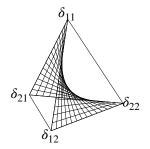


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- $T : \mathcal{P}(X) \to \mathcal{P}(Y)$  cannot have kernel  $\delta_{f(x)}(\cdot)$ .



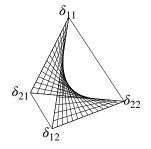
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- The dual is strictly convex:

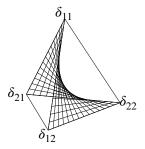
$$D^*_{KL}[u,q\otimes p] = \ln \int e^u q \otimes p$$



## Solution to Kantorovich's OTP

•  $\Gamma[q, p]$  is convex:

$$\pi_X[(1-t)w_1 + tw_2] = (1-t)q + tq = q$$



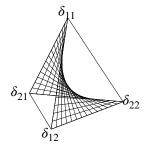
# Solution to Kantorovich's OTP

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 $\Gamma[q,p] = \{w : F[w,q \otimes p] \le 1\}$ 



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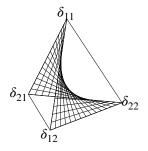
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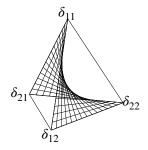
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Monge-Amper equation

$$q = p \circ \nabla \varphi |\nabla^2 \varphi|$$

where  $\varphi : X \to \mathbb{R} \cup \{\infty\}$  is convex, and  $\nabla \varphi : X \to Y$  is such that  $p = q \circ (\nabla \varphi)^{-1}$  (McCann, 1995; Villani, 2009).





Strict Inequalities

Theorem (Belavkin, 2013b)

• Let  $\{w(\beta)\}_u$  be a family of  $w(\beta) \in \mathcal{P}(X \otimes Y)$ 

maximizing  $\mathbb{E}_{w}\{u\}$  on sets  $\{w : F[w] \leq \lambda\}, \forall \lambda = F[w]$ 

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• If *F*<sup>\*</sup> is strictly convex, then

 $w(\beta) \in \partial \mathcal{P}(X \otimes Y) \text{ iff } \lambda \geq \sup F \text{ (i.e. } \beta \to \infty).$ 

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•  $F : \mathcal{P}(X \otimes Y) \to \mathbb{R} \cup \{\infty\}$  closed convex and minimized at

 $q \otimes p \in \partial F^*(0) \subset Int(\mathcal{P}(X \otimes Y))$ 

• If  $F^*$  is strictly convex, then

 $w(\beta) \in \partial \mathcal{P}(X \otimes Y) \text{ iff } \lambda \geq \sup F \text{ (i.e. } \beta \to \infty \text{).}$ 

**2** For any  $\sigma \in \partial \mathcal{P}(X \otimes Y)$  with  $F[\sigma] = F[w(\beta)] = \lambda$ 

$$\mathbb{E}_{\sigma}\{u\} < \mathbb{E}_{w(\beta)}\{u\}$$

Strict Inequalities

Theorem (Belavkin, 2013b)

• Let  $\{w(\beta)\}_u$  be a family of  $w(\beta) \in \mathcal{P}(X \otimes Y)$ 

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**2** For any  $\sigma \in \partial \mathcal{P}(X \otimes Y)$  with  $F[\sigma] = F[w(\beta)] = \lambda$ 

 $\mathbb{E}_{\sigma}\{u\} < \mathbb{E}_{w(\beta)}\{u\}$ 

**3** For any  $\sigma \in \partial \mathcal{P}(X \otimes Y)$  with  $\mathbb{E}_{\sigma}\{u\} = \mathbb{E}_{w(\beta)}\{u\} = v$ 

 $F[\sigma] > F[w(\beta)]$ 

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# Strict Bounds for Monge OTP

Corollary

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- Let  $w(\beta)$  is a solution to Shannon's OCP  $R_c[q](\lambda)$ .
- If  $w_f$  and  $w(\beta)$  have equal  $I_{w_f}\{x, y\} = I_{w(\beta)}\{x, y\} = \lambda < \sup I_w\{x, y\}$ , then

 $K_c[p,q](\lambda) > R_c[q](\lambda) > 0$ 

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• If  $w_f$  and  $w(\beta)$  achieve equal values  $K_c[p,q] = R_c[q](\lambda) = v > 0$ , then

$$K_c^{-1}[p,q](v) > R_c^{-1}[q](v)$$

References

Optimal transportation problems (OTPs)

Information and entropy

Optimal channel problem (OCP)

Dual formulation of OTP

Geometry of information divergence and optimization

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