Kantorovich optimal transport problem and Shannon's optimal channel problem

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In honor of
Shun-ichi Amari

Optimal transportation problems (OTPs)

Information and entropy

Optimal channel problem (OCP)

Geometry of information divergence and optimization

Dynamical OTP: Optimization of evolution

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Kantorovich's OTP

Optimal Transportation Problem (Kantorovich, 1939, 1942; Vasershtein, 1969; Dobrushin, 1970)

$$K_c(q,p) := \inf \left\{ \int_{X \times Y} c(x,y)\, dw : \pi_X w = q,\ \pi_Y w = p \right\}$$

where $c : X \times Y \to \mathbb{R}$ is a cost function (e.g. a metric).

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

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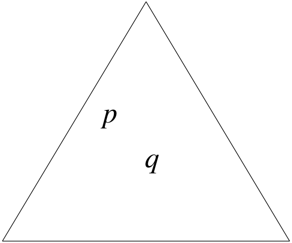

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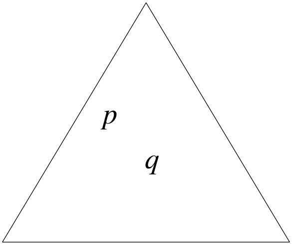

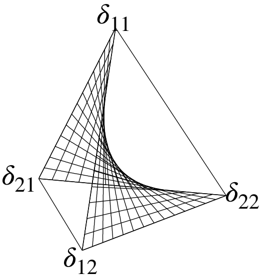

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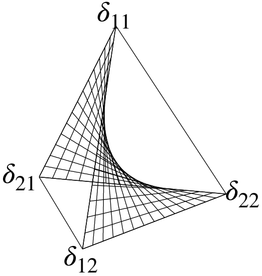

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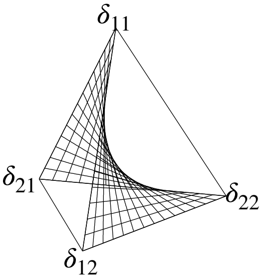
$$q \mapsto Tq = p = \int_X p(\cdot \mid x)\,dq$$



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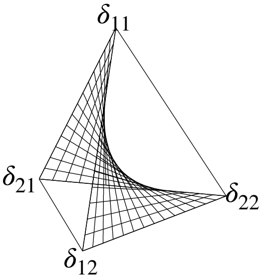

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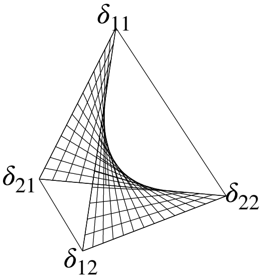
- T is determined by $w \in \mathcal{P}(X \otimes Y)$:

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



Monge OTP

Optimal Transportation Problem (Monge, 1781)

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

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

- $p(\cdot \mid x)$ 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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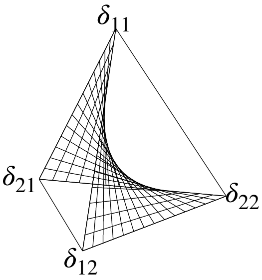
- $w_f \in \partial\mathcal{P}(X \otimes Y)$:

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



Shannon's Information and Entropy

KL-divergence (Kullback & Leibler, 1951)

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

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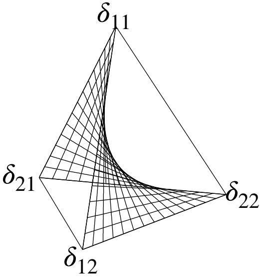

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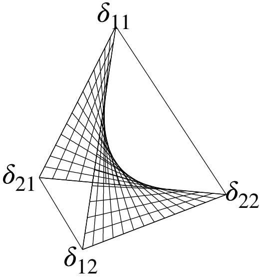
For $w \in \Gamma(q, p) \subset \mathcal{P}(X \otimes Y)$:

$$\begin{aligned} I_w\{x, y\} &:= D_{KL}(w, q \otimes p) \\ &= H(q) - H(q(x \mid y)) \\ &= H(p) - H(p(y \mid x)) \end{aligned}$$



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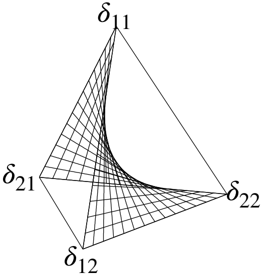
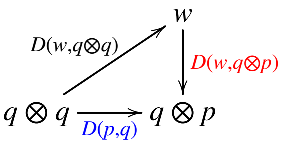


Entropy $H(p) = -\int \ln p\, dp$

$$H(p) := \sup_{w:\pi_Y w = p} I_w\{x,y\} = I_w\{y,y\}$$


w
D(w,q⊗q)
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q ⊗ q
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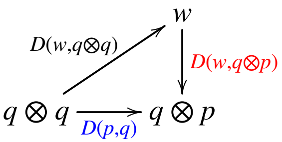
Theorem (Shannon-Pythagorean)

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

$$D_{KL}(w, q \otimes q) = D_{KL}(w, q \otimes p) + D_{KL}(p, q)$$

(Belavkin, 2013a)



Theorem (Shannon-Pythagorean)

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

$$D_{KL}(w, q \otimes q) = {\color{red} D_{KL}(w, q \otimes p)} + {\color{blue} D_{KL}(p, q)}$$

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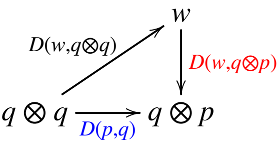

Proof.

$$D(w, q\otimes q) = \underbrace{D(w, q \otimes p)}_{\color{red} I_w\{x,y\}} + \underbrace{D(q \otimes p, q \otimes q)}_{\color{blue} D(p,q)} - \underbrace{\langle \ln q \otimes p - \ln q \otimes q, q \otimes p - w \rangle}_{0}$$

$$\ln q \otimes p - \ln q \otimes q = 1_X \otimes (\ln p - \ln q) \qquad \square$$

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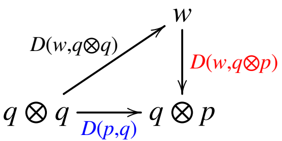

Proof.

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Cross-Information (Belavkin, 2013a)

$$D_{KL}(w, q \otimes q) = \underbrace{-\langle \ln q, p \rangle}_{\text{Cross-entropy}} - \underbrace{[H(p) - D_{KL}(w, q \otimes p)]}_{H(p(y|x))}$$

Shannon's OCP

Optimal Channel Problem (Shannon, 1948)

$$S_c(q, \lambda) := \inf \left\{ \int_{X \times Y} c(x, y)\, dw \, : \, \pi_X w = q, \; I_w\{x, y\} \leq \lambda \right\}$$

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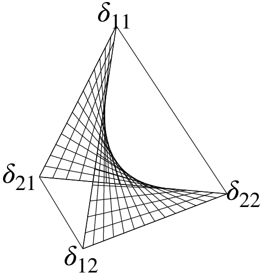

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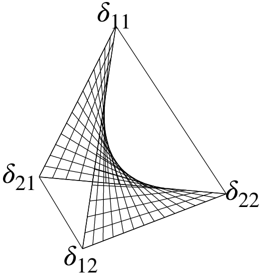
Exponential family solutions

- Optimal $T : \mathcal{P}(X) \to \mathcal{P}(Y)$ is defined by

$$w = e^{-\beta c - \ln Z}\, q \otimes p\,, \quad \beta^{-1} = -dS_c(q, \lambda)/d\lambda$$



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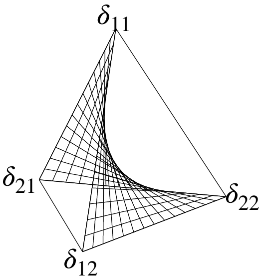

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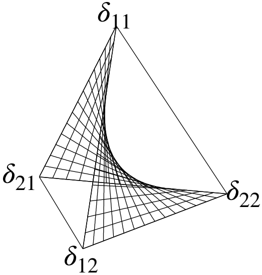

Value of Information (Stratonovich, 1965)

$$V(\lambda) := S_c(q, 0) - S_c(q, \lambda) = \sup\{\mathbb{E}_w\{u\} : I_w\{x, y\} \leq \lambda\}$$

Relation to Kantorovich OTP

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- q and p have entropies $H(q)$ and $H(p)$ and

$$0 \leq I_w\{x,y\} \leq \min[H(q), H(p)]$$

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

$$S_c(q, \lambda) \leq K_c(q,p)$$

Inverse Optimal Values

Inverse of the OCP Value

$$S_c^{-1}(q, v) := \inf\left\{ I_w\{x, y\} : \pi_X w = q, \int c\, dw \leq v \right\}$$

Inverse Optimal Values

Inverse of the OCP Value

$$S_c^{-1}(q, \upsilon) := \inf\left\{ I_w\{x, y\} : \pi_X w = q,\ \int c\, dw \leq \upsilon \right\}$$

Inverse of the OTP Value

$$K_c^{-1}(q, p, \upsilon) := \inf\left\{ I_w\{x, y\} : \pi_X w = q,\ \pi_Y w = p,\ \int c\, dw \leq \upsilon \right\}$$

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- These inverse values represent the smallest amount of Shannon's information required to achieve expected cost $\int c\, dw = \upsilon$.

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- These inverse values represent the smallest amount of Shannon's information required to achieve expected cost $\int c \, dw = \upsilon$.
- If $\upsilon = K_c(q, p)$, then

$$S_c^{-1}(q, \upsilon) \leq K_c^{-1}(q, p, \upsilon)$$

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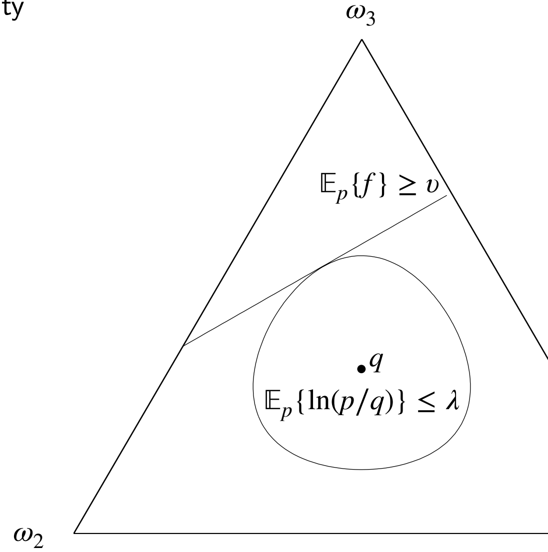
Problems on Conditional Extremum

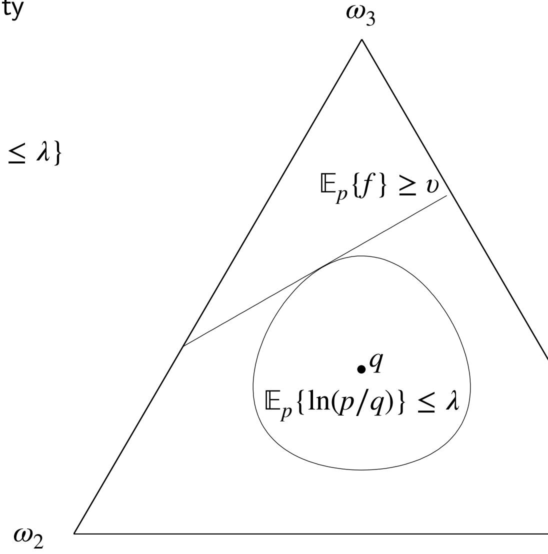
- $\mathbb{E}_p\{u\} = \langle u, p \rangle$ expected utility



Problems on Conditional Extremum

- $\mathbb{E}_p\{u\} = \langle u, p\rangle$ expected utility
- $v_u(\lambda) = -S_{-u}(q, \lambda)$ utility of information λ:

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



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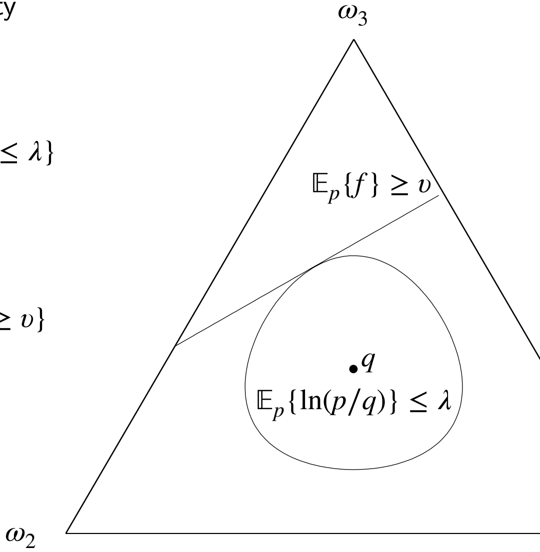

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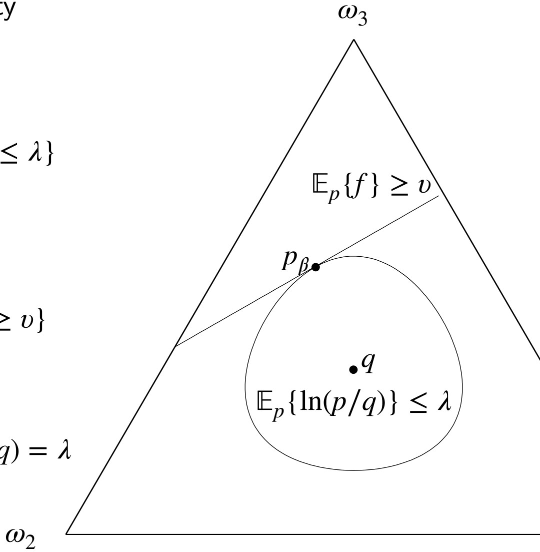
$$p(\beta) \in \partial F^*(\beta u, q)\,, \quad F(p(\beta), q) = \lambda$$



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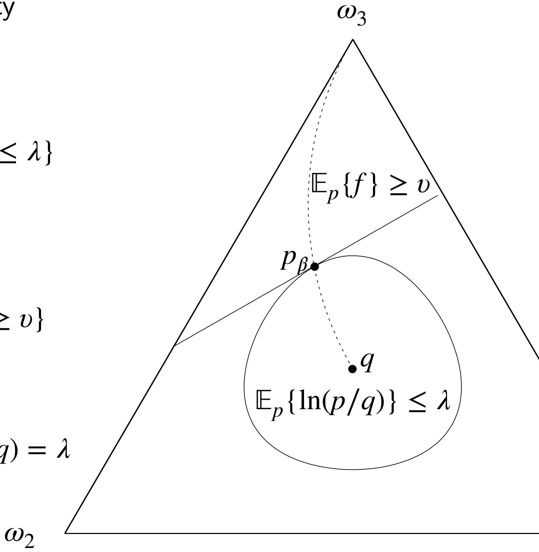

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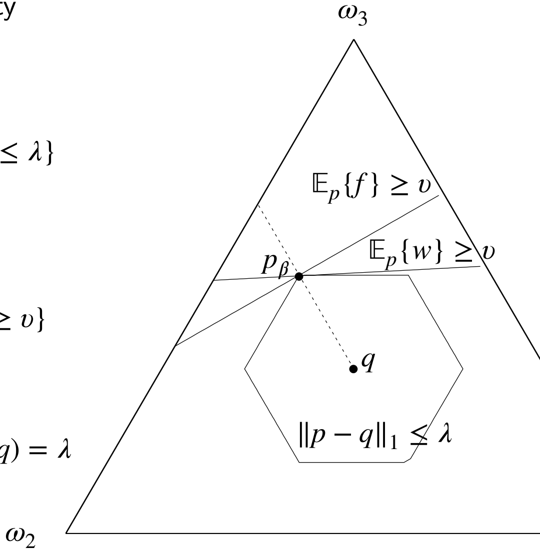
- $\lambda_u(\upsilon) = \upsilon_u^{-1}(\upsilon)$ information of utility υ:

$$\lambda_u(\upsilon) := \inf\{F(p, q) : \langle u, p \rangle \geq \upsilon\}$$

- $p(\beta)$ optimal solutions:

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



General Solution

- Lagrange function for $\upsilon_u(\lambda) := \sup\{\langle u, p\rangle : F(p,q) \leq \lambda\}$ $\big(\lambda_u(\upsilon) := \inf\{F(p,q) : \langle u, p\rangle \geq \upsilon\}\big)$:

$$\begin{aligned} L(p,\beta^{-1}) &= \langle u, p\rangle + \beta^{-1}[\lambda - F(p,q)] \\ \Big(L(p,\beta) &= F(p,q) + \beta[\upsilon - \langle u, p\rangle]\Big) \end{aligned}$$

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Example: Exponential Solution

- For $D_{KL}(p,q) = \langle \ln(p/q), p\rangle - \langle 1, p-q\rangle$:

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

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- Optimal solutions are gradients of $D^*_{KL}(u,q) = \ln\langle e^u, q\rangle$:

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

Solution to Shannon's OCP

- The solution for $I_w\{x,y\} = D_{KL}(w, q \otimes p) \leq \lambda$:

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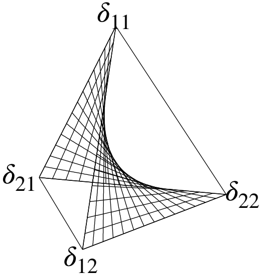

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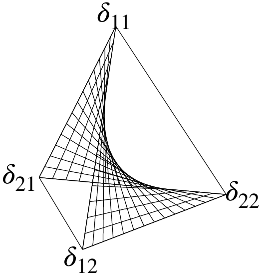

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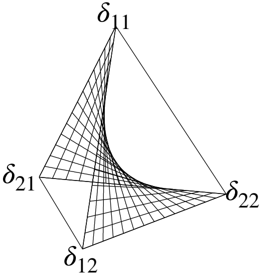

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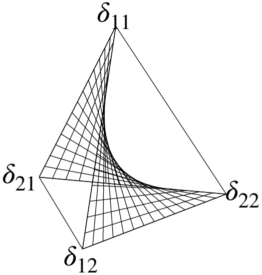
- The dual is strictly convex:

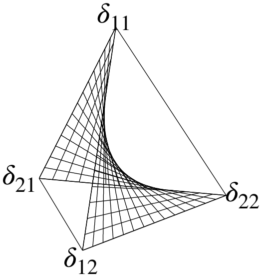
$$D^*_{KL}(u, q \otimes p) = \ln \int e^u\, q \otimes p$$



Solution to Kantorovich's OTP

- $\Gamma(q, p)$ is convex:

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



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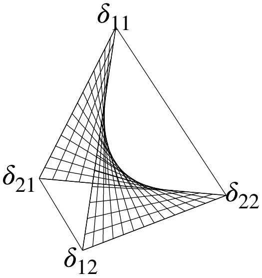

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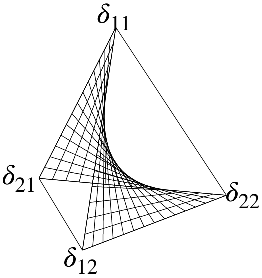

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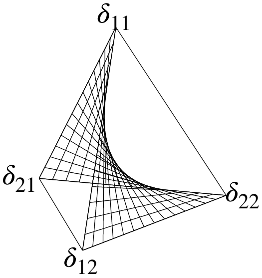

Monge-Amper equation

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

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* $w(\beta) \in \mathcal{P}(X \otimes Y)$

$$\textit{maximizing } \mathbb{E}_w\{u\} \textit{ on sets } \{w : F(w) \leq \lambda\}\,,\ \forall\, \lambda = F(w)$$

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Optimal Transport and the Expected Utility Principle

- Let $(X \times Y, \lesssim)$ be a set with preference relation (total pre-order).

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Theorem

Pre-ordered linear space $(L, \lesssim)$ satisfies (1), (2) and (3) if and only if $(L, \lesssim)$ has a utility representation by a closed linear functional $u : L \to \mathbb{R}$.

Dynamical Problems

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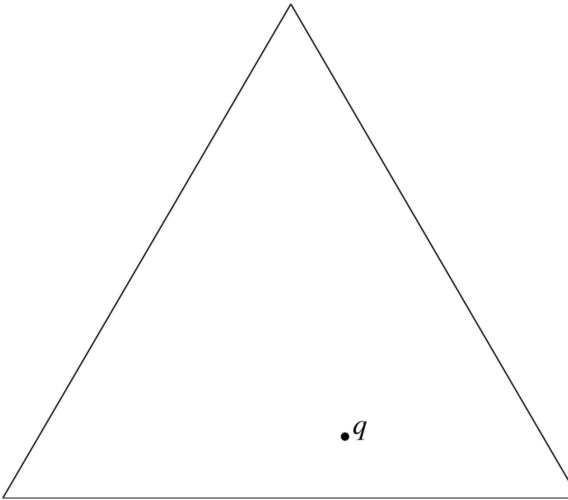

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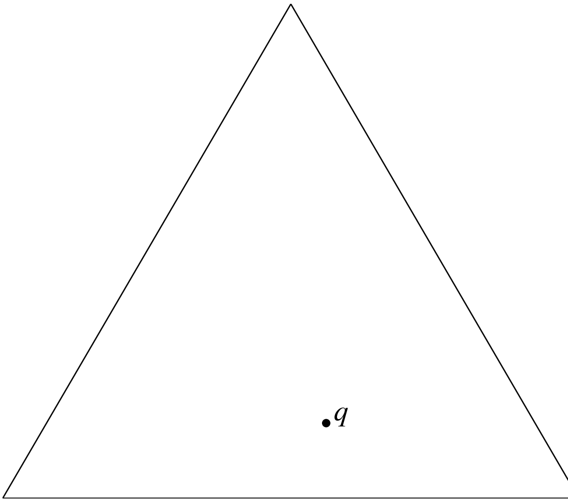

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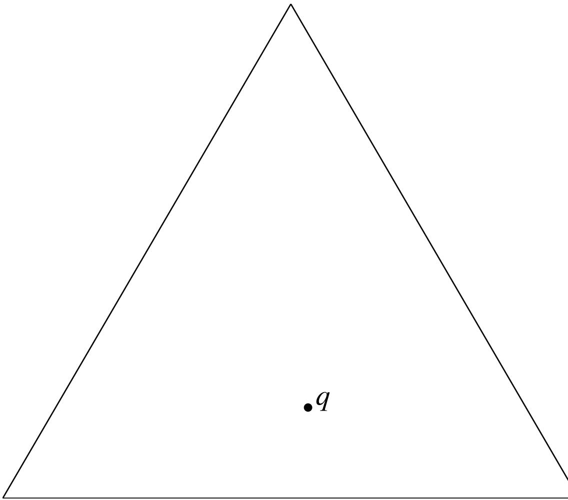

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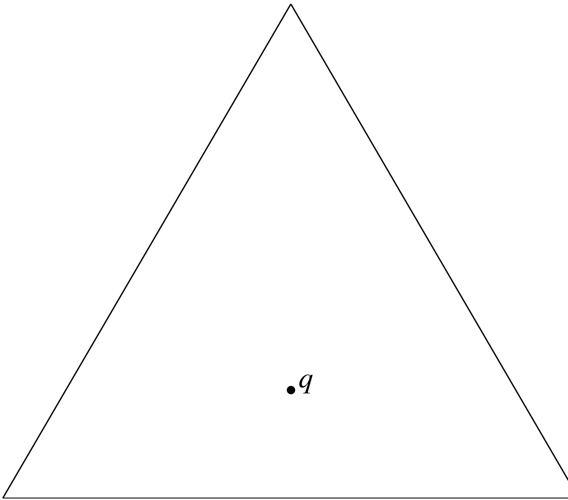

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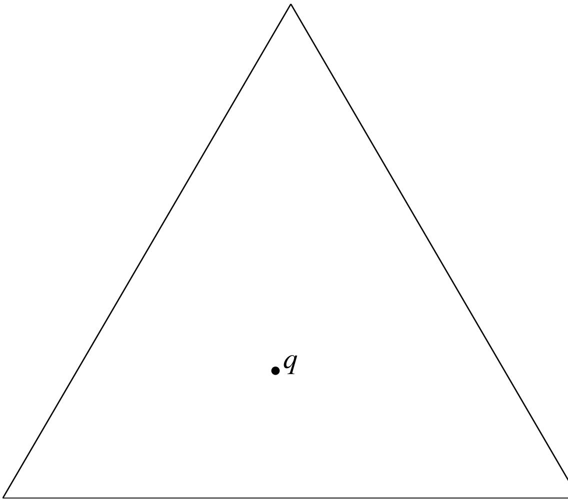

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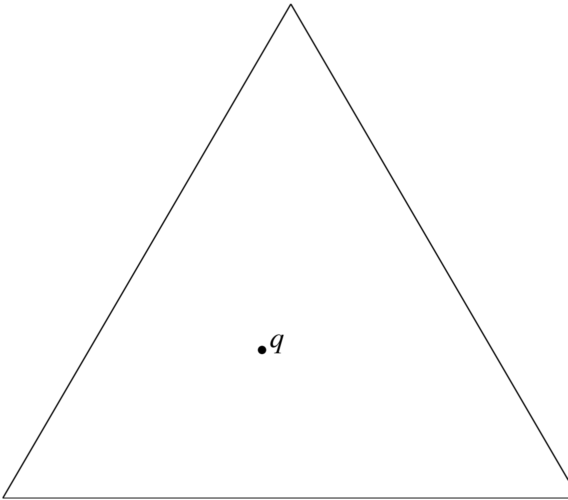

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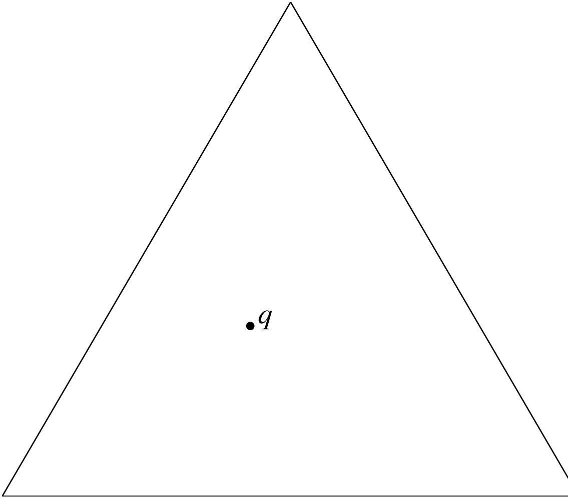

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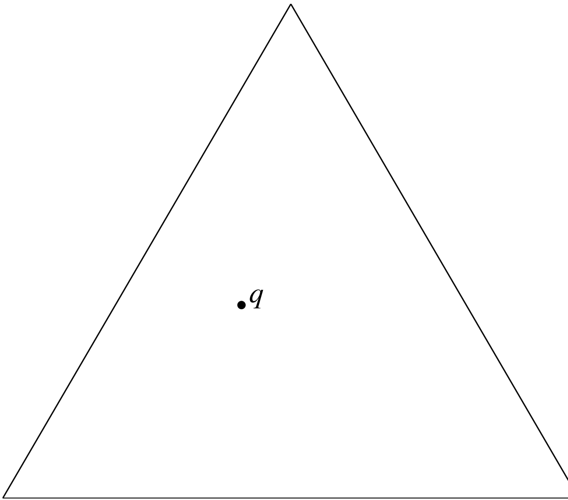

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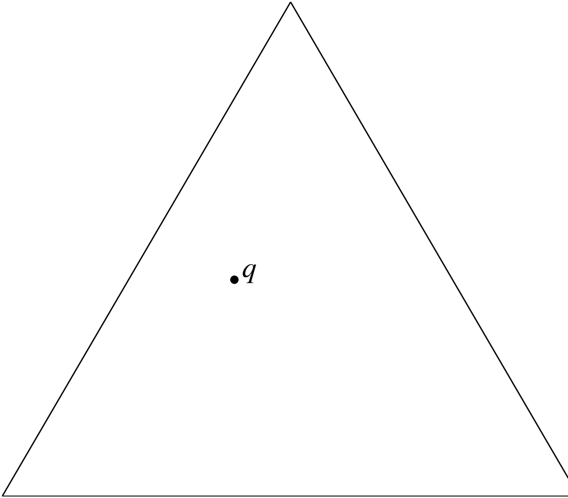

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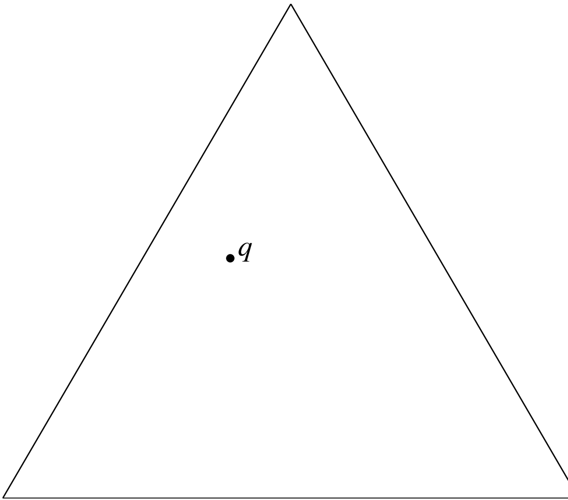

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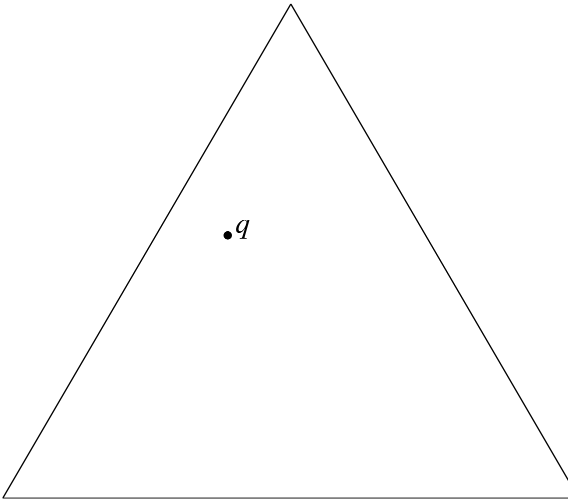

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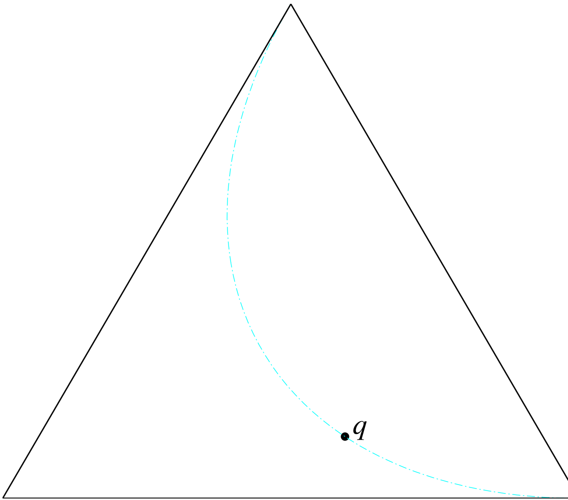

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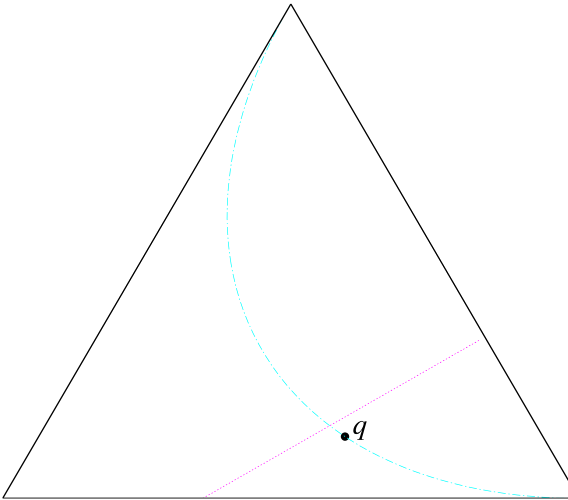

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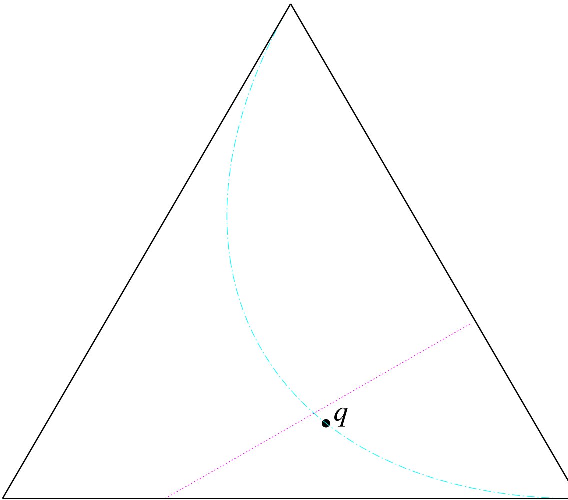

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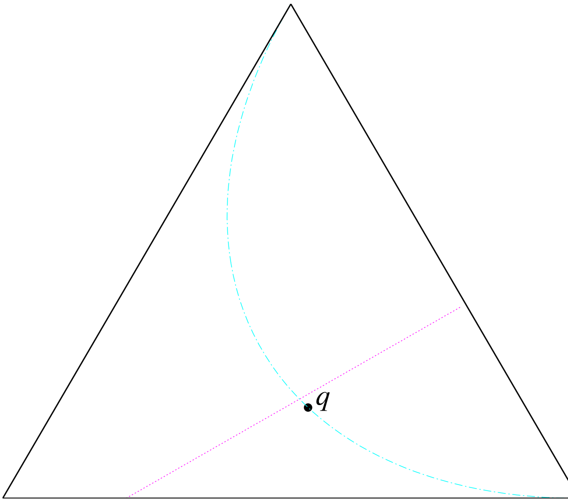

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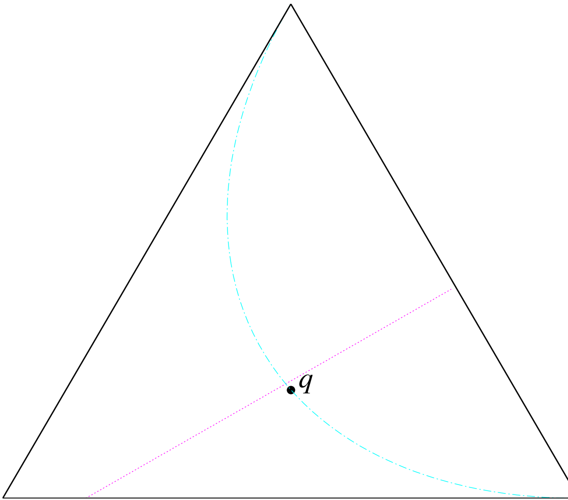

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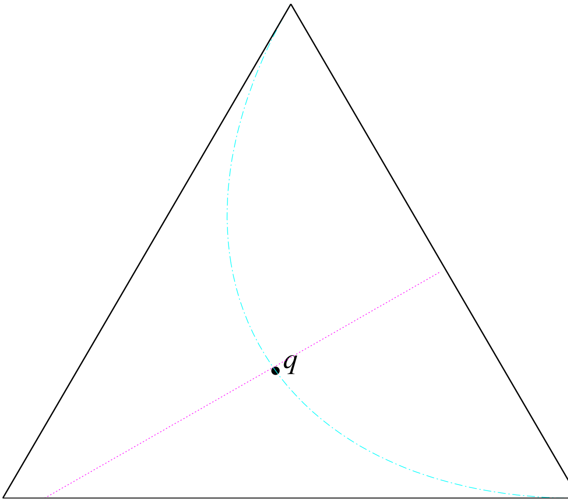

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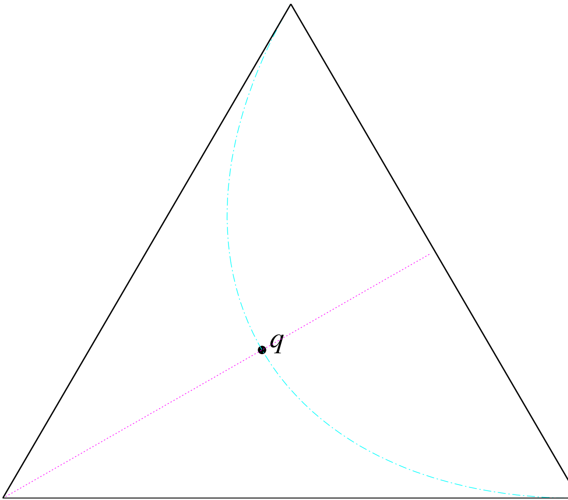

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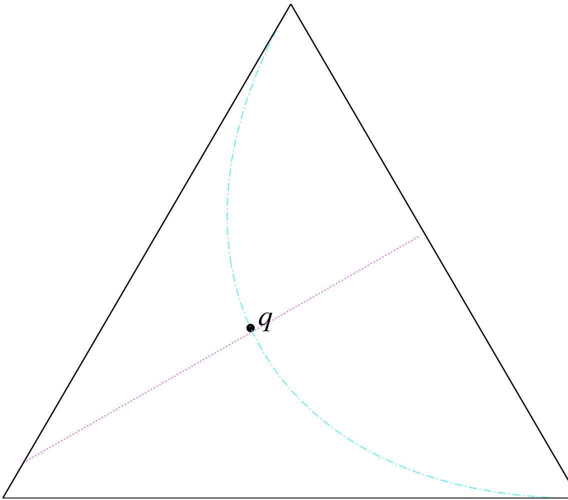

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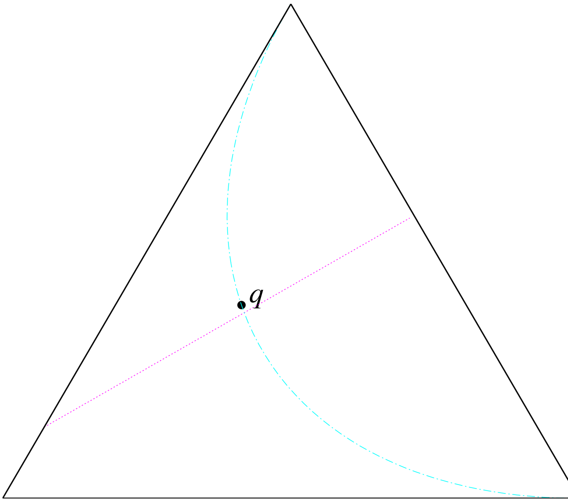

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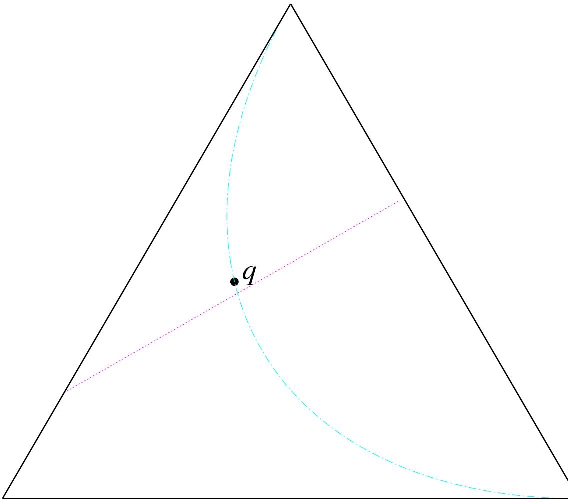

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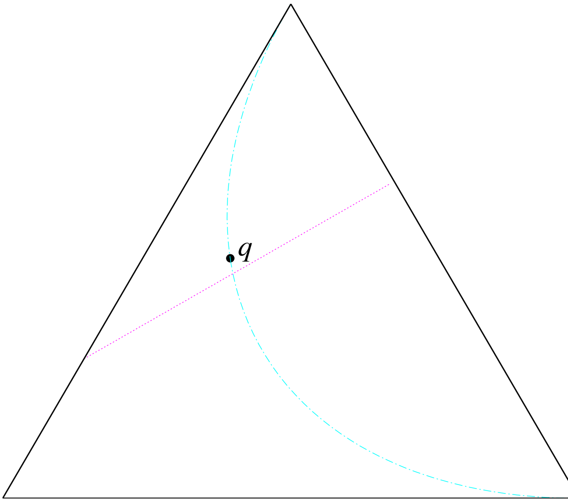

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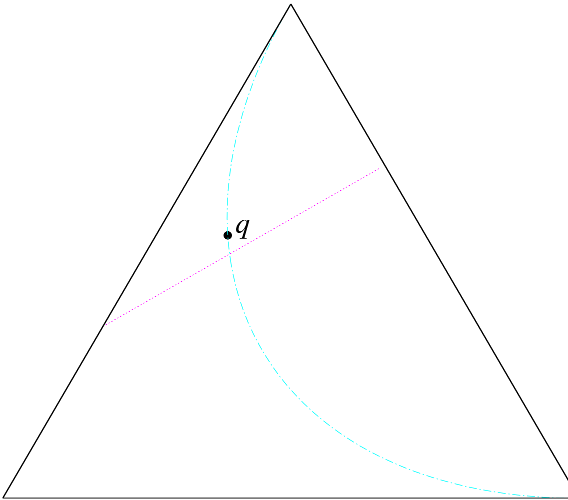
- Why not directly $q \mapsto Tq = \delta_\top$?



Example: Search in Hamming space $\{1, \dots, \alpha\}^l$

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- For $l \geq 2$

$$\log_2(l + 1) < l \log_2 \alpha$$

Optimal Control of Mutation Rate

- Optimal transition kernels are

$$P_\beta(y \mid x) = \frac{e^{-\beta \|y-x\|_H}}{[1+(\alpha-1)e^{-\beta}]^l} = \prod_{i=1}^{l} \frac{e^{-\beta(1-\delta_{x_i y_i})}}{1+(\alpha-1)e^{-\beta}}$$

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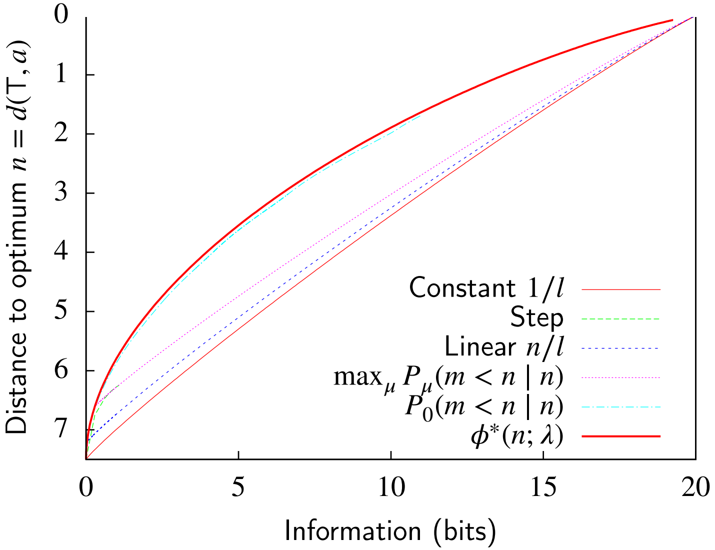
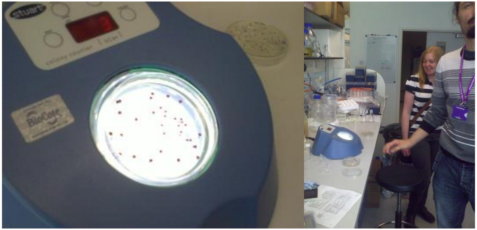
- The CDF method:

$$\mu(n) = \sum_{m=0}^{n-1} \binom{l}{m} \frac{(\alpha-1)^m}{\alpha^l}$$

Evolution of Fitness in Information



Mutation Rate Control in *E. coli*



- Used strains of *Escherichia coli* K-12 MG1665

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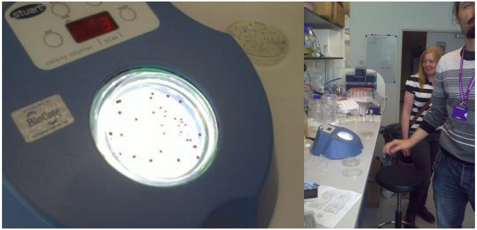

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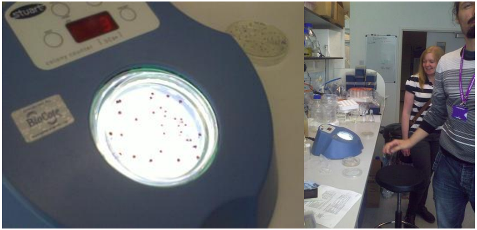

- Used strains of *Escherichia coli* K-12 MG1665
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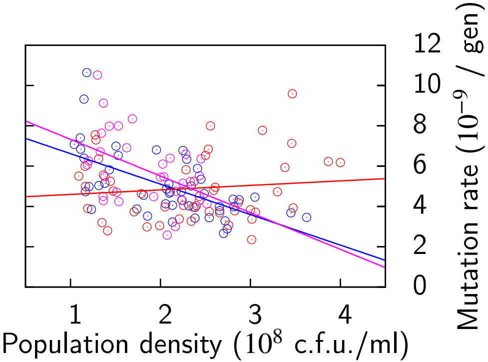
- Estimated mutation rates μ in *E.coli* strains grown in Davis minimal medium with different amount of glucose.

Experimental Results (Krašovec et al., 2014)



- Strong relationship between μ and density of cells ($p < .0001$).

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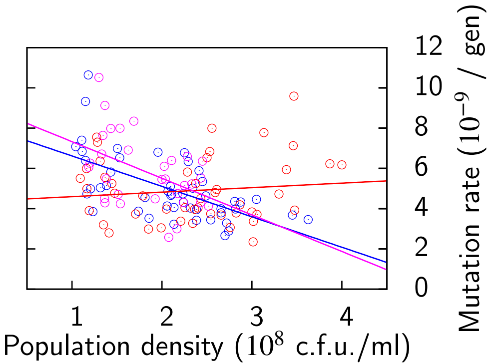

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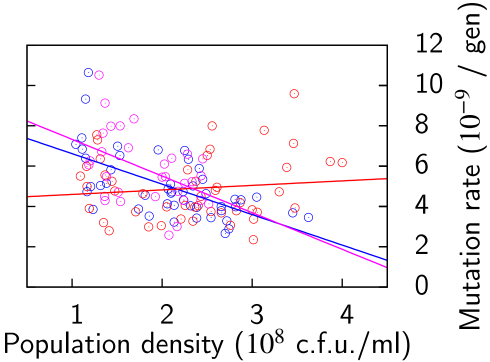

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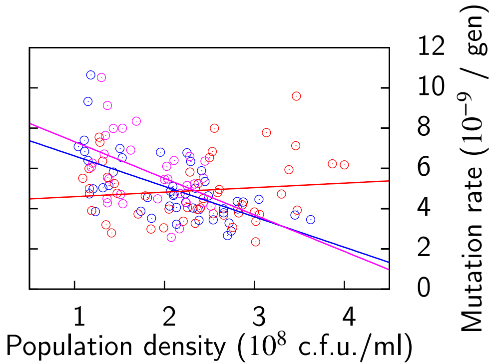

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Optimal transportation problems (OTPs)

Information and entropy

Optimal channel problem (OCP)

Geometry of information divergence and optimization

Dynamical OTP: Optimization of evolution

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